Hwk 4

February 1, 2018

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

        # Graphics
        import matplotlib as mpl
        import matplotlib.pyplot as plt
        import seaborn as sns
        from matplotlib import rc

        rc('text', usetex=True)
        rc('text.latex', preamble=r'\usepackage{cmbright}')
        rc('font', **{'family': 'sans-serif', 'sans-serif': ['Helvetica']})

        # Magic function to make matplotlib inline;
        %matplotlib inline

        # This enables SVG graphics inline.
        # There is a bug, so uncomment if it works.
        %config InlineBackend.figure_formats = {'png', 'retina'}

        # JB's favorite Seaborn settings for notebooks
        rc = {'lines.linewidth': 2,
              'axes.labelsize': 18,
              'axes.titlesize': 18,
              'axes.facecolor': 'DFDFE5'}
        sns.set_context('notebook', rc=rc)
        sns.set_style("dark")

        mpl.rcParams['xtick.labelsize'] = 16
        mpl.rcParams['ytick.labelsize'] = 16
        mpl.rcParams['legend.fontsize'] = 14
```

2   Implementation of Needleman Wunsch algorithm

The algorithm below works but is a little incomplete. At the moment it will fail if there are multiple optimal alignments, but this could be easily solved by choosing one optimal alignment at random. Alternatively, I could modify it by presenting all possible alignments, but I started this morning and ran out of time. All work below is my own.

```
In [9]: class needle:
            def __init__(self, a, b):
                """Initialize needle object"""
                self.a = ' ' + a
                self.b = ' ' + b
                self.m, self.x, self.g = 10, -1, -5
                self.make_mat()
                self.histories = {}

            def make_mat(self):
                """Initialize alignment matrix"""
                n, n2 = len(self.a), len(self.b)
                mat = np.zeros(shape=(n, n2))
                mat[:,0]= np.linspace(0, (n-1)*self.g, n)
                mat[0,:] = np.linspace(0, (n2-1)*self.g, n2)
                self.mat = mat

            def matcher(self, c1, c2):
                """For a pair of coordinates, if the pair matches,
                figure out whether they should be aligned or not"""
                if self.a[c1] == self.b[c2]:
                    return self.m
                else:
                    return self.x

            def submat(self, c1, c2):
                """Returns a 2x2 submatrix"""
                smat = self.mat[c1-1:c1+1, c2-1:c2+1]
                return smat

            def next_square(self, c1, c2):
                """Fill in the next 2x2 square"""
                smat = self.submat(c1, c2)
                # (c1,c2)-1 -> (c1, c2) is a possible match
                s00 = smat[0, 0] + self.matcher(c1, c2)
                # other two are gaps
                s10 = smat[1, 0] + self.g
                s01 = smat[0, 1] + self.g

                array = np.array([s00, s10, s01])
                score = np.max(array)
```

```python
            self.mat[c1, c2] = score
            self.histories[(c1, c2)] = np.where(array == score)[0]

    def fill_in(self):
        """Fill in the matrix"""
        for c1 in range(1, len(self.a)):
            for c2 in range(1, len(self.b)):
                self.next_square(c1, c2)

    def init_traceback(self):
        """Initialize the traceback parameters"""
        # coordinates of the maximum score(s)
        # note, np.where returns an x-coord array and a y-coord
        # array in a tuple if there is more than one entry
        c = np.where(np.max(self.mat[:,len(self.b)-1]) == self.mat)
        if len(c[0]) > 1:
            # there are multiple alignments
            print('uhoh')
        else:
            self.initial_coords = (c[0][0], c[1][0])
            begin = self.histories[self.initial_coords]

        self.begin = begin


    def trace(self, c1, c2, trace, Sa, Sb):
        """Figures out whether it is a gap or a mismatch or what"""
        if len(trace) == 1:
            if trace[0] == 0:
                return c1-1, c2-1, self.a[c1-1]+Sa, self.b[c1-1]+Sb
            if trace[0] == 1:
                return c1-1, c2, self.a[c1-1]+Sa, '-'+Sb
            else:
                return c1, c2 -1, '-'+Sa, self.b[c2-1]+Sb
        else:
            print('uhoh')

    def traceback(self):
        """
        Trace an alignment path.
        This function currently only works if there is a SINGLE
        allowable alignment...
        I could easily fix this by choosing a random alignment out of
        the multiple optimal ones
        """
        self.init_traceback()
        c = np.where(np.max(self.mat[:,len(self.b)-1]) == self.mat)
        c1_init = c[0][0]
```

```
                c2_init = c[1][0]
                C1, C2 = np.array([c1_init]), np.array([c2_init])
                F = True
                c1, c2 = c1_init, c2_init
                Sa = self.a[c1]
                Sb = self.b[c2]
                while F:
                    if (c1, c2) not in self.histories.keys():
                        F = False
                        continue
                    c1, c2, Sa, Sb = self.trace(c1, c2, self.histories[(c1, c2)], Sa, Sb)
                    C1, C2 = np.append(C1, [c1]), np.append(C2, [c2])
                self.C1 = C1
                self.C2 = C2

            def draw_alignments(self):
                """Draw the alignment as a matrix of zeros and 1's"""
                self.m = np.zeros(shape=(len(self.a), len(self.b)))
                for coord in zip(self.C1, self.C2):
                    self.m[coord[0], coord[1]] = 1
                print(self.m)

In [3]: wunsch = needle('atcg', 'atc')
        wunsch.fill_in()
        wunsch.mat

Out[3]: array([[  0.,   -5.,  -10.,  -15.],
               [ -5.,   10.,    5.,    0.],
               [-10.,    5.,   20.,   15.],
               [-15.,    0.,   15.,   30.],
               [-20.,   -5.,   10.,   25.]])
```

Here, I perform the traceback, and then draw the alignment as a matrix of zeros and ones.

```
In [4]: wunsch.traceback()
        wunsch.draw_alignments()

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

3   Implementation of a random number generator with a negative binomial distribution

For this problem, I relied heavily on this PDF, page 21.

A geometric random variable, Y_N can be generated from a `geom(p)` distribution by using the generator:

$$Y_i = \left\lfloor 1 + \frac{\log u_i}{\log 1 - p} \right\rfloor$$

The PDF I used claims that the negative binomial distribution with parameters p and n can be generated by calculating:

$$r + \sum_i^r Y_i(p)$$

However, when I compare my generator with the scipy generator, the functions are shifted and the correction that matches the curves exactly is:

$$\sum_i^r Y_i(p) - r$$

```python
In [5]: # define parameters to use
        n = 10
        p = .1
```
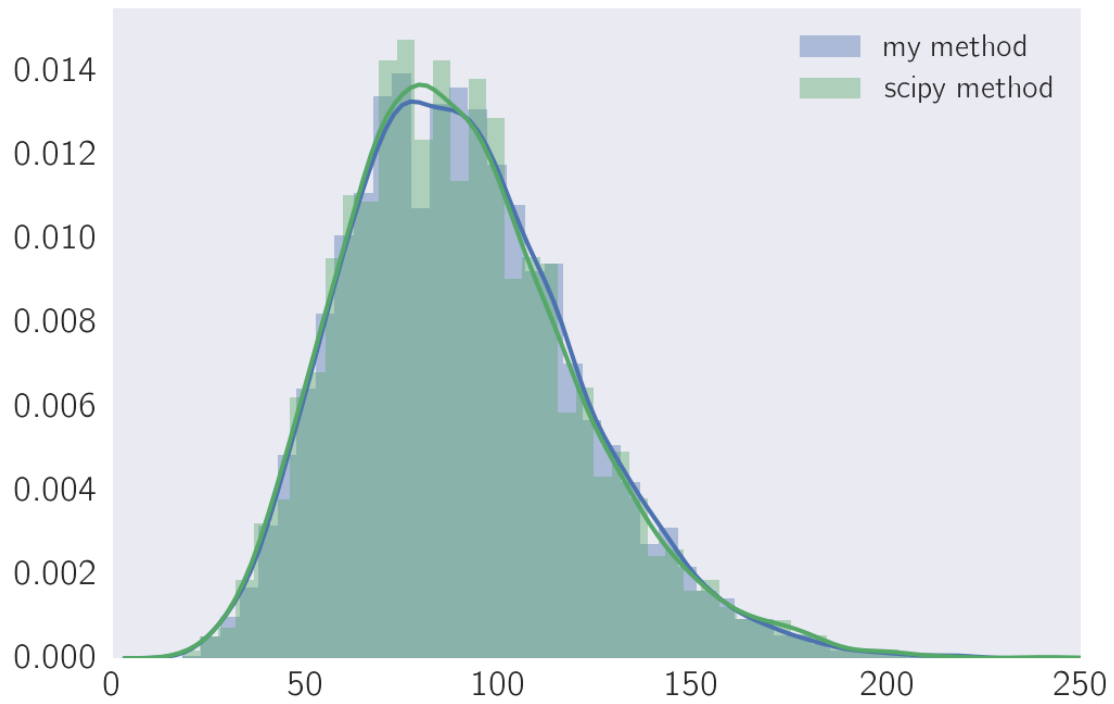
```python
In [6]: def bernoulli_generator(p):
            """Given a probability `p`, returns a geometrically distributed variable"""
            u = np.random.random()
            return np.floor(1 + np.log(u)/np.log(1-p))


        def neg_binom_generator(n, p):
            """Generates random numbers with a negative binomial distribution.
            The method used is to add `n` random bernoulli variables, then subtracts
            `n`."""
            return np.sum(np.array([bernoulli_generator(p) for i in range(n)])) - n
```

```python
In [7]: # make arrays for histograms
        iters = 10**4
        # my function
        x = np.array([neg_binom_generator(n, p) for i in range(iters)])
        # scipy function
        y = np.array([stats.nbinom.rvs(n, p, size=1) for i in range(iters)])
```

```python
In [8]: # plot
        ax = sns.distplot(x, label='my method')
        ax = sns.distplot(y, label='scipy method')
        plt.xlim(0, 250)
        plt.legend()
```

Out[8]: <matplotlib.legend.Legend at 0x105df3710>

In [ ]: