B-splinesCollocation_PoissonEq

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In [2]: """
        Created on Mon Apr 16 10:33:22 2018
        New basis function
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        """
        import numpy as np
        import matplotlib.pyplot as plt
        import scipy.linalg as spl
        import scipy.constants as spc
        import scipy.integrate as spi
        from bspline import Bspline
        from bspline.splinelab import aptknt

        def Vol(r):
            return(4/3*np.pi*r**3)

        def uniform_pot(r,R, Q=1): #see eq. (14) in Assignment PDF
            return(np.piecewise(r,[r<=R, r>R], [lambda x: Q/Vol(R), lambda x: 0]))

        def analytic_uniform_shell(r,R,Q=1):
            return(np.piecewise(r,[r<=R,r>R],[lambda x: Q/R*(3/2-x**2/(2*R**2)),lambda x: Q/x]

        def shell_pot(r,R_in,R_out,Q=1): #see eq. (15) in Assignment PDF
            return(np.piecewise(r,[r<R_in,(r>=R_in) & (r<=R_out),r>R_out], [lambda x: 0, lambd

        # Hydrogen wave functions according to Demtröder 3 page 149
        def H_psi_n1(r,Z=1,a0 = 1):
            return(1/np.sqrt(np.pi)* (Z/a0)**(3/2)* np.exp(-Z*r/a0) ) #n=1,l=0, m=0

        def H_psi_n2(r, Z = 1,a0=1):
            return(1/(4*np.sqrt(2*np.pi)) * (Z/a0)**(3/2)* (2-Z*r/a0) * np.exp(-Z*r/2*a0)) #n=

        R = 1; Delta = 1e-8; Q = 1; gap=0.2; el_charge = 1


        r = np.linspace(Delta,12,50) #Points where Splines and phi need to collocate
        '''
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for i in range(len(r)):
  if i == np.max(np.where(r<R)):
      print(i)
      r[i] = R-Delta
  if i == np.min(np.where(r>R)):
      print(i)
      r[i] = R+Delta
'''

knot_vector = aptknt(r, 3) #kreates knot points with Ghost points
basis = Bspline(knot_vector,3) #Object of basic spline vectors: basis(0) gives 0t'th ba


A1 = basis.collmat(r)  # Full collocation matrix, where points of agreement are knot p
A2 = basis.collmat(r, deriv_order=2) #2nd order derivative of Bspline matrix

c1 = np.zeros(np.size(A2[0,:])); c1[0] = 1 #Adding boundary conditions
c2 = np.zeros(np.size(A2[0,:])); c2[-1] = 1 #first coefficient is 0 and last one is Q
A2[0] = c1
A2[-1] = c2

pot = -r * 4*np.pi* uniform_pot(r,R)
pot[0] = 0 #Boundary condition: setting c0 to 0 because phi(r=0)=0
pot[-1] = Q  #if r goes to infty the potential goes to Q phi(r=infty) =Q

LUA2 = spl.lu_factor(A2) # Do LU decomposition, so switching to different potentials i

#Uniformely charged sphere
C = spl.lu_solve(LUA2,pot) #Solve the matrix equation with Bspline''(r)*c_n = roh(r) t
phi = np.dot(A1,C) # to get Potential phi one can use dotprouct. See eq. (11) in Assig

#Uniformely charged shell
pot_shell = -r*4*np.pi*shell_pot(r,R-gap,R+gap)
pot_shell[0] = 0
pot_shell[-1] = Q

C_shell = spl.lu_solve(LUA2,pot_shell)
phi_shell = np.dot(A1,C_shell)

#Checking for Normalization of the used wave functions: integral(4*pi*r**2*psi(r)**2*d
def H_psi_n1_norm(r,Z=1,a0 = 1):
    return(4*np.pi*r**2* (1/np.sqrt(np.pi)* (Z/a0)**(3/2)* np.exp(-Z*r/a0))**2 )
def H_psi_n2_norm(r, Z = 1,a0=1):
    return(4*np.pi*r**2* (1/(4*np.sqrt(2*np.pi)) * (Z/a0)**(3/2)* (2-Z*r/a0) * np.exp(

norm_psi_n1 = spi.quad(H_psi_n1_norm,0,1000)
norm_psi_n2 = spi.quad(H_psi_n2_norm,0,1000)
print('Norm_n1 = '+str(norm_psi_n1[0])+' Error= '+str(norm_psi_n1[1]))
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```
        print('Norm_n2 = '+str(norm_psi_n2[0])+' Error= '+str(norm_psi_n2[1]))

        #solve for Hydrogen atom
        pot_psi_n1 = -r*4*np.pi*el_charge*H_psi_n1(r)**2
        pot_psi_n1[0] = 0
        pot_psi_n1[-1] = el_charge
        C_psi_n1 = spl.lu_solve(LUA2,pot_psi_n1)
        phi_psi_n1 = np.dot(A1,C_psi_n1)


        pot_psi_n2 = -r*4*np.pi*el_charge*H_psi_n2(r)**2
        pot_psi_n2[0] = 0
        pot_psi_n2[-1] = el_charge
        C_psi_n2 = spl.lu_solve(LUA2,pot_psi_n2)
        phi_psi_n2 = np.dot(A1,C_psi_n2)
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Norm_n1 = 0.9999999999999999 Error= 1.0812512262409847e-13
Norm_n2 = 1.0 Error= 5.582255950060929e-11
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In [9]: for i in range(len(r)):
            plt.plot(r,basis(i))
        plt.show()
```

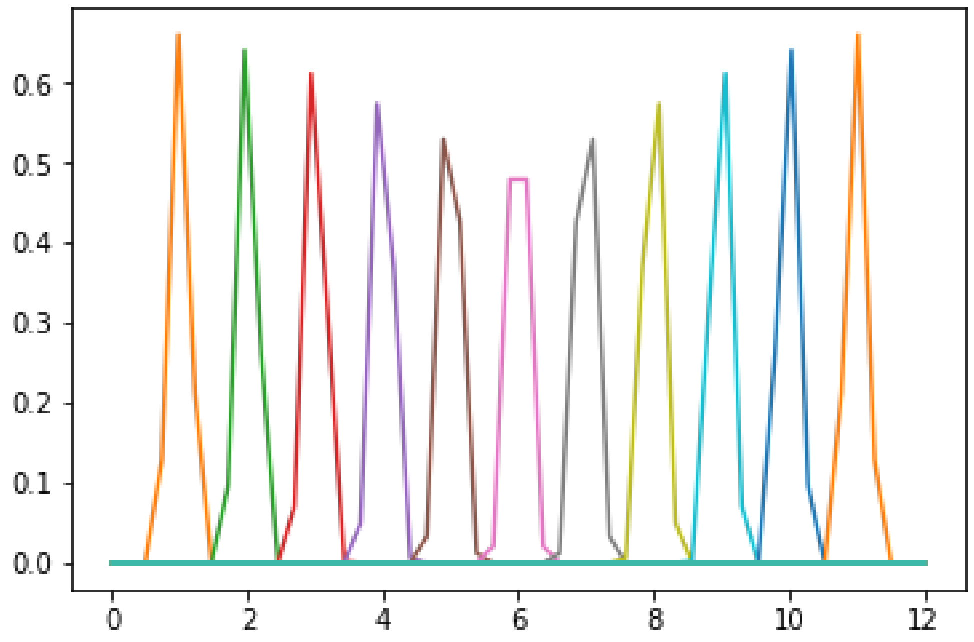

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(50, 50)
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In [11]: Ainv = spl.inv(A2)
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