Homework 4 - MCM

April 6, 2018

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In [41]: import numpy as np
         import matplotlib.pyplot as plt
         from matplotlib import cm
```

1 Homework 4

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```
In [21]: # code to generate transition matrix
         W = np.zeros((5, 5))
         W[0] = 0.5
         W[4, 4] = 0.5
         for i in range(4):
             W[i+1, i] = 0.5

In [22]: # transition matrix
         W

Out[22]: array([[0.5, 0.5, 0.5, 0.5, 0.5],
                [0.5, 0. , 0. , 0. , 0. ],
                [0. , 0.5, 0. , 0. , 0. ],
                [0. , 0. , 0.5, 0. , 0. ],
                [0. , 0. , 0. , 0.5, 0.5]])

In [23]: # code to generate eigenvalues and eigenvectors from transition matrix
         eigenValues, eigenVectors = np.linalg.eig(W)

In [24]: # the real component of the eigenvalues
         eigenValues.real

Out[24]: array([ 1.0000000e+00, -4.8513264e-05, -4.8513264e-05,  4.8513264e-05,
                 4.8513264e-05])

In [25]: # the real component of the eigenvectors
         eigenVectors.real

Out[25]: array([[ 8.62662186e-01,  1.29136450e-12,  1.29136450e-12,
                  1.29205783e-12,  1.29205783e-12],
```

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              [ 4.31331093e-01,  8.86518505e-13,  8.86518505e-13,
               -4.05111415e-13, -4.05111415e-13],
              [ 2.15665546e-01, -6.86114440e-05, -6.86114440e-05,
               -6.86114448e-05, -6.86114448e-05],
              [ 1.07832773e-01,  7.07141081e-01,  7.07141081e-01,
               -7.07072470e-01, -7.07072470e-01],
              [ 1.07832773e-01, -7.07072470e-01, -7.07072470e-01,
                7.07141081e-01,  7.07141081e-01]])
```

```
In [26]: # code to generate the steady state distribution from the first eigenvector
         eV1 = eigenVectors.real[:, 0]
         eV1 = np.abs(eV1) / np.linalg.norm(eV1, 1)
         ssd = eV1.reshape((5, 1))
```

```
In [27]: # the steady state distribution
         ssd
```

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Out[27]: array([[0.5   ],
                [0.25  ],
                [0.125 ],
                [0.0625],
                [0.0625]])
```

```
In [28]: # code for generating the expected value
         x = np.linspace(1, 5, 5)

         expectedValue = 0
         for i in range(len(x)):
             expectedValue = expectedValue + x[i]*ssd[i]
```

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In [29]: # the expected value
         expectedValue
```

```
Out[29]: array([1.9375])
```

2 Question 2

```
In [30]: def MultiDNorm(init, mu, sigma, mu2, sigma2):
             """the target distribution, x = [x1, x2],mu, mu2 = mean
             and sigma and sigma2 is the covariance matrix"""
             k = len(init)
             mu.reshape(k,1)
             mu2.reshape(k, 1)
             init.reshape(k,1)

             # exponential part
             v = np.exp(-0.5 * np.dot((init - mu).T,np.dot(np.linalg.inv(sigma), (init -mu)))
             # prefactor
```

```
        v = v/np.sqrt((2*np.pi)**k * np.linalg.det(sigma))

        # exponential part
        v2 = np.exp(-0.5 * np.dot((init - mu2).T,np.dot(np.linalg.inv(sigma2), (init -mu2))
        # prefactor
        v2 = v2/np.sqrt((2*np.pi)**k * np.linalg.det(sigma2))

        return 0.6*v + 0.4*v2
```

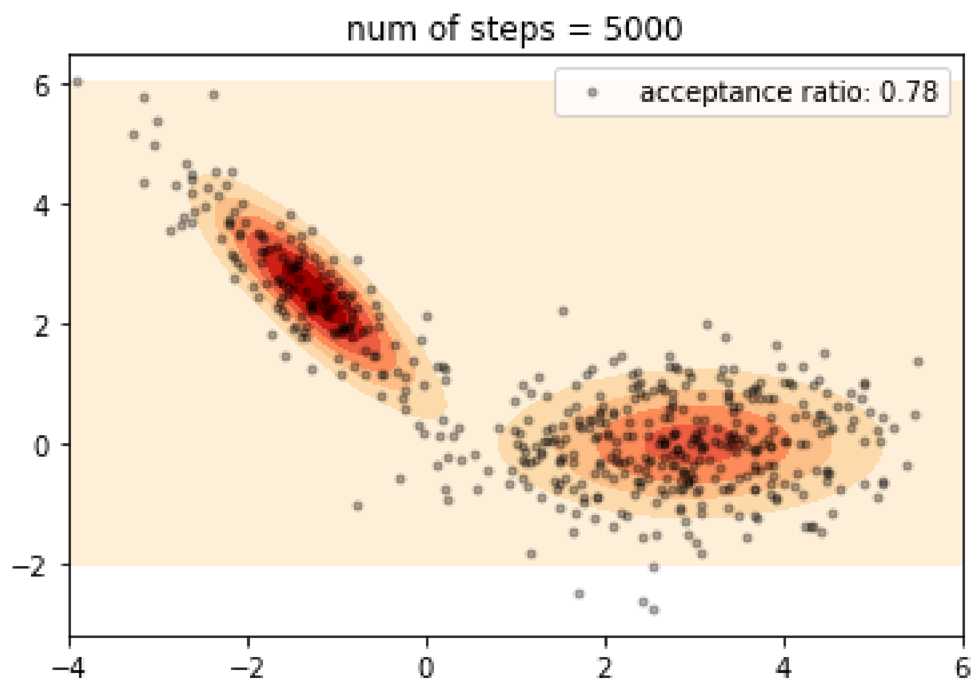
```
In [31]: def proposal_u(oldx, delta):
             newx = oldx + np.random.uniform(-delta, delta,oldx.shape)
             return newx

         def proposal_n(oldx, delta):
             newx = oldx + np.random.normal(-delta, delta,oldx.shape)
             return newx

         def metropolis_accept(newx, oldFuncVal, m, S, m2, S2, func):
             accept = False
             newFuncVal = func(newx, m, S, m2, S2)
             ratio = newFuncVal/(oldFuncVal + 1.0e-21)
             if ratio > 1.:
                 accept = True
             elif np.random.rand() < ratio:
                 accept = True

             return accept, newFuncVal
```

```
In [39]: def driver(x, delta, prop_flag, nsteps, thin=10):
             # target distribution parameters
             mu1 = np.array([3., 0.]).reshape(2,1)
             Sig1 = np.array([[1.5, 0], [0, 0.5]])
             mu2 = np.array([-1.25, 2.5]).reshape(2,1)
             Sig2 = np.array([[0.5, -0.6], [-0.6, 1.]])
             # initialize
             f = MultiDNorm(x, mu1, Sig1, mu2, Sig2)
             AccRatio = 0.0
             NumSucc  = 0
             recz     = np.zeros((int(nsteps/thin), 2)) # record
             # actual chain
             for iMCS in range(nsteps):
                 if prop_flag:
                     newx = proposal_u(x, delta)
                 else:
                     newx = proposal_n(x, delta)

                 accept, newf = metropolis_accept(newx, f, mu1,Sig1, mu2, Sig2, MultiDNorm)
```

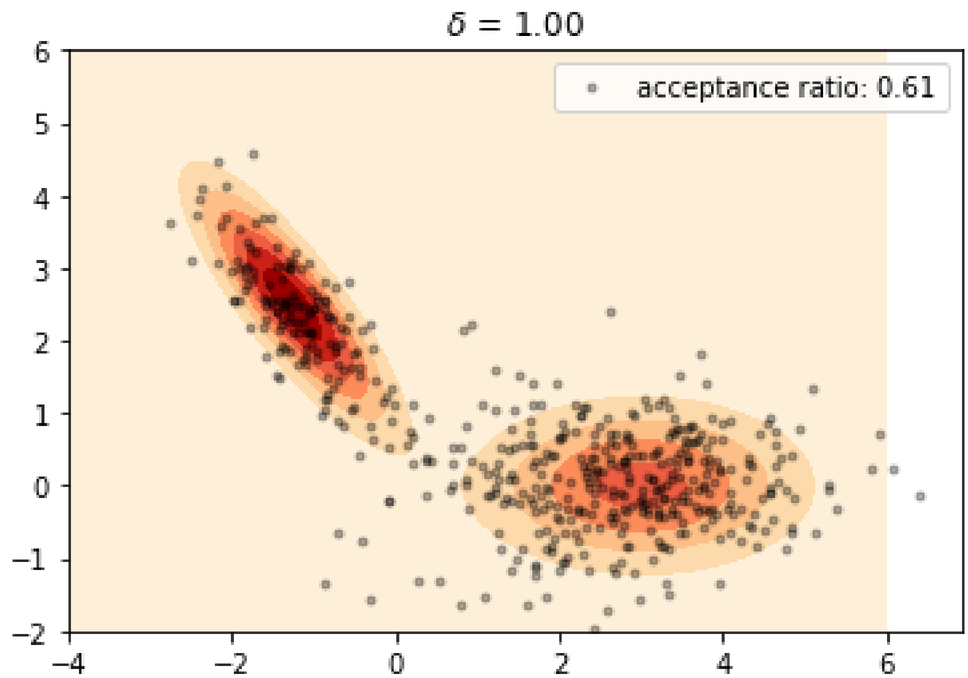
```
            if accept:
                NumSucc += 1
                x = newx
                f = newf

            if (iMCS % thin) == 0:
                recz[int(iMCS/thin)] = x.T

        AccRatio = float(NumSucc)/float(nsteps)

        x = np.linspace(-4,6,100)
        y = np.linspace(-2,6,100)
        X, Y = np.meshgrid(x,y)
        # FIX THIS LINE
        Z = np.zeros((100, 100))
        for i in range(len(X)):
            for j in range(len(Y)):
                init = np.vstack([X[i, j], Y[i, j]])
                Z[i, j] = MultiDNorm(init, mu1, Sig1, mu2, Sig2)

        return recz, AccRatio, X, Y, Z
```

In [126]:
```
#different trial runs (varying number of MC steps):
mc_steps = [ 1000, 5000,10000]
# fixed variables:
x2 = np.array([0., 0.]).reshape(2,1)
delta = 0.5
prop_flag = True
# times 4
recz, AccRatio, X, Y, Z =driver(x2, delta, prop_flag, mc_steps[1])

plt.plot(recz[:,0],recz[:,1],'k.', alpha=0.3, label = f'acceptance ratio: {AccRatio:0.

plt.title('num of steps = {:d}'.format(mc_steps[1]))
plt.legend()
plt.contourf(X, Y, Z, cmap=cm.OrRd)
```

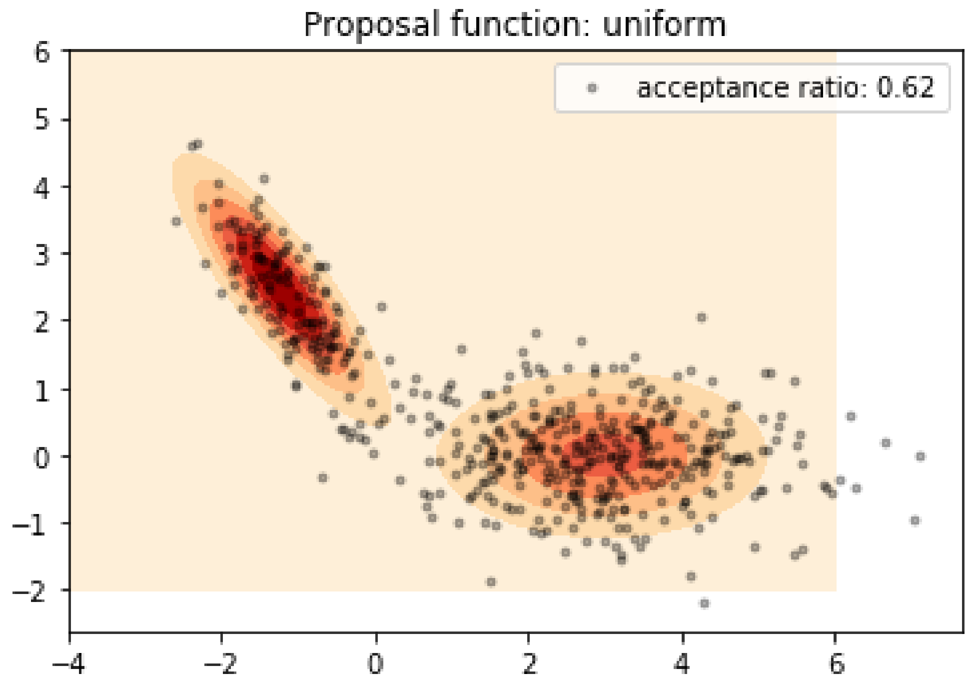
Out[126]:
```
<matplotlib.contour.QuadContourSet at 0x7fe6e6338f28>
```



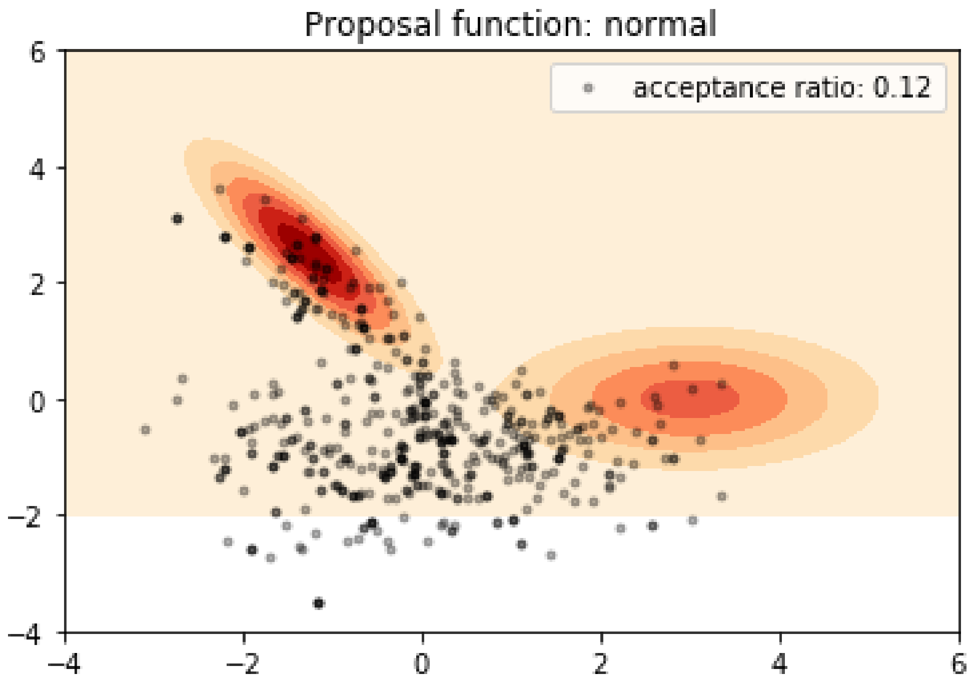

```
In [140]: # different trial runs (different delta)
          deltas = [0.3, 0.5, 1.0, 2.0]
          # fixed variables
          nsteps = 5000

          # times 4
          recz, AccRatio, X, Y, Z = driver(x2, deltas[2], prop_flag, nsteps)
          plt.plot(recz[:,0],recz[:,1],'k.', alpha=0.3, label = f'acceptance ratio: {AccRatio:0.

          plt.title('$\delta$ = {0:0.2f}'.format(deltas[2]))
          plt.legend()
          plt.contourf(X, Y, Z, cmap=cm.OrRd)

Out[140]: <matplotlib.contour.QuadContourSet at 0x7fe6e5c4e7f0>
```



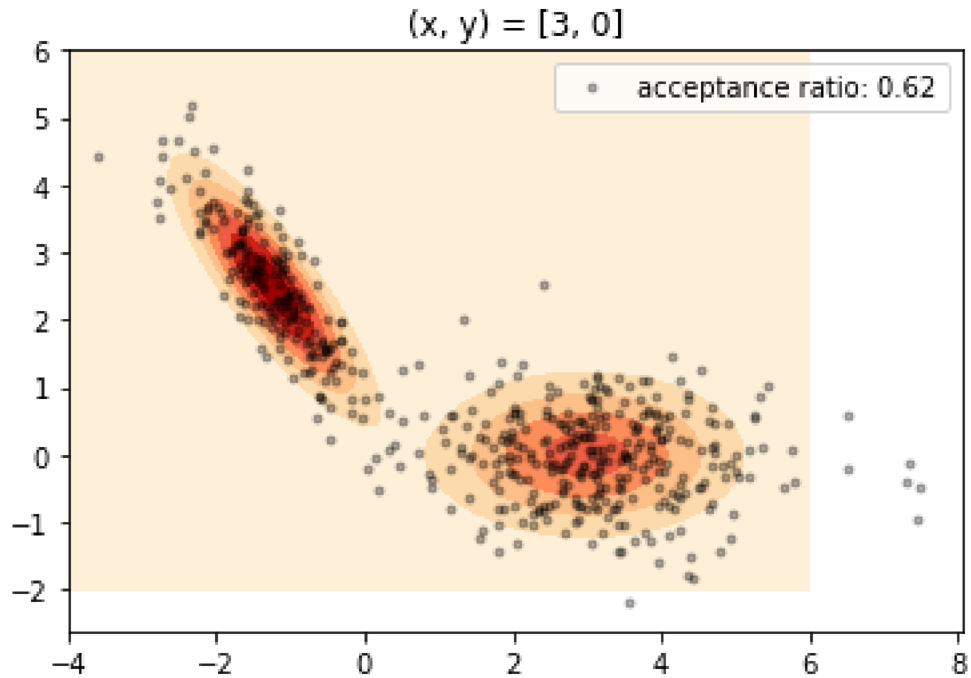

```
In [128]: # normal vs proposal function
          delta = 1.0

          recz, AccRatio, X, Y, Z = driver(x2, delta, True, nsteps)
          plt.plot(recz[:,0],recz[:,1],'k.', alpha=0.3, label = f'acceptance ratio: {AccRatio:0.

          plt.title('Proposal function: uniform')
          plt.legend()
          plt.contourf(X, Y, Z, cmap=cm.OrRd)

Out[128]: <matplotlib.contour.QuadContourSet at 0x7fe6e6224fd0>
```




```
In [129]: recz, AccRatio, X, Y, Z = driver(x2, delta, False, nsteps)
          plt.plot(recz[:,0],recz[:,1],'k.', alpha=0.3, label = f'acceptance ratio: {AccRatio:0.

          plt.title('Proposal function: normal')
          plt.legend()
          plt.contourf(X, Y, Z, cmap=cm.OrRd)

Out[129]: <matplotlib.contour.QuadContourSet at 0x7fe6e61a51d0>
```




```
In [144]: # different initial states
          x_vals = [[0,0],[-4,6],[6,-2],[-1,2], [3,0]]

          # times 5
          recz, AccRatio, X, Y, Z = driver(np.asarray(x_vals[4]).reshape(2,1), delta, prop_flag,
          plt.plot(recz[:,0],recz[:,1],'k.', alpha=0.3, label = f'acceptance ratio: {AccRatio:0.

          plt.title('(x, y) = {0}'.format(x_vals[4]))
          plt.legend()
          plt.contourf(X, Y, Z, cmap=cm.OrRd)

Out[144]: <matplotlib.contour.QuadContourSet at 0x7fe6e5aa7828>
```



Tune the parameters, until you are "visually" satisfied with the sampling. Report your observations, and try to explain them in terms of (a) the acceptance ratio, and (b) peaks exploration of both peaks?

Number of MC steps > When modifying the number of MC steps, I found that although the acceptance ratio was highest with 1000 steps (0.78), the contour plot was too sparse to be an acceptable exploration of peaks. With 5000 steps, the exploration of peaks was even and had about the same value of acceptance ratio (0.76)

Number of MC Steps	Acceptance Ratio
1000	0.78
10000	0.75
5000	0.76

The choice of δ > As the value of delta grew, the acceptance ratio decreased. However, upon visualization of the exploration of peaks, $\delta = 1.0$ appeared to have the best representation of both peaks

δ	Acceptance Ratio
0.3	0.89
0.5	0.79
1.0	0.59
2.0	0.37

Use a normal proposal function instead of uniform > The normal distribution does not sample from the right peak at all, while the uniform distribution samples from both equally.

Proposal distribution	Acceptance Ratio
uniform	0.61
normal	0.12

Different initial states > I used initial states with specific orientation to the peaks to test the acceptance ratio. (0, 0) is the closest to the center of the two peaks while (-4, 6) and (6,-2) are the opposite corners of the sampling space. (3, 0) and (-1,2) are the estimated center points of the peaks. Generally they range from 0.5-0.65 acceptance ratio, and as we know from class, if there are enough MC steps, variance in the initial state should have a negligent effect on the final acceptance ratio

x, y	Acceptance Ratio
(0,0)	0.61
(-4, 6)	0.55
(6, -2)	0.61
(3, 0)	0.62
(-1, 2)	0.61