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Sample solutions

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Part 0: Intro to Numpy/Scipy

[Numpy \(http://www.numpy.org/\)](http://www.numpy.org/) is a Python module that provides fast primitives for multidimensional arrays. It's well-suited to implementing numerical algebra algorithms, and for those can be much faster than Python's native list and dictionary types when you only need to store and operate on

Some of the material from this lesson is copied from the following, and more comprehensive, tutorial: [link \(http://www.scipy-lectures.org/intro/numpy/index.html\)](http://www.scipy-lectures.org/intro/numpy/index.html)

Quick demo. The recommended importing idiom is:

```
In [1]: import numpy as np
        print(np.__version__)

1.14.0
```

Creating a simple numpy array

```
In [2]: a = np.array([1,2,3,4])
        print(a)

[1 2 3 4]
```

Why bother with Numpy? A motivating example

We already have lists and dictionary types, which are pretty easy to use and very flexible. So why bother with this special type?

Exercise 0 (ungraded). One reason to consider Numpy is that it "can be much faster," as noted above. But how much faster is that? Run the example to see.

```
In [3]: n = 1000000

In [4]: L = range(n)
        %timeit [i**2 for i in L]

273 ms ± 3.44 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

In [5]: np.arange(10) # Moral equivalent to `range`

Out[5]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])

In [6]: A = np.arange(n)
        %timeit A**2

690 µs ± 2.34 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

Creating multidimensional arrays

Beyond simple arrays, Numpy supports multidimensional arrays. To do more than one dimension, call `numpy.array()` but nest each new dimension in a list. It's easiest to see by example.

```
In [7]: # Create a two-dimensional array of size 3 rows x 4 columns:
        B = np.array([[0, 1, 2, 3],
                      [4, 5, 6, 7],
                      [8, 9, 10, 11]])

        print(B)

[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]]

In [8]: print(B.ndim) # What does this do?
        print(B.shape) # What does this do?
        print(len(B)) # What does this do?

2
(3, 4)
3

In [9]: C1 = [[0, 1, 2, 3],
```

```

    [4, 5, 6, 7],
    [8, 9, 10, 11]]

C2 = [[12, 13, 14, 15],
      [16, 17, 18, 19],
      [20, 21, 22, 23]]

C = np.array([C1, C2])

print(C)
print(C.ndim)
print(C.shape)
print(len (C))

```

```

[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]
3
(2, 3, 4)
2

```

There are routines for creating various kinds of structured matrices as well, which are similar to those found in [MATLAB](http://www.mathworks.com/products/matlab/) (<http://www.mathworks.com/products/matlab/>) and [Octave](https://www.gnu.org/software/octave/) (<https://www.gnu.org/software/octave/>).

In [10]: `print(np.zeros((3, 4)))`

```

[[0. 0. 0. 0.]
 [0. 0. 0. 0.]
 [0. 0. 0. 0.]]

```

In [11]: `print(np.ones((3, 4)))`

```

[[1. 1. 1. 1.]
 [1. 1. 1. 1.]
 [1. 1. 1. 1.]]

```

In [12]: `print(np.eye(3))`

```

[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]

```

In [13]: `print(np.diag([1, 2, 3]))`

```

[[1 0 0]
 [0 2 0]
 [0 0 3]]

```

You can also create empty (uninitialized) arrays. What does the following produce?

In [14]: `A = np.empty((3, 4)) # An "empty" 3 x 4 matrix`
`print(A)`

```

[[1. 1. 1. 1.]
 [1. 1. 1. 1.]
 [1. 1. 1. 1.]]

```

Exercise 1 (ungraded). The following code creates an identity matrix in two different ways, which are found to be equal according to the assertic there is a subtle difference between the I and I_u matrices created below; can you spot it?

In [15]: `n = 3`
`I = np.eye(n)`

`print("==> I = eye(n):")`
`print(I)`

`u = [1] * n`
`I_u = np.diag(u)`

`print("\n==> u:\n", u)`
`print("==> I_u = diag (u):\n", I_u)`

`assert np.all(I_u == I)`

```

==> I = eye(n):
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]

```

```

==> u:

```

```
[1, 1, 1]
==> I_u = diag (u):
[[1 0 0]
 [0 1 0]
 [0 0 1]]
```

Answer. Give this some thought before you read the answer that follows!

The difference is in the element types. The `eye()` function returns an identity matrix and uses a floating-point type as the element type. By contrast, `diag()` expects a list of initializer values upon input, derives the element type from that input. In this case, `u` contains values that will be stored as integers, therefore, `diag()` constructs its output assuming integer elements.

Try running `print(I_u.dtype)` and `print(I.dtype)` to confirm that these element types differ.

Indexing and slicing

The usual 0-based slicing and indexing notation you know and love from lists is also supported for Numpy arrays. In the multidimensional case, natural multidimensional analogues with index ranges separated by commas.

```
In [16]: # Recall: C
print (C)

[[[ 0  1  2  3]
  [ 4  5  6  7]
  [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]
```

What part of `C` will the following slice extract? Run the code to find out.

```
In [17]: print (C[0, 2, :])

[ 8  9 10 11]
```

What will the following slice return? Run the code to find out.

```
In [18]: print (C[1, 0, ::-1])

[15 14 13 12]
```

Exercise 2 (5 points). Consider the following 6×6 matrix, which has 4 different subsets highlighted.

0	1	2	3	4	5
10	11	12	13	14	15
20	21	22	23	24	25
30	31	32	33	34	35
40	41	42	43	44	45
50	51	52	53	54	55

For each subset illustrated above, write an indexing or slicing expression that extracts the subset. Store the result of each slice into `Z_green`, `Z_orange`, and `Z_cyan`.

```
In [19]: Z= np.array([[0,1,2,3,4,5],[10,11,12,13,14,15],[20,21,22,23,24,25],[30,31,32,33,34,35],[40,41,42,43,44,45],[50,51,52,53,54,55]])

# Construct `Z_green`, `Z_red`, `Z_orange`, and `Z_cyan`:
### BEGIN SOLUTION
Z_orange = Z[0, 3:5]
Z_red = Z[:, 2]
Z_green = Z[2::2, ::2]
Z_cyan = Z[4:, 4:]
### END SOLUTION
```

```
In [20]: # Test cell: `check_Z`

print("==> Z:\n", Z)
assert (Z == np.array([np.arange(0, 6),
```

```

        np.arange(10, 16),
        np.arange(20, 26),
        np.arange(30, 36),
        np.arange(40, 46),
        np.arange(50, 56]])).all()

print("\n==> Orange slice:\n", Z_orange)
assert (Z_orange == np.array ([3, 4])).all()

print("\n==> Red slice:\n", Z_red)
assert (Z_red == np.array ([2, 12, 22, 32, 42, 52])).all()

print("\n==> Cyan slice:\n", Z_cyan)
assert (Z_cyan == np.array ([[44, 45], [54, 55]])).all()

print("\n==> Green slice:\n", Z_green)
assert (Z_green == np.array ([[20, 22, 24], [40, 42, 44]])).all()

print("\n(Passed!)")

```

```

==> Z:
[[ 0  1  2  3  4  5]
 [10 11 12 13 14 15]
 [20 21 22 23 24 25]
 [30 31 32 33 34 35]
 [40 41 42 43 44 45]
 [50 51 52 53 54 55]]

```

```

==> Orange slice:
[3 4]

```

```

==> Red slice:
[ 2 12 22 32 42 52]

```

```

==> Cyan slice:
[[44 45]
 [54 55]]

```

```

==> Green slice:
[[20 22 24]
 [40 42 44]]

```

```

(Passed!)

```

Slices are views

To help save memory, when you slice a Numpy array, you are actually creating a *view* into that array. That means modifications through the view the original array.

```

In [21]: print("==> Recall C: %s" % str(C.shape))
        print(C)

```

```

==> Recall C: (2, 3, 4)
[[[ 0  1  2  3]
   [ 4  5  6  7]
   [ 8  9 10 11]]

 [[12 13 14 15]
  [16 17 18 19]
  [20 21 22 23]]]

```

```

In [22]: C_view = C[1, 0::2, 1::2] # Question: What does this produce?
        print ("==> C_view: %s" % str (C_view.shape))
        print (C_view)

```

```

==> C_view: (2, 2)
[[13 15]
 [21 23]]

```

```

In [23]: C_view[:, :] = -C_view[::-1, ::-1] # Question: What does this do?
        print (C_view)

```

```

[[-23 -21]
 [-15 -13]]

```

```

In [24]: print (C)

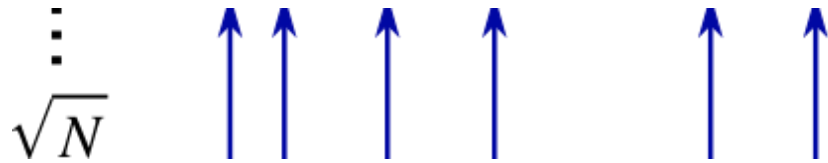
```

```

[[[ 0  1  2  3]
   [ 4  5  6  7]
   [ 8  9 10 11]]

 [[ 12 -23 14 -21]
  [ 16 17 18 19]
  [ 20 -15 22 -13]]]

```

That is, given a positive integer n , the algorithm iterates from $i \in \{2, 3, 4, \dots, \lfloor \sqrt{n} \rfloor\}$, repeatedly "crossing out" values that are strict multiple "Crossing out" means maintaining an array of, say, booleans, and setting values that are multiples of i to False.

```
In [31]: from math import sqrt

def sieve(n):
    """
    Returns the prime number 'sieve' shown above.

    That is, this function returns an array `X[0:n+1]`
    such that `X[i]` is true if and only if `i` is prime.
    """
    is_prime = np.empty(n+1, dtype=bool) # the "sieve"

    # Initial values
    is_prime[0:2] = False # {0, 1} are _not_ considered prime
    is_prime[2:] = True # All other values might be prime

    # Implement the sieving loop
    ### BEGIN SOLUTION
    for k in range(2, int(sqrt(n))+1):
        is_prime[2*k::k] = False
    ### END SOLUTION

    return is_prime

# Prints your primes
print("==> Primes through 20:\n", np.nonzero(sieve(20))[0])

==> Primes through 20:
[ 2  3  5  7 11 13 17 19]
```

```
In [32]: # Test cell: `prime_sieve_test`

is_prime = sieve(20)
assert len (is_prime) == 21
assert (is_prime == np.array([False, False, True, True, False, True, False, True, False, False, False,
True, False, False, False, True, False, True, False])).all()
```

Note: The contents below appears as "Part 1" in the Notebook 10 assignment.

Part 1: Supplemental Background on Numpy

This notebook is a quick overview of additional functionality in Numpy. It is intended to supplement the videos and the other parts of this assignnn **not** contain any exercises that you need to submit.

```
In [1]: import numpy as np
print(np.__version__)

1.14.0
```

Random numbers

Numpy has a rich collection of (pseudo) random number generators. Here is an example; see the documentation for [numpy.random\(\)](https://docs.scipy.org/doc/numpy/reference/routines.random.html) (<https://docs.scipy.org/doc/numpy/reference/routines.random.html>) for more details.

```
In [2]: A = np.random.randint(-10, 10, size=(4, 3)) # return random integers from -10 (inclusive) to 10 (exclus
print(A)

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
```

Aggregations or reductions

Suppose you want to reduce the values of a Numpy array to a smaller number of values. Numpy provides a number of such functions that *aggregate*. Examples of aggregations include sums, min/max calculations, and averaging, among others.

```
In [3]: print("np.max =", np.max(A),"; np.amax =", np.amax(A)) # np.max() and np.amax() are synonyms
        print("np.min =", np.min(A),"; np.amin =", np.amin(A)) # same
        print("np.sum =", np.sum(A))
        print("np.mean =", np.mean(A))
        print("np.std =", np.std(A))

np.max = 7 ; np.amax = 7
np.min = -10 ; np.amin = -10
np.sum = 3
np.mean = 0.25
np.std = 7.025252071396916
```

The above examples aggregate over all values. But you can also aggregate along a dimension using the optional axis parameter.

```
In [4]: print("Max in each column:", np.amax(A, axis=0)) # i.e., aggregate along axis 0, the rows, producing co
        print("Max in each row:", np.amax(A, axis=1)) # i.e., aggregate along axis 1, the columns, producing ro

Max in each column: [ 6  7  7]
Max in each row: [ 7  7  6 -2]
```

Universal functions

Universal functions apply a given function *elementwise* to one or more Numpy objects.

For instance, `np.abs(A)` takes the absolute value of each element.

```
In [5]: print(A, "\n==>\n", np.abs(A))

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
==>
[[ 5  7  6]
 [10  7  7]
 [ 6  3 10]
 [ 2  6 10]]
```

Some universal functions accept multiple, compatible arguments. For instance, here, we compute the *elementwise maximum* between two matrices, producing a new matrix C such that $c_{ij} = \max(a_{ij}, b_{ij})$.

The matrices must have compatible shapes, which we will elaborate on below when we discuss Numpy's *broadcasting rule*.

```
In [6]: print(A) # recall A

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
```

```
In [7]: B = np.random.randint(-10, 10, size=A.shape)
        print(B)

[[ 5  5 -5]
 [-6  9 -10]
 [-9 -3 -7]
 [ 3 -3  7]]
```

```
In [8]: C = np.maximum(A, B) # elementwise comparison
        print(C)

[[ 5  7  6]
 [-6  9  7]
 [ 6  3 -7]
 [ 3 -3  7]]
```

You can also build your own universal functions! For instance, suppose we want a way to compute, elementwise, $f(x) = e^{-x^2}$ and we have a scalar x . We can do so:

```
In [9]: def f(x):
        from math import exp
        return exp(-(x**2))
```


This function accepts one input (x) and returns a single output. The following will create a new Numpy universal function `f_np`. See the document `np.frompyfunc()` (<https://docs.scipy.org/doc/numpy/reference/generated/numpy.frompyfunc.html>) for more details.

```
In [10]: f_np = np.frompyfunc(f, 1, 1)

print(A, "\n=>\n", f_np(A))

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
=>
[[1.3887943864964021e-11 5.242885663363464e-22 2.3195228302435696e-16]
 [3.720075976020836e-44 5.242885663363464e-22 5.242885663363464e-22]
 [2.3195228302435696e-16 0.00012340980408667956 3.720075976020836e-44]
 [0.01831563888873418 2.3195228302435696e-16 3.720075976020836e-44]]
```

Broadcasting

Sometimes we want to combine operations on Numpy arrays that have different shapes but are *compatible*.

In the following example, we want to add 3 elementwise to every value in A.

```
In [11]: print(A)
print()
print(A + 3)

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]

[[ 8 10  9]
 [-7 10 10]
 [ 9  6 -7]
 [ 1 -3 -7]]
```

Technically, A and 3 have different shapes: the former is a 4×3 matrix, while the latter is a scalar (1×1). However, they are compatible because how to *extend*---or **broadcast**---the value 3 into an equivalent matrix object of the same shape in order to combine them.

To see a more sophisticated example, suppose each row `A[i, :]` are the coordinates of a data point, and we want to compute the centroid of a points (or center-of-mass, if we imagine each point is a unit mass). That's the same as computing the mean coordinate for each column:

```
In [12]: A_row_means = np.mean(A, axis=0)

print(A, "\n=>\n", A_row_means)

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
=>
[-0.25  2.75 -1.75]
```

Now, suppose you want to shift the points so that their mean is zero. Even though they don't have the same shape, Numpy will interpret `A - A_row_means` precisely this operation, effectively extending or "replicating" `A_row_means` into rows of a matrix of the same shape as A, in order to then perform subtraction.

```
In [13]: A_row_centered = A - A_row_means
A_row_centered

Out[13]: array([[ 5.25,  4.25,  7.75],
                [-9.75,  4.25,  8.75],
                [ 6.25,  0.25, -8.25],
                [-1.75, -8.75, -8.25]])
```

Suppose you instead want to mean-center the *columns* instead of the rows. You could start by computing column means:

```
In [14]: A_col_means = np.mean(A, axis=1)

print(A, "\n=>\n", A_col_means)

[[ 5  7  6]
 [-10  7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
```

```
=>
[ 6.          1.33333333 -0.33333333 -6.          ]
```

But the same operation will fail!

```
In [15]: A - A_col_means # Fails!
```

```
-----
ValueError                                Traceback (most recent call last)
<ipython-input-15-d3357eda1460> in <module>()
----> 1 A - A_col_means # Fails!
```

```
ValueError: operands could not be broadcast together with shapes (4,3) (4,)
```

The error reports that these shapes are not compatible. So how can you fix it?

Broadcasting rule. One way is to learn Numpy's convention for **broadcasting** ([https://docs.scipy.org/doc/numpy/reference/ufuncs.html#b](https://docs.scipy.org/doc/numpy/reference/ufuncs.html#broadcasting)). Numpy starts by looking at the shapes of the objects:

```
In [19]: print(A.shape, A_row_means.shape)

(4, 3) (3,)
```

These are compatible if, starting from *right to left*, the dimensions match **or** one of the dimensions is 1. This convention of moving from right to left as matching the *trailing dimensions*. In this example, the rightmost dimensions of each object are both 3, so they match. Since `A_row_means` has 1 dimension, it can be replicated to match the remaining dimensions of `A`.

By contrast, consider the shapes of `A` and `A_col_means`:

```
In [20]: print(A.shape, A_col_means.shape)

(4, 3) (4,)
```

In this case, per the broadcasting rule, the trailing dimensions of 3 and 4 do not match. Therefore, the broadcast rule fails. To make it work, we `reshape` `A_col_means` to have a unit trailing dimension. Use Numpy's `reshape()` (<https://docs.scipy.org/doc/numpy/reference/generated/numpy.reshape>) to convert `A_col_means` into a shape that has an explicit trailing dimension of size 1.

```
In [21]: A_col_means2 = np.reshape(A_col_means, (len(A_col_means), 1))
print(A_col_means2, "=>", A_col_means2.shape)

[[ 6.          ]
 [ 1.33333333]
 [-0.33333333]
 [-6.          ]] => (4, 1)
```

Now the trailing dimension equals 1, so it can be matched against the trailing dimension of `A`. The next dimension is the same between the two `ndarray`s. Numpy knows it can replicate accordingly.

```
In [22]: print("A - A_col_means2\n\n", A, "\n-", A_col_means2)
print("\n=>\n", A - A_col_means2)
```

```
A - A_col_means2

[[ 5  7  6]
 [-10 7  7]
 [ 6  3 -10]
 [-2 -6 -10]]
- [[ 6.          ]
   [ 1.33333333]
   [-0.33333333]
   [-6.          ]]

=>
[[ -1.          1.          0.          ]
 [-11.33333333  5.66666667  5.66666667]
 [  6.33333333  3.33333333 -9.66666667]
 [  4.          0.         -4.          ]]
```

Thought exercise. As a thought exercise, you might see if you can generalize and apply the broadcasting rule to a 3-way array.

Part 2: Dense matrix storage

This part of the lab is a brief introduction to efficient storage of matrices.

Exercise 0 (ungraded). Import Numpy!

```
In [1]: import numpy as np
print(np.__version__)

1.14.0
```

Dense matrix storage: Column-major versus row-major layouts

For linear algebra, we will be especially interested in 2-D arrays, which we will use to store matrices. For this common case, there is a subtle performance issue related to how matrices are stored in memory.

By way of background, physical storage---whether it be memory or disk---is basically one big array. And because of how physical storage is implemented, it turns out that it is much faster to access consecutive elements in memory than, say, to jump around randomly.

A matrix is a two-dimensional object. Thus, when it is stored in memory, it must be mapped in some way to the one-dimensional physical array. There are many possible mappings, but the two most common conventions are known as the *column-major* and *row-major* layouts:

 Exercise: Extract these slices

Exercise 1 (2 points). Let A be an $m \times n$ matrix stored in column-major format. Let B be an $m \times n$ matrix stored in row-major format.

Based on the preceding discussion, recall that these objects will be mapped to 1-D arrays of length mn , behind the scenes. Let's call the 1-D array representations \hat{A} and \hat{B} . Thus, the (i, j) element of A , a_{ij} , will map to some element \hat{a}_u of \hat{A} ; similarly, b_{ij} will map to some element \hat{b}_v of \hat{B} .

Determine formulae to compute the 1-D index values, u and v , in terms of $\{i, j, m, n\}$. Assume that all indices are 0-based, i.e., $0 \leq i \leq m - 1$, $0 \leq j \leq n - 1$, $0 \leq u, v \leq mn - 1$.

```
In [2]: def linearize_colmajor(i, j, m, n): # calculate `u`
        """
        Returns the linear index for the `(i, j)` entry of
        an `m`-by-`n` matrix stored in column-major order.
        """
        ### BEGIN SOLUTION
        return i + j*m
        ### END SOLUTION
```

```
In [3]: def linearize_rowmajor(i, j, m, n): # calculate `v`
        """
        Returns the linear index for the `(i, j)` entry of
        an `m`-by-`n` matrix stored in row-major order.
        """
        ### BEGIN SOLUTION
        return i*n + j
        ### END SOLUTION
```

```
In [4]: # Test cell: `calc_uv_test`

# Quick check (not exhaustive):
assert linearize_colmajor(7, 4, 10, 20) == 47
assert linearize_rowmajor(7, 4, 10, 20) == 144

assert linearize_colmajor(10, 8, 86, 26) == 698
assert linearize_rowmajor(10, 8, 86, 26) == 268

assert linearize_colmajor(8, 34, 17, 40) == 586
assert linearize_rowmajor(8, 34, 17, 40) == 354

assert linearize_colmajor(32, 48, 37, 55) == 1808
assert linearize_rowmajor(32, 48, 37, 55) == 1808

assert linearize_colmajor(24, 33, 57, 87) == 1905
assert linearize_rowmajor(24, 33, 57, 87) == 2121

assert linearize_colmajor(10, 3, 19, 74) == 67
assert linearize_rowmajor(10, 3, 19, 74) == 743

print("(Passed.)")

(Passed.)
```

Requesting a layout in Numpy

requesting a layout in Numpy

In Numpy, you can ask for either layout. The default in Numpy is row-major.

Historically numerical linear algebra libraries were developed assuming column-major layout. This layout happens to be the default when you declare an array in the Fortran programming language. By contrast, in the C and C++ programming languages, the default convention for a 2-D array is row-major. So the Numpy default is the C/C++ convention.

In your programs, you can request either order of Numpy using the order parameter. For linear algebra operations (common), we recommend using the column-major convention.

In either case, here is how you would create column- and row-major matrices.

```
In [5]: n = 5000
A_colmaj = np.ones((n, n), order='F') # column-major (Fortran convention)
A_rowmaj = np.ones((n, n), order='C') # row-major (C/C++ convention)
```

Exercise 2 (1 point). Given a matrix A , write a function that scales each column, $A(:,j)$ by j . Then compare the speed of applying that function to row and column major order.

```
In [6]: def scale_colwise(A):
        """Given a Numpy matrix `A`, visits each column `A[:, j]`
        and scales it by `j`."""
        assert type(A) is np.ndarray

        n_cols = A.shape[1] # number of columns
        ### BEGIN SOLUTION
        for j in range(n_cols):
            A[:, j] *= j
        ### END SOLUTION
        return A
```

```
In [7]: # Test (timing) cell: `scale_colwise_test`

# Measure time to scale a row-major input column-wise
%timeit scale_colwise(A_rowmaj)

# Measure time to scale a column-major input column-wise
%timeit scale_colwise(A_colmaj)

311 ms ± 3.08 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
28.3 ms ± 202 µs per loop (mean ± std. dev. of 7 runs, 10 loops each)
```

Python vs. Numpy example: Matrix-vector multiply

Look at the definition of matrix-vector multiplication from [Da Kuang's linear algebra notes \(https://www.dropbox.com/s/f410k9fgd7iesdv/kuang-lir-dl=0\)](https://www.dropbox.com/s/f410k9fgd7iesdv/kuang-lir-dl=0). Let's benchmark a matrix-vector multiply in native Python, and compare that to doing the same operation in Numpy.

First, some setup. (What does this code do?)

```
In [8]: # Dimensions; you might shrink this value for debugging
n = 2500
```

```
In [9]: # Generate random values, for use in populating the matrix and vector
from random import gauss

# Native Python, using Lists
A_py = [gauss(0, 1) for i in range(n*n)] # Assume: Column-major
x_py = [gauss(0, 1) for i in range(n)]
```

```
In [10]: # Convert values into Numpy arrays in column-major order
A_np = np.reshape(A_py, (n, n), order='F')
x_np = np.reshape(x_py, (n, 1), order='F')
```

```
In [11]: # Here is how you do a "matvec" in Numpy:
%timeit A_np.dot(x_np)

928 µs ± 124 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

Exercise 3 (3 points). Implement a matrix-vector product that operates on native Python lists. Assume the 1-D **column-major** storage of the matrix A .

```
In [12]: def matvec_py(m, n, A, x):
        """
        Native Python-based matrix-vector multiply, using Lists.
        The dimensions of the matrix A are m-by-n, and x is a
        vector of length n.
        """
        assert type(A) is list and all([type(aij) is float for aij in A])
        assert type(x) is list
        assert len(x) == n
```

```

assert len(A) >= (m*n)

y = [0.] * m
### BEGIN SOLUTION
for j in range(n):
    for i in range(m):
        y[i] += A[i + j*m] * x[j]
### END SOLUTION
return y

```

```

In [13]: # Test cell: `matvec_py_test`

# Estimate a bound on the difference between these two
EPS = np.finfo(float).eps # "machine epsilon"
CONST = 10.0 # Some constant for the error bound
dy_max = CONST * n * EPS

print (""=> Error bound estimate:
        C*n*eps
        == %g*%g*%g
        == %g
        "" % (CONST, n, EPS, dy_max))

# Run the Numpy version and your code
y_np = A_np.dot (x_np)
y_py = matvec_py (n, n, A_py, x_py)

# Compute the difference between these
dy = y_np - np.reshape (y_py, (n, 1), order='F')
dy_norm = np.linalg.norm (dy, ord=np.inf)

# Summarize the results
from IPython.display import display, Math

comparison = "\leq" if dy_norm <= dy_max else ">"
display (Math (
    r' ||y_{\textrm{np}} - y_{\textrm{py}}||_{\infty}'
    r' = \textrm{\%g} \%s \textrm{\%g} \ (\textrm{estimated bound})'
    % (dy_norm, comparison, dy_max)
))

if n <= 4: # Debug: Print all data for small inputs
    print ("@A_np:\n", A_np)
    print ("@x_np:\n", x_np)
    print ("@y_np:\n", y_np)
    print ("@A_py:\n", A_py)
    print ("@x_py:\n", x_np)
    print ("@y_py:\n", y_py)
    print ("@dy:\n", dy)

# Trigger an error on likely failure
assert dy_norm <= dy_max
print("\n(Passed!)")

```

```

==> Error bound estimate:
        C*n*eps
        == 10*2500*2.22045e-16
        == 5.55112e-12

```

$$||y_{\text{np}} - y_{\text{py}}||_{\infty} = 6.6791\text{e-}13 \leq 5.55112\text{e-}12 \text{ (estimated bound)}$$

```

(Passed!)

```

```

In [14]: %timeit matvec_py (n, n, A_py, x_py)

1.66 s ± 30.6 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)

```

Fin! If you've reached this point and everything executed without error, you can submit this part and move on to the next one.

Part 3: Sparse matrix storage

This part is about sparse matrix storage in Numpy/Scipy.

Note: When you submit this notebook to the autograder, there will be a time-limit of about 180 seconds (3 minutes). If your notebook takes more time than that to run, it's likely you are not writing efficient enough code.

Start by running the following code cell to get some of the key modules you'll need.

In [1]:

```
import sys
print(sys.version)

from random import sample # Used to generate a random sample

import numpy as np
print(np.__version__)

import pandas as pd
print(pd.__version__)

from IPython.display import display

# Custom benchmarking code
%load_ext autoreload
%autoreload 2

from cse6040bench import benchit
```

3.7.5 (default, Dec 18 2019, 06:24:58)
[GCC 5.5.0 20171010]
1.19.4
1.1.2

Sample data

For this part, you'll need to download the dataset below. It's a list of pairs of strings. The strings, it turns out, correspond to anonymized Yelp! users (*a*, *b*) exists if user *a* is friends on Yelp! with user *b*.

Exercise 0 (ungraded). Verify that you can obtain the dataset and take a peek by running the two code cells that follow.

In [2]:

```
import requests
import os
import hashlib
import io

local_filename = './resource/asnlib/publicdata/UserEdges-1M.csv'
checksum = '4668034bbcd2fa120915ea2d15eafa8d'
with io.open(local_filename, 'r', encoding='utf-8', errors='replace') as f:
    body = f.read()
    body_checksum = hashlib.md5(body.encode('utf-8')).hexdigest()
    assert body_checksum == checksum, \
        "Data file '{}' has incorrect checksum: '{}' instead of '{}'".format(local_filename,
                                                                              body_checksum,
                                                                              checksum)

    print("==> Checksum test passes: {}".format(checksum))

print("==> '{}' is ready!\n".format(local_filename))
print("(Auxiliary files appear to be ready.)")

==> Checksum test passes: 4668034bbcd2fa120915ea2d15eafa8d
==> './resource/asnlib/publicdata/UserEdges-1M.csv' is ready!

(Auxiliary files appear to be ready.)
```

In [3]:

```
# Peek at the data:
edges_raw = pd.read_csv(local_filename)
display(edges_raw.head ())
print("...\n`edges_raw` has {} entries.".format(len(edges_raw)))
```

	Source	Target
0	18kPq7GPye-YQ3LyKyAZPw	rpOyqD_893cqmDAtJLbdog
1	18kPq7GPye-YQ3LyKyAZPw	4U9kSBLuBDU391x6bxU-YA
2	18kPq7GPye-YQ3LyKyAZPw	fHtTaujcyKvXglE33Z5ylw
3	18kPq7GPye-YQ3LyKyAZPw	8J4IIYcqBIFch8T90N923A
4	18kPq7GPye-YQ3LyKyAZPw	wy6l_zUo7SN0qrvNRWgySw

...
`edges_raw` has 1000000 entries.

Evidently, this dataframe has one million entries.

Exercise 1 (ungraded). Explain what the following code cell does.

```
In [4]: edges_raw_trans = pd.DataFrame({'Source': edges_raw['Target'],
                                         'Target': edges_raw['Source']})
edges_raw_symm = pd.concat([edges_raw, edges_raw_trans])
edges = edges_raw_symm.drop_duplicates()

V_names = set(edges['Source'])
V_names.update(set(edges['Target']))

num_edges = len(edges)
num_verts = len(V_names)
print("==> |V| == {}, |E| == {}".format(num_verts, num_edges))

==> |V| == 107456, |E| == 882640
```

Answer. Give this question some thought before peeking at our suggested answer, which follows.

Recall that the input dataframe, `edges_raw`, has a row (a, b) if a and b are friends. But here is what is unclear at the outset: if (a, b) is an entry in (b, a) also an entry? The code in the above cell effectively figures that out, by computing a dataframe, `edges`, that contains both (a, b) and (b, a) , additional duplicates, i.e., no copies of (a, b) .

It also uses sets to construct a set, `V_names`, that consists of all the names. Evidently, the dataset consists of 107,456 unique names and 441,322 pairs, or 882,640 pairs when you "symmetrize" to ensure that both (a, b) and (b, a) appear.

Graphs

One way a computer scientist thinks of this collection of pairs is as a *graph*: [\(https://en.wikipedia.org/wiki/Graph_\(discrete_mathematics%29\)\)](https://en.wikipedia.org/wiki/Graph_(discrete_mathematics%29))

The names or user IDs are *nodes* or *vertices* of this graph; the pairs are *edges*, or arrows that connect vertices. That's why the final output object `V_names` (for vertex names) and `edges` (for the vertex-to-vertex relationships). The process or calculation to ensure that both (a, b) and (b, a) are edges is sometimes referred to as *symmetrizing* the graph: it ensures that if an edge $a \rightarrow b$ exists, then so does $b \rightarrow a$. If that's true for all edges, the graph is *undirected*. The Wikipedia page linked to above explains these terms with some examples and helpful pictures, so take a moment to read the material before moving on.

We'll also refer to this collection of vertices and edges as the *connectivity graph*.

Sparse matrix storage: Baseline methods

Let's start by reminding ourselves how our previous method for storing sparse matrices, based on nested default dictionaries, works and perform

```
In [5]: def sparse_matrix(base_type=float):
        """Returns a sparse matrix using nested default dictionaries."""
        from collections import defaultdict
        return defaultdict(lambda: defaultdict (base_type))

def dense_vector(init, base_type=float):
    """
    Returns a dense vector, either of a given length
    and initialized to 0 values or using a given list
    of initial values.
    """
    # Case 1: `init` is a list of initial values for the vector entries
    if type(init) is list:
        initial_values = init
        return [base_type(x) for x in initial_values]

    # Else, case 2: `init` is a vector length.
    assert type(init) is int
    return [base_type(0)] * init
```

Exercise 2 (3 points). Implement a function to compute $y \leftarrow Ax$. Assume that the keys of the sparse matrix data structure are integers in the interval $[0, s-1]$ where s is the number of rows or columns as appropriate.

Hint: Recall that you implemented a *dense* matrix-vector multiply in Part 2. Think about how to adapt that same piece of code when the structure for storing A has changed to the sparse representation given in this exercise.

```
In [6]: def spmv(A, x, num_rows=None):
        if num_rows is None:
            num_rows = max(A.keys()) + 1
        y = dense_vector(num_rows)

        # Recall: y = A*x is, conceptually,
        # for all i, y[i] == sum over all j of (A[i, j] * x[j])
        ### BEGIN SOLUTION
        for i, row_i in A.items():
            s = 0.
            for j, val in row_i.items():
                s += val * x[j]
```

```

    for j, a_ij in row_1.items():
        s += a_ij * x[j]
    y[i] = s
    ### END SOLUTION
    return y

```

In [7]: `# Test cell: `spmv_baseline_test``

```

# / 0.   -2.5   1.2 \   / 1. \   / -1.4 \
# / 0.1   1.    0.  / * / 2. / = / 2.1 /
# \ 6.   -1.    0.  /   \ 3. /   \ 4.0 /

```

```

A = sparse_matrix ()
A[0][1] = -2.5
A[0][2] = 1.2
A[1][0] = 0.1
A[1][1] = 1.
A[2][0] = 6.
A[2][1] = -1.

```

```

x = dense_vector ([1, 2, 3])
y0 = dense_vector ([-1.4, 2.1, 4.0])

```

`# Try your code:`

```
y = spmv(A, x)
```

```
max_abs_residual = max([abs(a-b) for a, b in zip(y, y0)])
```

```

print ("==> A:", A)
print ("==> x:", x)
print ("==> True solution, y0:", y0)
print ("==> Your solution, y:", y)
print ("==> Residual (infinity norm):", max_abs_residual)
assert max_abs_residual <= 1e-14

```

```
print ("\n(Passed.)")
```

```

==> A: defaultdict(<function sparse_matrix.<locals>.<lambda> at 0x7fa06b203d40>, {0: defaultdict(<class
{1: -2.5, 2: 1.2}), 1: defaultdict(<class 'float'>, {0: 0.1, 1: 1.0}), 2: defaultdict(<class 'float'>,
-1.0)})})
==> x: [1.0, 2.0, 3.0]
==> True solution, y0: [-1.4, 2.1, 4.0]
==> Your solution, y: [-1.4000000000000004, 2.1, 4.0]
==> Residual (infinity norm): 4.440892098500626e-16

```

(Passed.)

Next, let's convert the edges input into a sparse matrix representing its connectivity graph. To do so, we'll first want to map names to integers.

In [8]:

```

id2name = {} # id2name[id] == name
name2id = {} # name2id[name] == id

```

```

for k, v in enumerate (V_names):
    # for debugging
    if k <= 5: print ("Name %s -> Vertex id %d" % (v, k))
    if k == 6: print ("...")

    id2name[k] = v
    name2id[v] = k

```

```

Name kp0eLSH_znMi-oWeo-tgmA -> Vertex id 0
Name IqYAc0tPG4Z9yzTEcD7hnw -> Vertex id 1
Name v2T0Tq3CnuAexorjj_Ikhg -> Vertex id 2
Name zD_5k650Z3CtyR9pvIwRXA -> Vertex id 3
Name 69QrMQfbjqjFWeBqb7_TWg -> Vertex id 4
Name fpzt05WgsrJCTk-zre5_fw -> Vertex id 5
...

```

Exercise 3 (3 points). Given `id2name` and `name2id` as computed above, convert edges into a sparse matrix, `G`, where there is an entry `G[s][t]` wherever an edge `(s, t)` exists.

Note - This step might take time for the kernel to process as there are 1 million rows

In [9]:

```
G = sparse_matrix()
```

```

### BEGIN SOLUTION
for i in range(len(edges)): # edges is the table above
    s = edges['Source'].iloc[i]
    t = edges['Target'].iloc[i]
    s_id = name2id[s]
    t_id = name2id[t]
    G[s_id][t_id] = 1.0
### END SOLUTION

```



```
In [10]: # Test cell: `edges2spmat1_test`

G_rows_nnz = [len(row_i) for row_i in G.values()]
print ("G has {} vertices and {} edges.".format(len(G.keys()), sum(G_rows_nnz)))

assert len(G.keys()) == num_verts
assert sum(G_rows_nnz) == num_edges

# Check a random sample
for k in sample(range(num_edges), 1000):
    i = name2id[edges['Source'].iloc[k]]
    j = name2id[edges['Target'].iloc[k]]
    assert i in G
    assert j in G[i]
    assert G[i][j] == 1.0

print ("\n(Passed.)")

G has 107456 vertices and 882640 edges.

(Passed.)
```

Exercise 4 (3 points). In the above, we asked you to construct G using integer keys. However, since we are, after all, using default dictionaries, use the vertex *names* as keys. Construct a new sparse matrix, H, which uses the vertex names as keys instead of integers.

```
In [11]: H = sparse_matrix()
#### BEGIN SOLUTION
for i in range(len(edges)): # edges is the table above
    s = edges['Source'].iloc[i]
    t = edges['Target'].iloc[i]
    H[s][t] = 1.0
#### END SOLUTION
```

```
In [12]: # Test cell: `create_H_test`

H_rows_nnz = [len(h) for h in H.values()]
print("`H` has {} vertices and {} edges.".format(len(H.keys()), sum(H_rows_nnz)))

assert len(H.keys()) == num_verts
assert sum(H_rows_nnz) == num_edges

# Check a random sample
for i in sample(G.keys(), 100):
    i_name = id2name[i]
    assert i_name in H
    assert len(G[i]) == len(H[i_name])

print ("\n(Passed.)")

`H` has 107456 vertices and 882640 edges.

(Passed.)
```

Exercise 5 (3 points). Implement a sparse matrix-vector multiply for matrices with named keys. In this case, it will be convenient to have vectors named keys; assume we use dictionaries to hold these vectors as suggested in the code skeleton, below.

Hint: Go back to **Exercise 2** and see what you did there. If it was implemented well, a modest change to the solution for Exercise 2 is all you need here.

```
In [13]: def vector_keyed(keys=None, values=0, base_type=float):
    if keys is not None:
        if type(values) is not list:
            values = [base_type(values)] * len(keys)
        else:
            values = [base_type(v) for v in values]
        x = dict(zip(keys, values))
    else:
        x = {}
    return x

def spmv_keyed(A, x):
    """Performs a sparse matrix-vector multiply for keyed matrices and vectors."""
    assert type(x) is dict

    y = vector_keyed(keys=A.keys(), values=0.0)
    ### BEGIN SOLUTION
    for i, A_i in A.items():
        for j, a_ij in A_i.items():
            y[i] += a_ij * x[j]
    ### END SOLUTION
    return y
```

```
In [14]: # Test cell: `spmv_keyed_test`

#   'row':  / 0.   -2.5   1.2 \   / 1. \   / -1.4 \
#   'your': / 0.1   1.    0.  / * / 2. / = / 2.1 /
#   'boat': \ 6.    -1.    0.  /   \ 3. /   \ 4.0 /

KEYS = ['row', 'your', 'boat']

A_keyed = sparse_matrix ()
A_keyed['row']['your'] = -2.5
A_keyed['row']['boat'] = 1.2
A_keyed['your']['row'] = 0.1
A_keyed['your']['your'] = 1.
A_keyed['boat']['row'] = 6.
A_keyed['boat']['your'] = -1.

x_keyed = vector_keyed (KEYS, [1, 2, 3])
y0_keyed = vector_keyed (KEYS, [-1.4, 2.1, 4.0])

# Try your code:
y_keyed = spmv_keyed (A_keyed, x_keyed)

# Measure the residual:
residuals = [(y_keyed[k] - y0_keyed[k]) for k in KEYS]
max_abs_residual = max ([abs (r) for r in residuals])

print ("==> A_keyed:", A_keyed)
print ("==> x_keyed:", x_keyed)
print ("==> True solution, y0_keyed:", y0_keyed)
print ("==> Your solution:", y_keyed)
print ("==> Residual (infinity norm):", max_abs_residual)
assert max_abs_residual <= 1e-14

print ("\n(Passed.)")
```

```
==> A_keyed: defaultdict(<function sparse_matrix.<locals>.<lambda> at 0x7fa05e6ac200>, {'row': defaultdict
'float'>, {'your': -2.5, 'boat': 1.2}}, 'your': defaultdict(<class 'float'>, {'row': 0.1, 'your': 1.0}))
efaultdict(<class 'float'>, {'row': 6.0, 'your': -1.0}))
==> x_keyed: {'row': 1.0, 'your': 2.0, 'boat': 3.0}
==> True solution, y0_keyed: {'row': -1.4, 'your': 2.1, 'boat': 4.0}
==> Your solution: {'row': -1.4000000000000004, 'your': 2.1, 'boat': 4.0}
==> Residual (infinity norm): 4.440892098500626e-16
```

```
(Passed.)
```

Let's benchmark `spmv()` against `spmv_keyed()` on the full data set. Do they perform differently?

If this benchmark or any of the subsequent ones take an excessively long time to run, including autograder failure, then it's likely you have implemented `spmv_keyed` efficiently. You'll need to look closely and ensure your implementation is not doing something that leads to excessive running time or memory consumption, which might happen if you don't really understand how dictionaries work.

```
In [15]: x = dense_vector ([1.] * num_verts)
          benchit('spmv(G, x)', scope=globals());

          x_keyed = vector_keyed (keys=[v for v in V_names], values=1.)
          benchit('spmv_keyed(H, x_keyed)', scope=globals());

Timing result: (5 trials) x (10 runs) in 7.345442164980341 secs
==> 0.14690884329960682 secs per run
Timing result: (5 trials) x (1 runs) in 1.6500538300606422 secs
==> 0.3300107660121284 secs per run
```

Alternative formats:

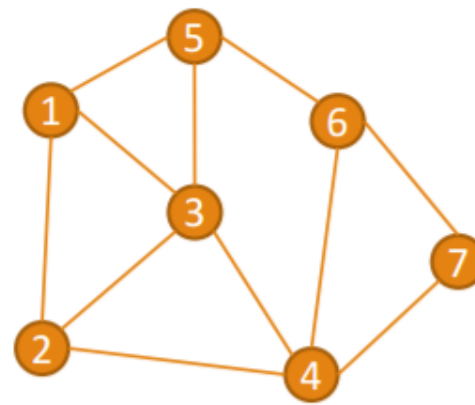
Take a look at the following slides: [link \(https://www.dropbox.com/s/4fwq21dy60g4w4u/cse6040-matrix-storage-notes.pdf?dl=0\)](https://www.dropbox.com/s/4fwq21dy60g4w4u/cse6040-matrix-storage-notes.pdf?dl=0). These slides cover two list-based sparse matrix formats known as *coordinate format* (COO) and *compressed sparse row* (CSR). We will also discuss them briefly.

Coordinate Format (COO)

In this format we store three lists, one each for rows, columns and the elements of the matrix. Look at the below picture to understand how these are formed.

Coordinate (COO) format

The triplets can be stored as 3 arrays: rows, cols, values.



	1	2	3	4	5
1		1	1		
2	1		1	1	
3	1	1		1	
4		1	1		
5	1		1		
6				1	
7				1	

```
rows = [0, 0, 0, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 5, 5, 5, 6, 6]
```

```
cols = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]
```

```
values = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

Note: 0-based arrays

Exercise 6 (3 points). Convert the `edges[:]` data into a coordinate (COO) data structure in native Python using three lists, `coo_rows[:]`, `coo_cols[:]`, `coo_vals[:]`, to store the row indices, column indices, and matrix values, respectively. Use integer indices and set all values to 1.

Hint - Think of what rows, columns and values mean conceptually when you relate it with our dataset of edges

```
In [16]: ### BEGIN SOLUTION
coo_rows = [name2id[s] for s in edges['Source']]
coo_cols = [name2id[t] for t in edges['Target']]
coo_vals = [1.0]*len(edges)
### END SOLUTION
```

```
In [17]: # Test cell: `create_coo_test`

assert len (coo_rows) == num_edges
assert len (coo_cols) == num_edges
assert len (coo_vals) == num_edges
assert all ([v == 1. for v in coo_vals])

# Randomly check a bunch of values
coo_zip = zip (coo_rows, coo_cols, coo_vals)
for i, j, a_ij in sample (list (coo_zip), 1000):
    assert (i in G) and j in G[i]

print ("\n(Passed.)")

(Passed.)
```

Exercise 7 (3 points). Implement a sparse matrix-vector multiply routine for COO implementation.

```
In [18]: def spmv_coo(R, C, V, x, num_rows=None):
        """
        Returns y = A*x, where A has 'm' rows and is stored in
        COO format by the array triples, (R, C, V).
        """
        assert type(x) is list
        assert type(R) is list
        assert type(C) is list
        assert type(V) is list
        assert len(R) == len(C) == len(V)
        if num_rows is None:
            num_rows = max(R) + 1

        y = dense_vector(num_rows)

        ### BEGIN SOLUTION
        for i, j, a_ij in zip(R, C, V):
            y[i] += a_ij * x[j]
        ### END SOLUTION

        return y
```

```
In [19]: # Test cell: `spmv_coo_test`

# / 0. -2.5 1.2 \ / 1. \ / -1.4 \
# | 0.1 1. 0. | * | 2. | = | 2.1 |
# \ 6. -1. 0. / \ 3. / \ 4.0 /

A_coo_rows = [0, 0, 1, 1, 2, 2]
A_coo_cols = [1, 2, 0, 1, 0, 1]
A_coo_vals = [-2.5, 1.2, 0.1, 1., 6., -1.]

x = dense_vector([1, 2, 3])
y0 = dense_vector([-1.4, 2.1, 4.0])

# Try your code:
y_coo = spmv_coo(A_coo_rows, A_coo_cols, A_coo_vals, x)

max_abs_residual = max ([abs(a-b) for a, b in zip(y_coo, y0)])

print("==> A_coo:", list(zip(A_coo_rows, A_coo_cols, A_coo_vals)))
print("==> x:", x)
print("==> True solution, y0:", y0)
print("==> Your solution:", y_coo)
print("==> Residual (infinity norm):", max_abs_residual)
assert max_abs_residual <= 1e-15

print("\n(Passed.)")

==> A_coo: [(0, 1, -2.5), (0, 2, 1.2), (1, 0, 0.1), (1, 1, 1.0), (2, 0, 6.0), (2, 1, -1.0)]
==> x: [1.0, 2.0, 3.0]
==> True solution, y0: [-1.4, 2.1, 4.0]
==> Your solution: [-1.4000000000000004, 2.1, 4.0]
==> Residual (infinity norm): 4.440892098500626e-16

(Passed.)
```

Let's see how fast this is...

```
In [20]: x = dense_vector([1.] * num_verts)
benchit('spmv_coo(coo_rows, coo_cols, coo_vals, x)', scope=globals());

Timing result: (5 trials) x (10 runs) in 9.597134733980056 secs
==> 0.19194269467960112 secs per run
```

Compressed Sparse Row Format

This format tries to compress the sparse matrix further compared to COO format. Suppose you have the following coordinate representation of A where you sort by row index:

```
rows = [0, 0, 0, 1, 1, 1, 2, 2, 2, 2, 3, 3, 3, 3, 4, 4, 4, 5, 5, 5, 6, 6]
cols = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]
values = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
```

If there are nnz nonzeros, then this representation requires $3*nnz$ units of storage since it needs three arrays, each of length nnz .

Observe that when we sort by row index, values are repeated wherever there is more than one nonzero in a row. The idea behind CSR is to exploit redundancy. From the sorted COO representation, we keep the column indices and values as-is. Then, instead of storing every row index, we just store the *offset* of each row in those two lists, which we'll refer to as the *row pointers*, stored as the list `rowptr`, below:

```
cols = [1, 2, 4, 0, 2, 3, 0, 1, 3, 4, 1, 2, 5, 6, 0, 2, 5, 3, 4, 6, 3, 5]
values = [1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1]
rowptr = [0, 3, 6, 10, 14, 17, 20, 22]
```

If the sparse matrix has n rows, then the `rowptr` list has $n+1$ elements, where the last element (`rowptr[-1] == rowptr[n]`) is nnz . (Why might the last element be nnz ?)

Exercise 8 (3 points). Complete the function, `coo2csr(coo_rows, coo_cols, coo_vals)`, below. The inputs are three Python lists corresponding to a sparse matrix in COO format, like the example illustrated above. Your function should return a triple, `(csr_ptrs, csr_inds, csr_vals)`, corresponding to the same matrix but stored in CSR format, again, like what is shown above, where `csr_ptrs` would be the row pointers (`rowptr`), `csr_inds` would be the column indices (`colind`), and `csr_vals` would be the values (`values`).

To help you out, we show how to calculate `csr_inds` and `csr_vals`. You need to figure out how to compute `csr_ptrs`. The function is set up to return three lists.

Your solution needs to handle *empty rows*, too. See the second test cell for an example.

```
In [21]: def coo2csr(coo_rows, coo_cols, coo_vals):
        from operator import itemgetter
```

```

C = sorted(zip(coo_rows, coo_cols, coo_vals), key=itemgetter(0))
nnz = len(C)
assert nnz >= 1

csr_inds = [j for _, j, _ in C]
csr_vals = [a_ij for _, _, a_ij in C]

# Your task: Compute `csr_ptrs`
### BEGIN SOLUTION
def solution_0(C): # "Basic"
    C_rows = [i for i, _, _ in C] # Sorted row indices
    ptrs = [] # Output
    i_previous = None # ID of the previously visited row
    for k, i in enumerate(C_rows):
        if i_previous is None: # `i` is the first row
            ptrs += [0] * (i+1) # `i` may be greater than 0!
        elif i != i_previous: # `i` is a new row index
            ptrs += [k] * (i - i_previous) # handles all-zero rows
        i_previous = i
    ptrs += [len(C_rows)]
    return ptrs

def solution_1(C): # Advanced!
    from collections import Counter
    from itertools import accumulate
    C_rows = [i for i, _, _ in C] # sorted rows
    row_counts = Counter(C_rows)
    num_rows = (C_rows[-1]+1) if C_rows else 0
    offsets = [row_counts.get(i, 0) for i in range(-1, num_rows)]
    return list(accumulate(offsets))

def solution_2(C): # Cuter version of `solution_0`
    from itertools import chain
    C_rows = [i for i, _, _ in C] # sorted rows
    ptrs = ( [[0] * (C_rows[0] + 1)] \
             + [[i] * (C_rows[i]-C_rows[i-1]) for i in range(1, nnz)] \
             + [[len(C)]] )
    return [i for i in chain.from_iterable(ptrs)] #flatten the nested list

csr_ptrs = solution_0(C)
### END SOLUTION

return csr_ptrs, csr_inds, csr_vals

```

In [22]: # Test cell 0: `create_csr_test` (1 point)

```

csr_ptrs, csr_inds, csr_vals = coo2csr(coo_rows, coo_cols, coo_vals)

assert type(csr_ptrs) is list, "`csr_ptrs` is not a list."
assert type(csr_inds) is list, "`csr_inds` is not a list."
assert type(csr_vals) is list, "`csr_vals` is not a list."

assert len(csr_ptrs) == (num_verts + 1), "`csr_ptrs` has {} values instead of {}".format(len(csr_ptrs),
)
assert len(csr_inds) == num_edges, "`csr_inds` has {} values instead of {}".format(len(csr_inds), num_e
assert len(csr_vals) == num_edges, "`csr_vals` has {} values instead of {}".format(len(csr_vals), num_e
assert csr_ptrs[num_verts] == num_edges, "`csr_ptrs[{}]" == {} instead of {}".format(num_verts, csr_ptr
], num_edges)

# Check some random entries
for i in sample(range(num_verts), 10000):
    assert i in G
    a, b = csr_ptrs[i], csr_ptrs[i+1]
    msg_prefix = "Row {} should have these nonzeros: {}".format(i, G[i])
    assert (b-a) == len(G[i]), "{}", which is {} nonzeros; instead, it has just {}".format(msg_prefix,
-a)
    assert all([(j in G[i]) for j in csr_inds[a:b]]), "{}. However, it may have missing or incorrect co
s: csr_inds[{}:{}] == {}".format(msg_prefix, a, b, csr_inds[a:b])
    assert all([(j in csr_inds[a:b] for j in G[i].keys())]), "{}. However, it may have missing or incor
indices: csr_inds[{}:{}] == {}".format(msg_prefix, a, b, csr_inds[a:b])

print ("\n(Passed.)")

```

(Passed.)

In [23]: # Test cell 1: case with empty rows (1 point)

```

#           B           csr_ptrs

# / 0 0 0 0 0 0 0 \           0
# | 0 0 0 0 0 0 0 |           0
# | 1 0 0 1 0 1 0 |           0
# | 0 0 0 0 0 0 0 | --> 3
# | 0 0 0 0 0 0 0 |           3
# | 0 1 0 0 1 0 1 |           3
# \ 0 0 1 1 0 0 0 /           6
#                               8

```

B coo_rows = [2, 2, 2, 5, 5, 5, 6, 6]

```

B_coo_rows = [2, 2, 2, 5, 5, 5, 6, 6]
B_coo_cols = [5, 0, 3, 1, 4, 6, 2, 3]
B_coo_vals = [1, 1, 1, 1, 1, 1, 1, 1]
B_csr_ptrs = [0, 0, 0, 3, 3, 3, 6, 8]

csr_ptrs, _, _ = coo2csr(B_coo_rows, B_coo_cols, B_coo_vals)

print(f'COO format:\n\tcoo_rows = {B_coo_rows} \n\tcoo_cols = {B_coo_cols} \n\tcoo_vals = {B_coo_vals}')
print(f'\nCSR pointers:')
print(f'==> True solution: {B_csr_ptrs}')
print(f'==> Your solution: {csr_ptrs}\n')

assert csr_ptrs == B_csr_ptrs
print("\n(Passed!)")

```

```

COO format:
    coo_rows = [2, 2, 2, 5, 5, 5, 6, 6]
    coo_cols = [5, 0, 3, 1, 4, 6, 2, 3]
    coo_vals = [1, 1, 1, 1, 1, 1, 1, 1]

```

```

CSR pointers:
==> True solution: [0, 0, 0, 3, 3, 3, 6, 8]
==> Your solution: [0, 0, 0, 3, 3, 3, 6, 8]

```

(Passed!)

```

In [24]: # Test cell 2: Spot-check some rows (1 point)

# Given the COO format of our dataset of edges, we will empty randomly selected 3 consecutive rows:
i = np.random.randint(num_verts-3)
idx = np.concatenate((np.where(np.array(coo_rows)==i)[0], np.where(np.array(coo_rows)==i+1)[0],
                        np.where(np.array(coo_rows)==i+2)[0]), axis=0)
coo_rows_empty = np.delete(np.array(coo_rows), idx).tolist()
coo_cols_empty = np.delete(np.array(coo_cols), idx).tolist()
coo_vals_empty = np.delete(np.array(coo_vals), idx).tolist()

# Output of coo2csr:
csr_ptrs_empty, _, _ = coo2csr(coo_rows_empty, coo_cols_empty, coo_vals_empty)

assert max(csr_ptrs_empty) == num_edges - len(idx), f'The largest entry of your output is {max(csr_ptrs
tead of {num_edges - len(idx)}'
assert len(csr_ptrs_empty) == num_verts + 1, f'Your output has {len(csr_ptrs_empty)} entries instead of
1}.'

# Check the CSR format by converting back to COO format:
coo_rows_converted = [(csr_ptrs_empty[i+1] - csr_ptrs_empty[i]) * [i] for i in range(len(csr_ptrs_empty
from itertools import chain
coo_rows_converted = [i for i in chain.from_iterable(coo_rows_converted)]

assert sorted(coo_rows_empty) == coo_rows_converted, "The function doesn't handle the empty rows correc
print ("\n(Passed.)")

(Passed.)

```

Exercise 9 (3 points). Now implement a CSR-based sparse matrix-vector multiply.

```

In [25]: def spmv_csr(ptr, ind, val, x, num_rows=None):
    assert type(ptr) == list
    assert type(ind) == list
    assert type(val) == list
    assert type(x) == list
    if num_rows is None: num_rows = len(ptr) - 1
    assert len(ptr) >= (num_rows+1) # Why?
    assert len(ind) >= ptr[num_rows] # Why?
    assert len(val) >= ptr[num_rows] # Why?

    y = dense_vector(num_rows)
    ### BEGIN SOLUTION
    for i in range(num_rows):
        for k in range(ptr[i], ptr[i+1]):
            y[i] += val[k] * x[ind[k]]
    ### END SOLUTION
    return y

```

```

In [26]: # Test cell: `spmv_csr_test`

# / 0.   -2.5   1.2 \ / 1. \ / -1.4 \
# / 0.1   1.    0.  / * / 2. / = / 2.1 /
# \ 6.   -1.    0.  / \ 3. / \ 4.0 /

A_csr_ptrs = [ 0,      2,      4,      6]
A_csr_cols = [ 1,    2,    0,    1,    0,    1]
A_csr_vals = [-2.5, 1.2, 0.1, 1., 6., -1.]

x = dense_vector([1, 2, 3])

```

```
y0 = dense_vector([-1.4, 2.1, 4.0])

# Try your code:
y_csr = spmv_csr(A_csr_ptrs, A_csr_cols, A_csr_vals, x)

max_abs_residual = max([abs(a-b) for a, b in zip(y_csr, y0)])

print ("==> A_csr_ptrs:", A_csr_ptrs)
print ("==> A_csr_{cols, vals}:", list(zip(A_csr_cols, A_csr_vals)))
print ("==> x:", x)
print ("==> True solution, y0:", y0)
print ("==> Your solution:", y_csr)
print ("==> Residual (infinity norm):", max_abs_residual)
assert max_abs_residual <= 1e-14

print ("\n(Passed.)")

==> A_csr_ptrs: [0, 2, 4, 6]
==> A_csr_{cols, vals}: [(1, -2.5), (2, 1.2), (0, 0.1), (1, 1.0), (0, 6.0), (1, -1.0)]
==> x: [1.0, 2.0, 3.0]
==> True solution, y0: [-1.4, 2.1, 4.0]
==> Your solution: [-1.4000000000000004, 2.1, 4.0]
==> Residual (infinity norm): 4.440892098500626e-16

(Passed.)
```

```
In [27]: x = dense_vector([1.] * num_verts)
        benchit('spmv_csr(csr_ptrs, csr_inds, csr_vals, x)', scope=globals());

Timing result: (5 trials) x (100000 runs) in 2.1117000339436345 secs
==> 4.223400067887269e-06 secs per run
```

Using Scipy's implementations

What you should have noticed is that the list-based COO and CSR formats do not really lead to sparse matrix-vector multiply implementations that are faster than the dictionary-based methods. Let's instead try Scipy's native COO and CSR implementations.

```
In [28]: import numpy as np
        import scipy.sparse as sp

        A_coo_sp = sp.coo_matrix((coo_vals, (coo_rows, coo_cols)))
        A_csr_sp = A_coo_sp.tocsr() # Alternatively: sp.csr_matrix((val, ind, ptr))
        x_sp = np.ones(num_verts)

        print ("\n==> COO in Scipy:")
        benchit('A_coo_sp.dot(x_sp)', scope=globals());

        print ("\n==> CSR in Scipy:")
        benchit('A_csr_sp.dot(x_sp)', scope=globals());

==> COO in Scipy:
Timing result: (5 trials) x (100 runs) in 1.3383243959979154 secs
==> 0.0026766487919958307 secs per run

==> CSR in Scipy:
Timing result: (5 trials) x (100 runs) in 1.0643295320915058 secs
==> 0.0021286590641830115 secs per run
```

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