11_Root_finding

March 17, 2016

1 11 Root finding and Trial-and-Error search

We want to find the roots $x_0$of

$$f(x_0) = 0$$

```
In [2]: import numpy as np
        import matplotlib
        import matplotlib.pyplot as plt
        %matplotlib inline
        matplotlib.style.use('ggplot')
```

1.1 Bisection

(Demonstrate algorithm on board).

```
In [3]: import numpy as np
```

1.1.1 Trial functions

Define two functions to work with; finding the roots amounts to solving a transcendental equation:

$$f(x) = 2\cos x - x = 0 \tag{1}$$

The following solution comes up for the energy eigenvalues of the bound particle states in the finite square well in quantum mechanics I:

$$f(E) = \sqrt{V_0 - E}\tan\sqrt{V_0 - E} - \sqrt{E} = 0 \tag{2}$$

(V_0 is the depth of the well potential. This solution is for even states.)

```
In [93]: def f(x):
             return 2*np.cos(x) - x

         def well(E, V0=10):
             return np.sqrt(V0 - E)*np.tan(np.sqrt(V0 - E)) - np.sqrt(E)
```

1.1.2 Implementation of the bisection algorithm

```
In [114]: def bisection(f, xminus, xplus, Nmax=100, eps=1e-14):
              for iteration in range(Nmax):
                  x = (xplus + xminus)/2
                  fx = f(x)
                  if f(xplus) * fx > 0:
                      # root is not between xplus and x
                      xplus = x
                  else:
                      xminus = x
                  if np.abs(fx) < eps:
                      break
              else:
                  print("bisect: no root found after {0} iterations (eps={1}); "
                        "best guess is {2} with error {3}".format(Nmax, eps, x, fx))
                  x = None
              return x
```

1.1.3 Testing with $f(x)$

```
In [21]: x0 = bisection(f, 0, 7)
         print(x0)
```

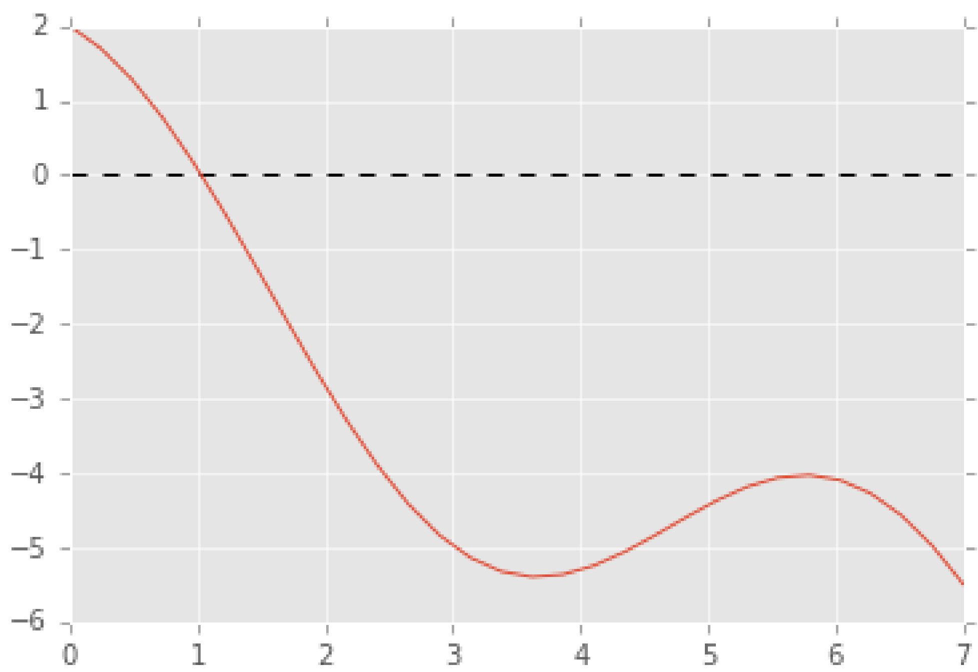
```
1.029866529322259
```

```
In [18]: f(x0)
```

```
Out[18]: -6.6613381477509392e-16
```

```
In [20]: X = np.linspace(0, 7, 30)
         plt.plot(X, np.zeros_like(X), 'k--')
         plt.plot(X, f(X))
```

```
Out[20]: [<matplotlib.lines.Line2D at 0x11734bf60>]
```



1.1.4 Activity

1. Find solutions for the square well for $V_0 = 10$
2. Plot `well(E, V_0=10)` for $0 < E < 11$ and check your solution graphically.
3. Vary the bracketing range to find all roots.

```
In [94]: E1 = bisection(well, 0, 10)
         print(E1)
```

```
0.004019262453329175
```

```
In [95]: well(E1)
```

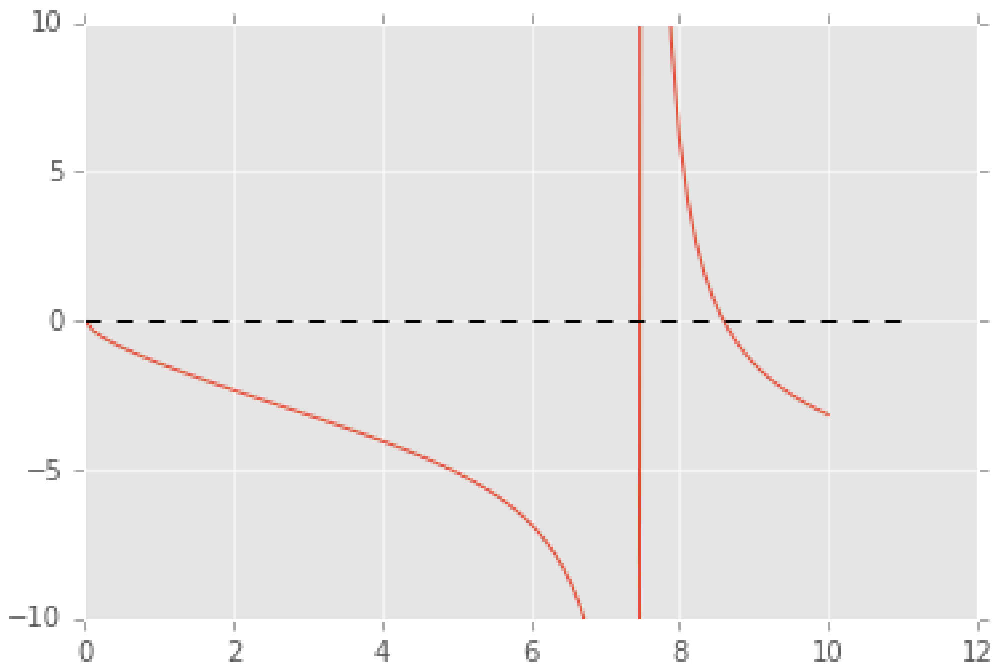
```
Out[95]: 5.6898930012039273e-16
```

```
In [96]: E_values = np.linspace(0, 11, 100)
```

```
In [97]: plt.plot(E_values, well(E_values, V0=10))
         plt.plot(E_values, np.zeros_like(E_values), 'k--')
         plt.ylim(-10,10)
```

```
/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
```

```
Out[97]: (-10, 10)
```




```
In [115]: E2 = bisection(well, 8.5, 10)
          print(E2)
          print(well(E2))
```

```
8.59278527522984
-3.5527136788e-15
```

Alternative form of the well Alternative form of the equation for the well:

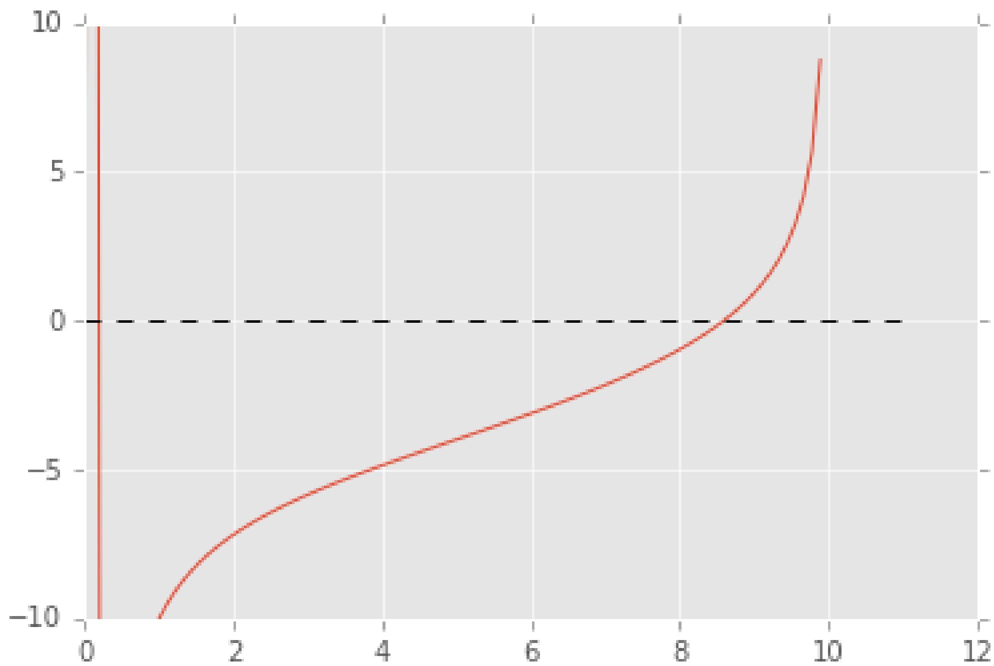
$$f(E) = \sqrt{E} \cot \sqrt{V_0 - E} - \sqrt{V_0 - E} = 0$$

In [74]:
```
def well2(E, V0=10):
    return np.sqrt(E) / np.tan(np.sqrt(V0 - E)) - np.sqrt(V0 - E)
```

In [76]:
```
E_values = np.linspace(0, 11, 100)
plt.plot(E_values, well2(E_values, V0=10))
plt.plot(E_values, np.zeros_like(E_values), 'k--')
plt.ylim(-10,10)
```

```
/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
  from ipykernel import kernelapp as app
/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
  from ipykernel import kernelapp as app
```

Out[76]: (-10, 10)



In [79]:
```
E0 = bisection(well2, 0, 0.1)
print(E0)
print(well2(E0))
print(well(E0))
```

```
0.0040192624533292465
-4.4408920985e-16
-0.137137438953
```

In [116]:
```
E1 = bisection(well2, 8, 9.9)
print(E1)
print(well2(E1))
print(well(E1))
```

```
8.592785275229836
-4.4408920985e-15
1.11022302463e-14
```

1.1.5 Additional activity: deeper well

Find bound states for a well with $V_0 = 20$

Use lambda functions (anonymous or "on-the-fly" functions) or define a new function `well20()`:

```
In [117]: def well20(E):
              return well(E, V0=20)
```

```
In [118]: bisection(well20, 0, 5, Nmax=10)
```

```
bisect: no root found after 10 iterations (eps=1e-14); best guess is 0.0048828125 with error 18.1396147
```

For experts: using anonynmous functions (same thing as above but saves typing... possibly at the cost of lack of clarity):

```
In [120]: bisection(lambda E: well(E, V0=20), 0, 5, Nmax=10)
```

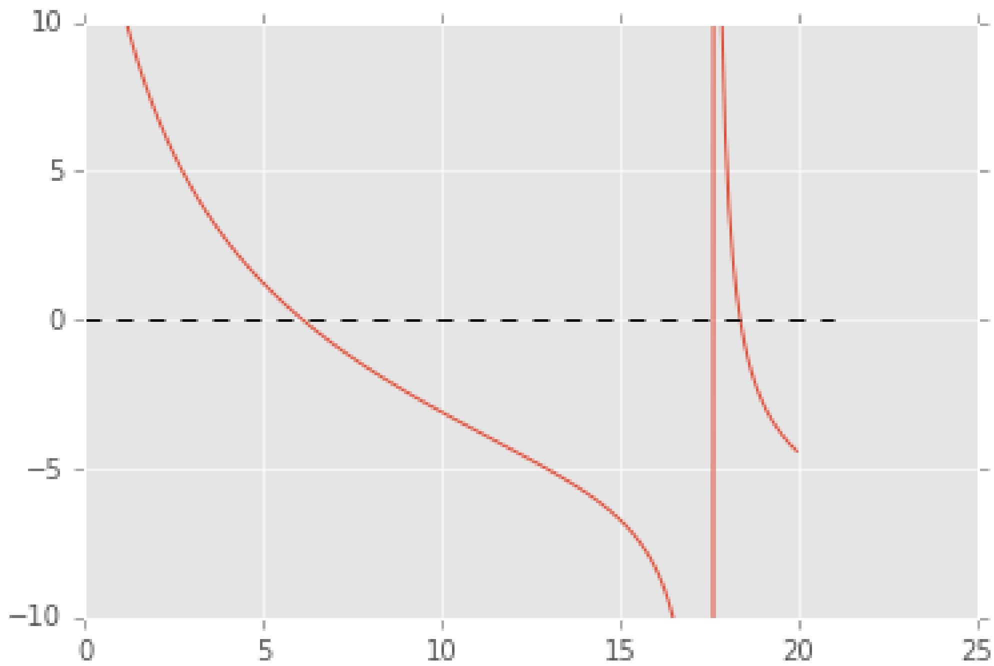
```
bisect: no root found after 10 iterations (eps=1e-14); best guess is 0.0048828125 with error 18.1396147
```

plot to get a better idea

```
In [121]: E_values = np.linspace(0, 21, 200)
          plt.plot(E_values, well20(E_values))
          plt.plot(E_values, np.zeros_like(E_values), 'k--')
          plt.ylim(-10,10)
```

```
/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
```

```
Out[121]: (-10, 10)
```



```
In [123]: bisection(well20, 0, 10)
```

```
Out[123]: 6.108467017547632
```

```
In [127]: bisection(well20, 17, 20, eps=1e-13)
```

```
Out[127]: 18.360519852466737
```

1.2 Newton-Raphson

(Demonstrate algorithm on board)

1.2.1 Activity: Implement Newton-Raphson

1. Implement the Newton-Raphson algorithm
2. Test with $f(x)$ and the well for $V_0 = 10$.
3. Bonus: test performance of `newton_raphson()` against `bisection()`.

```
In [113]: def newton_raphson(f, x, h=3e-1, Nmax=100, eps=1e-14):
              for iteration in range(Nmax):
                  fx = f(x)
                  if np.abs(fx) < eps:
                      break
                  df = (f(x + h/2) - f(x - h/2))/h
                  Delta_x = -fx/df
                  x += Delta_x
              else:
                  print("Newton-Raphson: no root found after {0} iterations (eps={1}); "
                        "best guess is {2} with error {3}".format(Nmax, eps, x, fx))
                  x = None
              return x
```

```
In [72]: newton_raphson(f, 0)
```

```
Out[72]: 1.0298665293222589
```

```
In [137]: newton_raphson(well, 0.3, eps=1e-14)
```

```
Newton-Raphson: no root found after 100 iterations (eps=1e-14); best guess is nan with error nan

/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
/opt/local/Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site-packages/ipykernel/__main
```

Can't get it to converge for the first root. Second root works:

```
In [138]: newton_raphson(well, 9, eps=1e-14)
```

```
Out[138]: 8.5927852752298381
```

Note that bisection is more robust and finds the first root:

```
In [139]: bisection(well, 0, 1)
```

```
Out[139]: 0.0040192624533297305
```

```
In [140]: %timeit newton_raphson(well, 9)
```

1000 loops, best of 3: 302 µs per loop

```
In [141]: %timeit bisection(well, 8, 9)
```

1000 loops, best of 3: 984 µs per loop

```
In [ ]:
```