Help

Course > Module 2: The computational analysis of data > Assignment: Notebook 10 due Nov 6 at 11:59 UTC > Sample solutions

## Sample solutions

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part1 (Score: 9.0 / 9.0)

Test cell (Score: 5.0 / 5.0)
 Test cell (Score: 1.0 / 1.0)
 Test cell (Score: 3.0 / 3.0)

Important note! Before you turn in this lab notebook, make sure everything runs as expected:

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Make sure you fill in any place that says YOUR CODE HERE or "YOUR ANSWER HERE."

## Part 1: Intro to Numpy/Scipy

Numpy (http://www.numpy.org/) is a Python module that provides fast primitives for multidimensional arrays. It's well-suited to implementing numerical linear 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 numerical data.

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

Quick demo. The recommended importing idiom is:

```
In [1]: import numpy as np
```

## 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 experiment below to see.

```
In [3]: n = 1000000
```

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

1 loop, best of 3: 502 ms per loop

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

100 loops, best of 3: 3.53 ms per loop
```

## Creating multidimensional arrays

Beyond simple arrays, Numpy supports multidimensional arrays. To do more than one dimension, call numpy.array() but nest each new dimension within 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]
         [4567]
         [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?
        (3, 4)
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]]]
        (2, 3, 4)
```

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

```
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?

Exercise 1 (ungraded). The following code creates an identity matrix in two different ways, which are found to be equal according to the assertion. But in fact 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(), which 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

#### HINGAINS WING SHORINS

The usual 0-based slicing and indexing notation you know and love from lists is also supported for Numpy arrays. In the multidimensional case, including their 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  $6 \times 6$  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\_red, z\_orange, and z\_cyan.

```
==> 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 will modify the original array.

```
In [21]: print("==> Recall C: %s" % str(C.shape))
         print(C)
         ==> Recall C: (2, 3, 4)
         [[[ 0 1 2 3]
          [4567]
           [ 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)
```

You can force a copy using the .copy() method:

```
In [25]: C_copy = C[1, 0::2, 1::2].copy ()
    C_copy[:, :] = -C_copy[::-1, ::-1]
    print ("==> C_view:")
    print (C_view)

    print ("\n==> C_copy:")
    print (C_copy)

==> C_view:
    [[-23 -21]
    [-15 -13]]

==> C_copy:
    [[13 15]
    [21 23]]
```

And to check whether two Numpy array variables point to the same object, you can use the numpy.may\_share\_memory() function:

```
In [26]: print ("C and C_view share memory: %s" % np.may_share_memory (C, C_view))
    print ("C and C_copy share memory: %s" % np.may_share_memory (C, C_copy))

C and C_view share memory: True
C and C_copy share memory: False
```

#### Indirect addressing

Two other common ways to index a Numpy array are to use a boolean mask or to use a set of integer indices.

Before looking at how to use a boolean mask for indexing, let's create one.

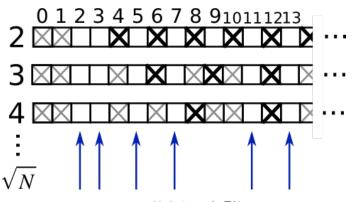
Exercise 3 (1 point). Given the input array, x[:], above, create an array,  $mask_mult_3[:]$  such that  $mask_mult_3[i]$  is true only if x[i] is a positive multiple of 3.

```
In [29]: Student's answer (Top)

mask_mult_3 = (x > 0) & (x % 3 == 0)
```

```
In [30]:
         Grade cell: mask mult 3 test
                                                                                  Score: 1.0 / 1.0 (Top)
         # Test cell: `mask_mult_3_test`
         print ("x:", x)
         print ("mask_mult_3:", mask_mult_3)
         print ("==> x[mask_mult_3]:", x[mask_mult_3])
         inv_mask_mult_3 = np.invert (mask_mult_3)
         assert ((x[mask_mult_3] % 3) == np.zeros (sum (mask_mult_3))).all ()
         assert (((x[inv_mask_mult_3] % 3) != np.zeros (sum (inv_mask_mult_3))) | (x[inv_mask_mu
         lt_3] == 0)).all ()
         x: [10 3 8 0 19 10 11 9 10 6 0 12 7 14 17]
         mask_mult_3:
         [False True False False False False True False True False True
          False False False]
         ==> x[mask_mult_3]: [ 3 9 6 12]
```

Exercise 4 (3 points). Complete the prime number sieve algorithm, which is illustrated below.



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 multiples of i. "Crossing out" means maintaining an array of, say, booleans, and setting values that are multiples of i to False.

```
In [31]:
                                                                                                 (Top)
         Student's answer
          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
              for k in range(2, int(sqrt(n))):
                  is_prime[(2*k):(n+1):k] = False
              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]

#### part2 (Score: 6.0 / 6.0)

Test cell (Score: 2.0 / 2.0)
 Test cell (Score: 1.0 / 1.0)
 Test cell (Score: 3.0 / 3.0)

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## Part 2: Dense matrix storage

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

Exercise 0 (ungraded). Import Numpy!

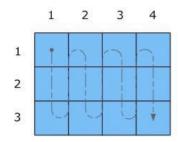
```
In [1]: import numpy as np
```

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

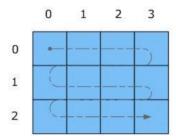
For linear algebra, we will be especially interested in 2-D arrays, which we will use to store matrices. For this common case, there is a subtle performance issue related to how matrices are stored in memory.

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:



A: Column-major order (Fortran-style)



B: Row-major order (C-style) Source: software.intel.com

**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.,  $0 \le i \le m-1$ ,  $0 \le j \le n-1$ , and  $0 \le u$ ,  $v \le mn-1$ .

```
In [2]: Student's answer (Top)

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.

"""

return i + j*m
```

```
In [4]:
        Grade cell: calc_uv_test
                                                                                    Score: 2.0 / 2.0 (Top)
         # 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.)")
```

#### Requesting a layout in Numpy

(Passed.)

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 a 2-D 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 layout. 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 matrices in row and column major order.

```
In [6]: Student's answer (Top)

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
    for j in range(n_cols):
        A[:, j] *= j
    return A
```

```
In [7]: Grade cell: scale_colwise_test

# 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)
```

```
1 loop, best of 3: 606 ms per loop

The slowest run took 11.02 times longer than the fastest. This could mean that an interme diate result is being cached.

1 loop, best of 3: 31.5 ms per loop
```

## Python vs. Numpy example: Matrix-vector multiply

Look at the definition of matrix-vector multiplication from <u>Da Kuang's linear algebra notes</u> (<a href="https://www.dropbox.com/s/f410k9fgd7iesdv/kuang-linalg-notes.pdf?dl=0">https://www.dropbox.com/s/f410k9fgd7iesdv/kuang-linalg-notes.pdf?dl=0</a>). 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)

100 loops, best of 3: 3.06 ms per loop
```

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.

```
In [13]:
                                                                                                  Score: 3.0 / 3.0 (Top)
           Grade cell: matvec_py_test
           # 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 "\gt"</pre>
           display (Math (
                    r' \hspace{0.1cm} |\hspace{0.1cm} y_{\text{\tiny{$1$}}} - y_{\text{\tiny{$1$}}} |\hspace{0.1cm} y_{\text{\tiny{$1$}}}| \hspace{0.1cm} |\hspace{0.1cm} y_{\text{\tiny{$1$}}}|
                     r' = \text{textrm}(g) %s \text{textrm}(g) (\text{textrm}(estimated bound})'
                     % (dy_norm, comparison, dy_max)
           if n <= 4: # Debug: Print all data for small inputs</pre>
                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</pre>
           print("\n(Passed!)")
```

```
==> Error bound estimate: C*n*eps == 10*2500*2.22045e-16 == 5.55112e-12 ||y_{np} - y_{py}||_{\infty} = 1.13687e-13 \le 5.55112e-12 \text{ (estimated bound)} (Passed!)

In [14]: \$timeit matvec_py (n, n, A_py, x_py) 1 loop, best of 3: 2.95 s per loop
```

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

```
part3 (Score: 24.0 / 24.0)
```

- 1. Test cell (Score: 0.0 / 0.0)
- 2. Test cell (Score: 0.0 / 0.0)
- 3. Test cell (Score: 3.0 / 3.0)
- 4. Test cell (Score: 3.0 / 3.0)
- 5. Test cell (Score: 3.0 / 3.0)
- 6. Test cell (Score: 3.0 / 3.0)
- 7. Test cell (Score: 3.0 / 3.0)
- 8. Test cell (Score: 3.0 / 3.0)
- 9. Test cell (Score: 3.0 / 3.0)
- 10. Test cell (Score: 3.0 / 3.0)

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## Part 3: Sparse matrix storage

This part is about sparse matrix storage in Numpy/Scipy. Start by running the following code cell to get some of the key modules you'll need.

```
In [1]: import numpy as np
   import pandas as pd
   from random import sample # Used to generate a random sample
   from IPython.display import display
```

#### 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! user IDs; a pair (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 [21: Grade cells download Score: 0.0 / 0.0 (Ton)
```

--- L-1- | GIAGE CEII, GOWIITOAG

00010. 0.0 / 0.0 (10p)

```
import requests
         import os
         import hashlib
         import io
         def is vocareum():
             return os.path.exists('.voc')
         file = 'UserEdges-1M.csv'
         if is vocareum():
             url = 'https://cse6040.gatech.edu/datasets/{}'.format(file)
             local_filename = '../resource/lib/publicdata/{}'.format(file)
         else:
             local_filename = file
             url = 'https://github.com/cse6040/labs-fa17/raw/master/datasets/{}'.format(file)
         if os.path.exists(local_filename):
            print("[{}]\n==> '{}' is already available.".format(url, local_filename))
             print("[{}] Downloading...".format(url))
             r = requests.get(url)
             with open(local_filename, 'w', encoding=r.encoding) as f:
                 f.write(r.text)
         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, \
                     "Downloaded 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))
        [https://github.com/cse6040/labs-fa17/raw/master/datasets/UserEdges-1M.csv]
        ==> 'UserEdges-1M.csv' is already available.
        ==> Checksum test passes: 4668034bbcd2fa120915ea2d15eafa8d
        ==> 'UserEdges-1M.csv' is ready!
In [3]: Grade cell: peek
                                                                                   Score: 0.0 / 0.0 (Top)
         # 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.

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 this table, is (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), with no 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 441,320 unique 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*: <a href="https://en.wikipedia.org/wiki/Graph\_(discrete\_mathematics">https://en.wikipedia.org/wiki/Graph\_(discrete\_mathematics</a>))

The names or user IDs are *node*s or *vertices* of this graph; the pairs are *edges*, or arrows that connect vertices. That's why the final output objects are named  $v_n$  ames (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 contained in edges is sometimes referred to as *symmetrizing* the graph: it ensures that if an edge  $a \to b$  exists, then so does  $b \to a$ . If that's true for all edges, then the graph is *undirected*. The Wikipedia page linked to above explains these terms with some examples and helpful pictures, so take a moment to review that 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 performs.

```
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  $\lceil 0,s \rangle$  where s is the number of rows or columns as appropriate.

```
In [7]: | Grade cell: spmv_baseline_test
                                                                                         Score: 3.0 / 3.0 (Top)
          # Test cell: `spmv_baseline_test`
             / 0. -2.5 1.2 \ / 1. \ / -1.4 \ | 0.1 1. 0. | = | 2. | = | 2.1 |
                           0. | = | 2. | = | 2.1 |
0. / \ 3. / \ 4.0 /
             ١ 6.
                     -1.
          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</pre>
         print ("\n(Passed.)")
         ==> A: defaultdict(<function sparse matrix.<locals>.<lambda> at 0x10761fbf8>, {0: default
```

```
==> A: defaultdict(<function sparse_matrix.<locals>.<lambda> at 0x10761fbf8>, {0: default dict(<class 'float'>, {1: -2.5, 2: 1.2}), 1: defaultdict(<class 'float'>, {0: 0.1, 1: 1.0}), 2: defaultdict(<class 'float'>, {0: 6.0, 1: -1.0})))
==> x: [1.0, 2.0, 3.0]
==> True solution, y0: [-1.4, 2.1, 4.0]
==> Your solution, y: [-1.400000000000004, 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
name?id = {} # name?id!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 CLS4cITfvt8ex0ckFr17Eg -> Vertex id 0
Name tQcsgxvBnL6FwgiIuCSbSg -> Vertex id 1
Name i-XxQeVD0wH0_chARIMQXw -> Vertex id 2
Name HKnZ2i_fLupIiT05QDAaYw -> Vertex id 3
Name quT3zHVSdqxS9DF5MKNTLA -> Vertex id 4
Name _4vcsFR5Uy1RdgvRILg23Q -> 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] == 1.0 wherever an edge (s, t) exists.

```
In [10]: Grade cell: edges2spmat1_test

# 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.)")
```

**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, we could also use the vertex *names* as keys. Construct a new sparse matrix, H, which uses the vertex names as keys instead of integers.

G has 107456 vertices and 882640 edges.

(Passed.)

H[s][t] = 1.0

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 that also have named keys; assume we use dictionaries to hold these vectors as suggested in the code skeleton, below.

```
In [13]:
                                                                                                 (Top)
         Student's answer
          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 aparse matrix-vector multiply for keyed matrices and vectors."""
              assert type(x) is dict
              y = vector_keyed(keys=x.keys(), values=0.0)
              for i, A_i in A.items():
                  for j, a_ij in A_i.items():
                      y[i] += a_ij * x[j]
              return v
```

```
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 <= le-14

print ("\n(Passed.)")</pre>
```

```
==> A_keyed: defaultdict(<function sparse_matrix.<locals>.<lambda> at 0x10759e730>, {'row': defaultdict(<class 'float'>, {'your': -2.5, 'boat': 1.2}), 'your': defaultdict(<class 'float'>, {'row': 0.1, 'your': 1.0}), 'boat': defaultdict(<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?

```
In [15]: x = dense_vector ([1.] * num_verts)
%timeit spmv (G, x)

x_keyed = vector_keyed (keys=[v for v in V_names], values=1.)
%timeit spmv_keyed (H, x_keyed)

1 loop, best of 3: 422 ms per loop
1 loop, best of 3: 729 ms per loop
```

#### Alternative formats:

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

#### **Coordinate Format (COO)**

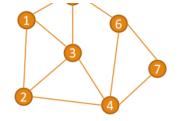
In this format we store three lists, one each for rows, columns and the elements of the matrix. Look at the below picture to understand how these lists are formed.

# Coordinate (COO) format

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







1		1	1		1		
2	1		1	1			
3	1	1		1	1		
4		1	1			1	1
5	1		1			1	
6				1	1		1
7				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[:], and coo\_vals[:], to store the row indices, column indices, and matrix values, respectively. Use integer indices and set all values to 1.

```
In [17]: Grade cell: create_coo_test

# 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]: Student's answer (Top)

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 type(V) is list assert len(R) == len(C) == len(V)
```

```
num_rows is None:
    num_rows = max(R) + 1

y = dense_vector(num_rows)
for i, j, a_ij in zip(R, C, V):
    y[i] += a_ij * x[j]
return y
```

```
In [19]:
                                                                                  Score: 3.0 / 3.0 (Top)
         Grade cell: spmv_coo_test
          # Test cell: `spmv_coo_test`
             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</pre>
         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: [-1.400000000000004, 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)
%timeit spmv_coo(coo_rows, coo_cols, coo_vals, x)

1 loop, best of 3: 545 ms per loop
```

#### **Compressed Sparse Row Format**

This is similar to the COO format excpet that it is much more compact and takes up less storage. Look at the picture below to understand more about this representation

## Compressed sparse row (CSR) format

Suppose a sparse matrix has nnz nonzero entries.

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

The COO format needs 3nnz elements to store the matrix. Can we do better?

When the nonzeros are stored row by row, we can compress the above storage:

This CSR format needs 2nnz+n elements to store the matrix.

Exercise 8 (3 points). Now create a CSR data structure, again using native Python lists. Name your output CSR lists csr\_ptrs, csr\_inds, and csr\_vals.

It's easiest to start with the COO representation. We've given you some starter code.

```
In [21]: Student's answer
                                                                                                    (Top)
          from operator import itemgetter
          C = sorted(zip(coo_rows, coo_cols, coo_vals), key=itemgetter(0))
          nnz = len(C)
          assert nnz >= 1
          assert (C[-1][0] + 1) == num verts # Why?
          csr_inds = [j for _, j, _ in C]
csr_vals = [a_ij for _, _, a_ij in C]
          # Your task: Compute `csr ptrs`
          ### BEGIN SOLUTION
          C_rows = [i for i, _,
                                  _ in C] # sorted row indices
          csr_ptrs = [0] * (num_verts + 1)
          cur_row = -1 # current row (initially an invalid index, -1)
          for k, row in enumerate(C_rows):
              if row != cur row: # Found a new row index
                   csr ptrs[row] = k # Record location
                   cur_row = row
          # Some rows might have been empty. The
          # next step fills those in.
          from itertools import accumulate
          csr_ptrs = list(accumulate(csr_ptrs, max))
          # Lastly, the boundary element:
          csr_ptrs[-1] = nnz
          ### END SOLUTION
```

```
assert len(csr_inds) == num_edges, " csr_inds  nas {} values instead or {}".format(len(
csr_inds), num_edges)
assert len(csr_vals) == num_edges, "`csr_vals` has {} values instead of {}".format(len(
csr vals), num edges)
assert csr_ptrs[num_verts] == num_edges, "`csr_ptrs[{}]` == {} instead of {}".format(nu
m verts, csr ptrs[num verts], 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 {}.".for
mat(msg_prefix, len(G[i]), b-a)
   assert all([(j in G[i]) for j in csr inds[a:b]]), "{}. However, it may have missing
or incorrect column indices: csr_inds[{}:{}] == {}".format(msg_prefix, a, b, csr_inds[a
:b1)
   assert all([(j in csr_inds[a:b] for j in G[i].keys())]), "{}. However, it may have
missing or incorrect column indices: csr_inds[{}:{}] == {}".format(msg_prefix, a, b, cs
r_inds[a:b])
print ("\n(Passed.)")
```

(Passed.)

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

```
In [23]: Student's answer
                                                                                                (Top)
          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)
              for i in range(num_rows):
                  for k in range(ptr[i], ptr[i+1]):
                      y[i] += val[k] * x[ind[k]]
              return y
```

```
In [24]: Grade cell: spmv_csr_test
                                                                              Score: 3.0 / 3.0 (Top)
         # Test cell: `spmv_csr_test`
            \ 6. -1.
         A_csr_ptrs = [0,
                                 2.
                                         4.
         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 ("==> Vour colution."
```

```
print ("==> Residual (infinity norm):", max_abs_residual)
assert max_abs_residual <= le-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: [-1.400000000000004, 2.1, 4.0]
==> Residual (infinity norm): 4.440892098500626e-16

(Passed.)

In [25]: x = dense_vector([1.] * num_verts)
%timeit spmv_csr(csr_ptrs, csr_inds, csr_vals, x)

1 loop, best of 3: 346 ms per loop
```

## **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 much faster than the dictionary-based methods. Let's instead try Scipy's native COO and CSR implementations.

```
In [26]: 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)
```

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