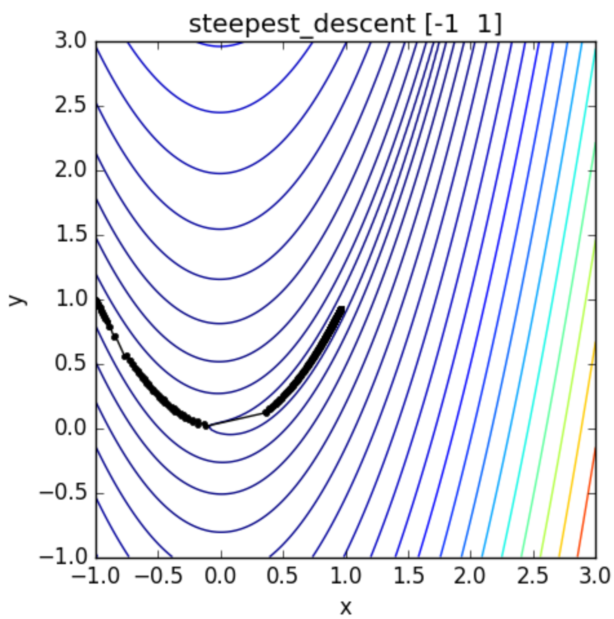
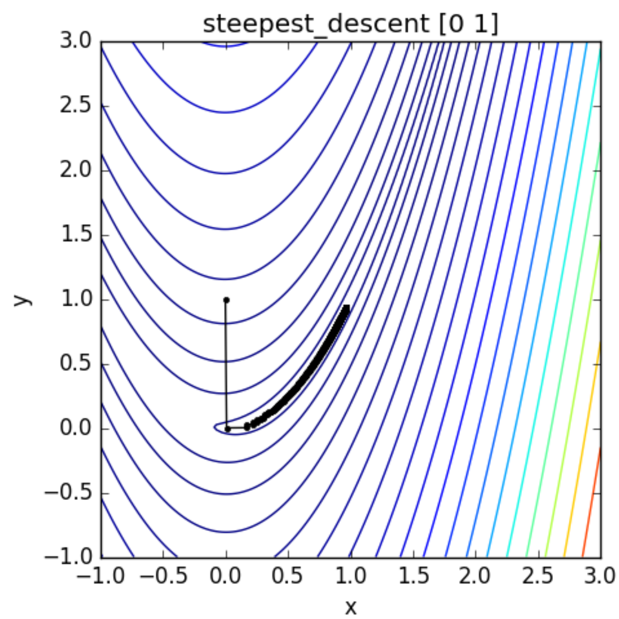
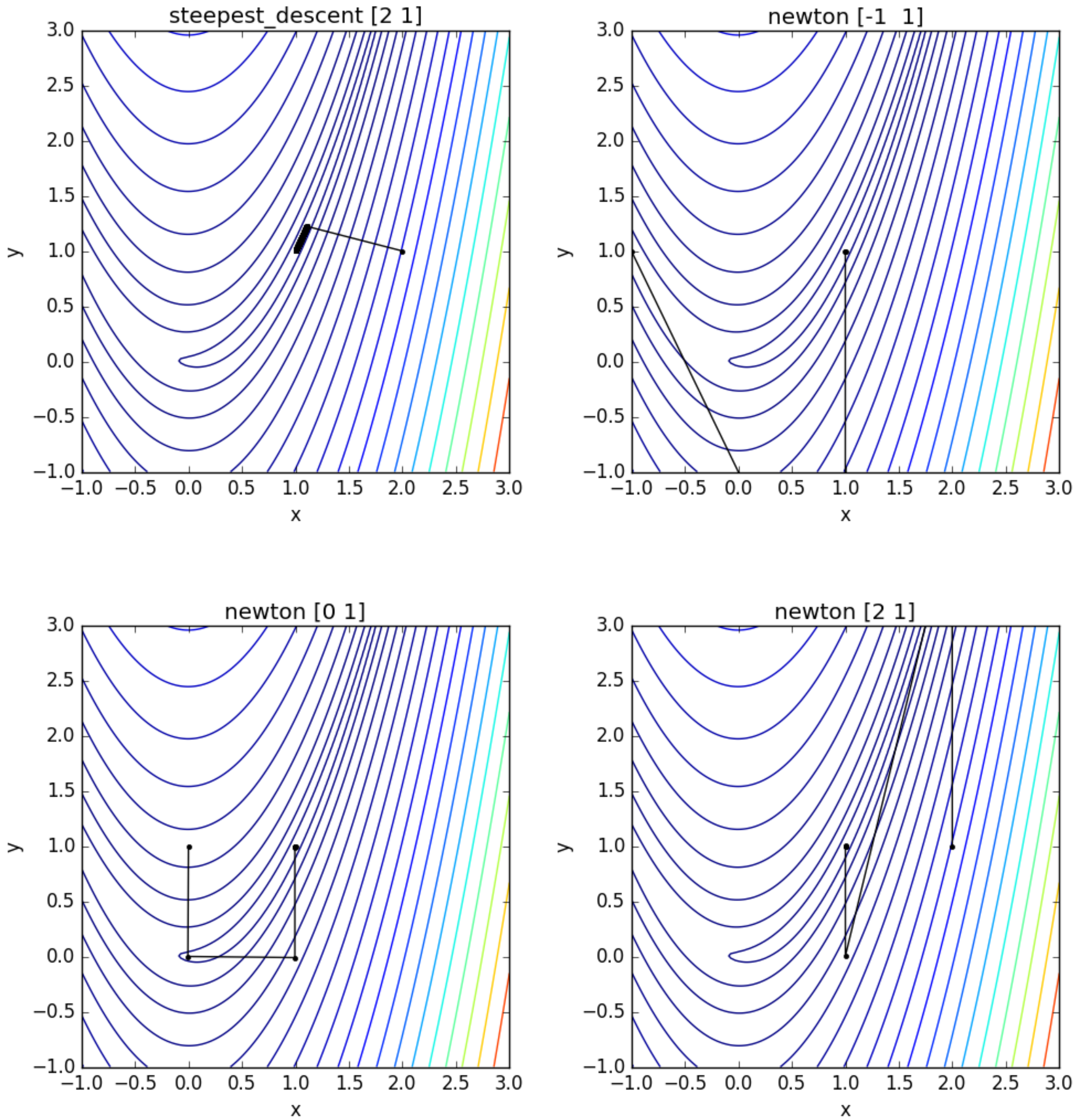
Shawn Pan - AM205 Homework 5 Code is attached as separate files.

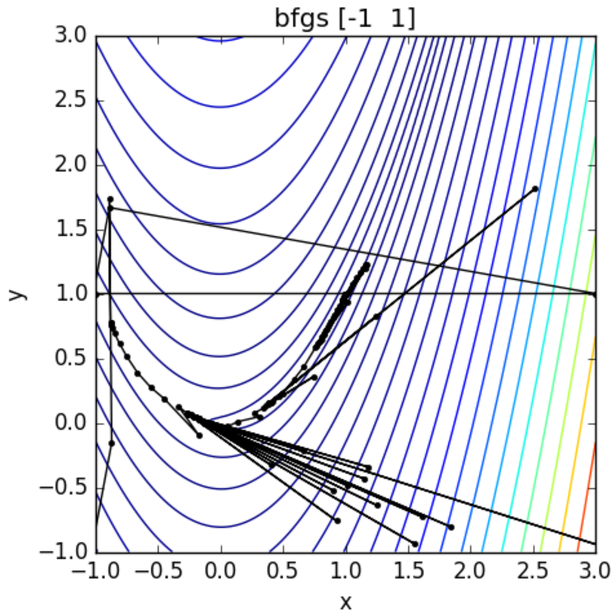
Problem 1

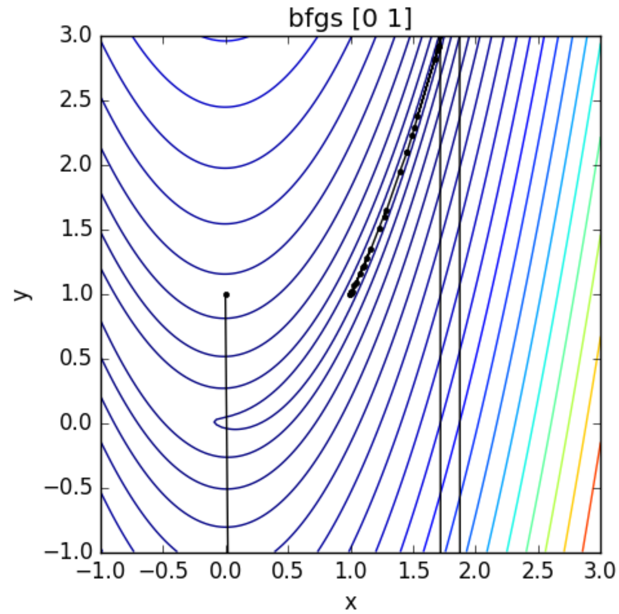
Method	Starting Point	Steps	Final Point
Steepest Descent	(-1, 1)	2000	(0.962, 0.926)
Steepest Descent	(0, 1)	2000	(0.967, 0.934)
Steepest Descent	(2, 1)	980	(1, 1)
Newton	(-1, 1)	3	(1, 1)
Newton	(0, 1)	6	(1, 1)
Newton	(2, 1)	6	(1, 1)
BFGS	(-1, 1)	124	(1, 1)
BFGS	(0, 1)	38	(1, 1)
BFGS	(2, 1)	45	(1, 1)

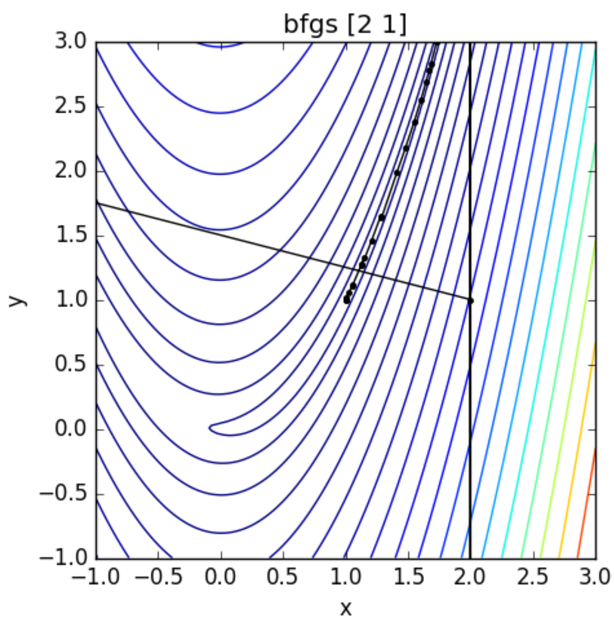





steepest_descent [2 1]
newton [-1 1]
newton [0 1]
newton [2 1]
x
y
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0


bfgs [-1 1]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
y
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0
x


bfgs [0 1]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
y
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0
x


bfgs [2 1]
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
y
−1.0 −0.5 0.0 0.5 1.0 1.5 2.0 2.5 3.0
x

Problem 2

(a)

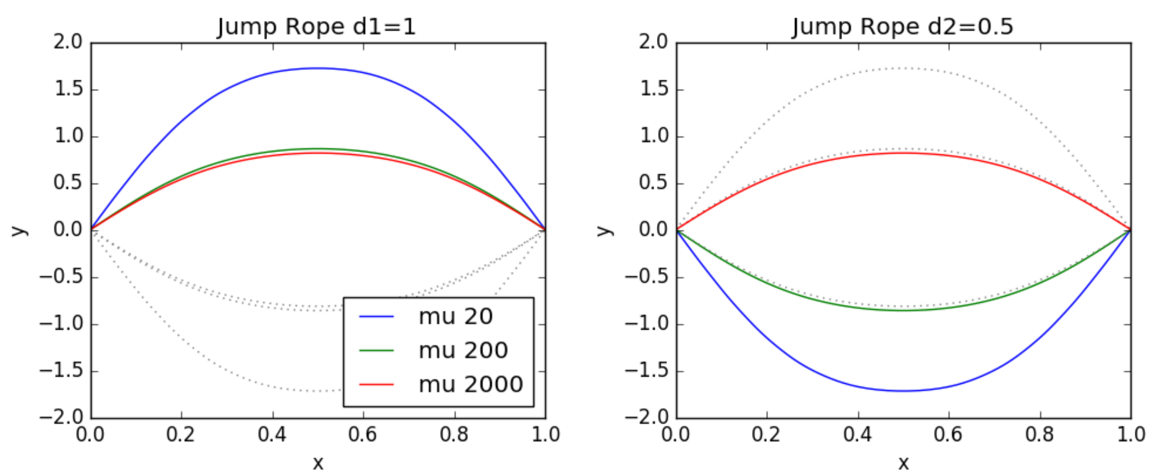
Some convenient intermediate terms:

$$
\begin{aligned}
\frac{dx}{ds} &= \frac{L}{R} + \sum_{k=1}^{20} \frac{\pi k c_k}{R} \cos \frac{\pi k s}{R} \\
\frac{dy}{ds} &= \sum_{k=1}^{20} \frac{\pi k d_k}{R} \cos \frac{\pi k s}{R} \\
\frac{\partial}{\partial c_i} \frac{dx}{ds} &= \frac{\pi i}{R} \cos \frac{\pi i s}{R} \\
\frac{\partial}{\partial d_i} \frac{dy}{ds} &= \frac{\pi i}{R} \cos \frac{\pi i s}{R} \\
\frac{\partial y}{\partial d_i} &= \sin \frac{\pi i s}{R} \\
A &= \sqrt{\left(\tfrac{dx}{ds}\right)^2 + \left(\tfrac{dy}{ds}\right)^2}
\end{aligned}
$$

Gradient components (expressed with intermediate terms above):

$$
\begin{aligned}
\frac{\partial r}{\partial c_i} &= \int_0^R \mu(2)\,(A-1)\,\frac{1}{2A}(2)\left(\frac{dx}{ds}\right)\left(\frac{\partial}{\partial c_i}\frac{dx}{ds}\right) ds \\
&= \int_0^R 2\mu \frac{A-1}{A}\left(\frac{dx}{ds}\right)\left(\frac{\partial}{\partial c_i}\frac{dx}{ds}\right) ds \\
\frac{\partial r}{\partial d_i} &= \int_0^R \left[2\mu \frac{A-1}{A}\left(\frac{dy}{ds}\right)\left(\frac{\partial}{\partial d_i}\frac{dy}{ds}\right) - 2\rho\omega^2 y \left(\frac{\partial y}{\partial d_i}\right)\right] ds
\end{aligned}
$$

(b/c)



$\mu = 2000$ appears to converge to the same solution, while $\mu = 20$ and $\mu = 200$ appear to converge to alternate solutions reflected across the x-axis. Because all y terms in the residual function are squared, the problem is symmetric and the reflected solutions (shown in grey) have the same energy.

Problem 3

(a)

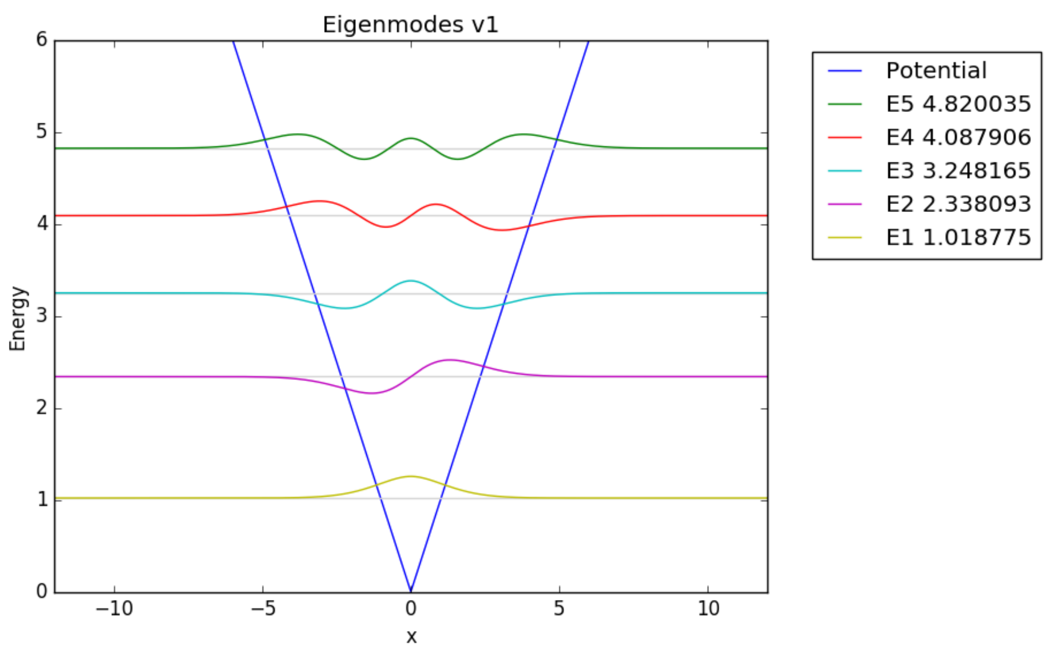
We will the centered finite difference approximation:

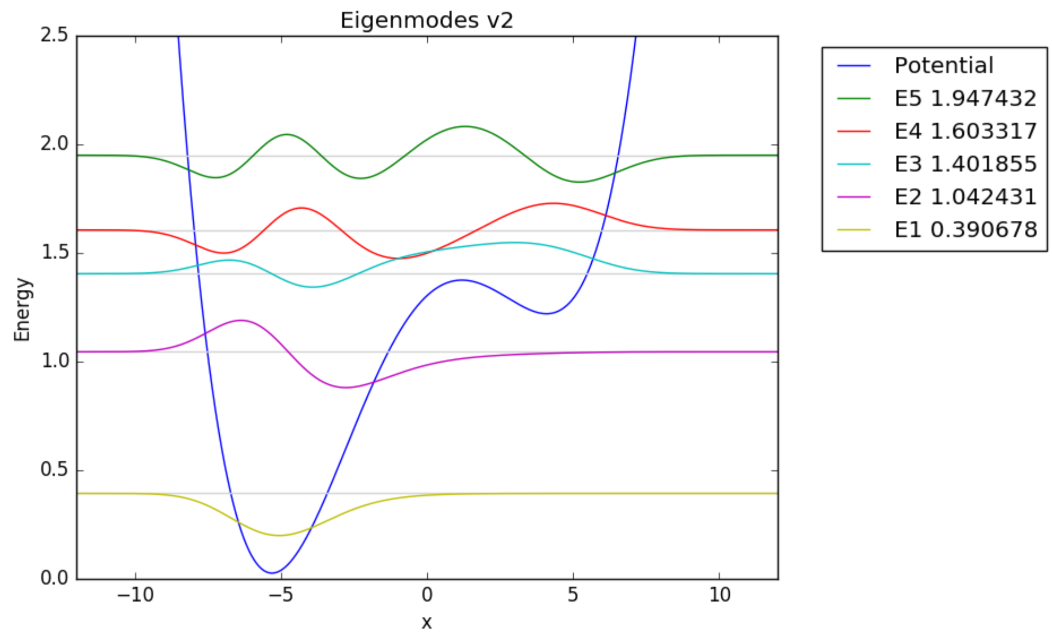
$$\frac{\partial^2 \Psi}{\partial x^2} \approx \frac{\Psi(x-h) - 2\Psi(x) + \Psi(x+h)}{h^2}$$

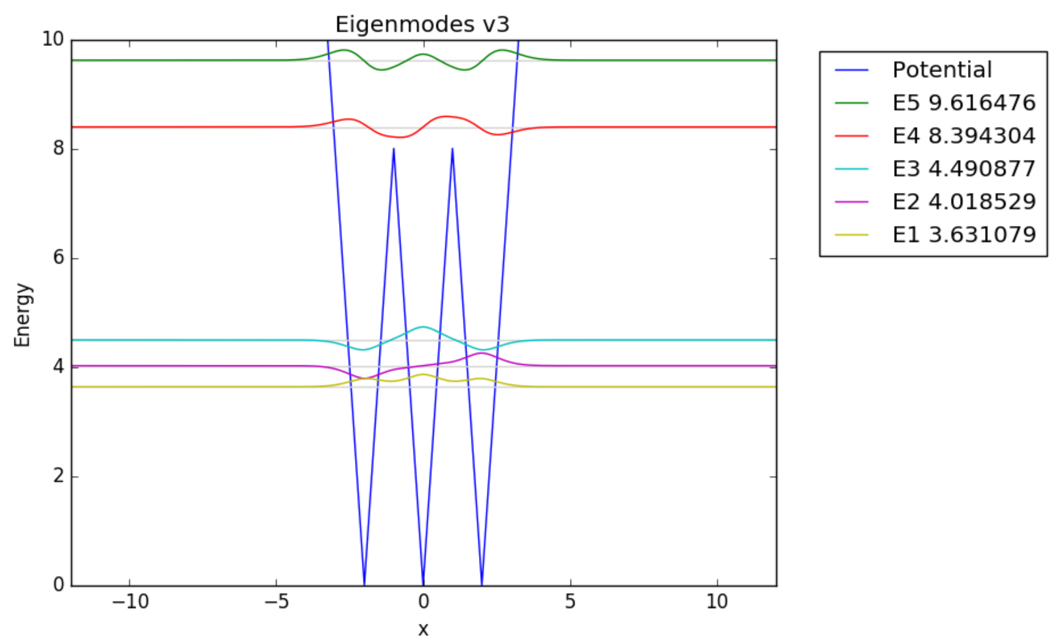
We can express the equation as $H\Psi = E\Psi$, where H is the following matrix with v_i as the potential evaluated on the grid point i.

$$\begin{pmatrix} \frac{2}{h^2} + v_0 & \frac{-1}{h^2} & 0 & 0 & \dots & 0 & 0 \\ \frac{-1}{h^2} & \frac{2}{h^2} + v_1 & \frac{-1}{h^2} & 0 & \dots & 0 & 0 \\ 0 & \frac{-1}{h^2} & \frac{2}{h^2} + v_2 & \frac{-1}{h^2} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \frac{-1}{h^2} & \frac{2}{h^2} + v_{1920} \end{pmatrix}$$

Note that truncating the first and last rows is conveniently equavalent to enforcing the zero Dirichlet boundary conditions. (Technically, this enforces $\Psi(-12-h) = 0$ and $\Psi(12+h) = 0$, but shifting one step doesn't change the numerical result.)







(b)

Probability particle lies between 0 and 6 for v_2.

```
Energies [ 0.39068  1.04243  1.40185  1.60332  1.94743]
Probability [  3.07578e-04   2.99542e-02   7.86516e-01   3.99204e-01   5.33140e-01]
```