Assignment 4: Collocation method with B-splines

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1 Introduction

The Poisson equation plays a big role in electrostatics, describing how electric potentials arise from given charge distributions.

In this report, we apply the collocation method with B-splines to solve the Poisson equation under spherical symmetry for three charge distributions: a uniformly charged sphere, a spherical shell, and the electron density of the hydrogen atom in its ground state.

We compare our numerical results with known analytical solutions in order to analyse the accuracy of the method.

2 Theory and Methods

2.1 Poisson Equation and Spherical Symmetry

The objective is to numerically solve the Poisson equation with spherical symmetry for different charge distributions using the collocation method with B-splines.

In spherical symmetry the Poisson equation reads:

$$\nabla^2 V(r) = -\frac{4\pi\rho(r)}{4\pi\varepsilon_0}, \tag{1}$$

where:

$$\nabla^2 V(r) = \frac{\partial^2 V(r)}{\partial r^2} + \frac{2}{r}\frac{\partial V(r)}{\partial r}. \tag{2}$$

If we choose to write

$$V(r) = \frac{\varphi(r)}{r} \tag{3}$$

we get:

$$\nabla^2 V(r) = \frac{1}{r}\frac{\partial^2 \varphi(r)}{\partial r^2} = \frac{4\pi\rho(r)}{4\pi\varepsilon_0} \tag{4}$$

i.e.

$$\frac{\partial^2 \varphi(r)}{\partial r^2} = -r\frac{4\pi\rho(r)}{4\pi\varepsilon_0} \tag{5}$$

which we solve using the collocation method with B-splines. We set $\frac{1}{4\pi\varepsilon_0} = 1$.

2.2 B-splines: Construction and Properties

B-splines are piecewise polynomial basis functions defined over a partitioned interval using a sequence of *knots* $\{t_i\}$. A B-spline of order k has degree: $k-1$. The zeroth degree B-splines are piecewise constants:

$$B_i^{k=1}(r) = \begin{cases} 1, & t_i \leq r < t_{i+1} \\ 0, & \text{otherwise} \end{cases} \tag{6}$$

and higher-order B-splines are defined recursively via the Cox-de Boor formula:

$$B_i^k(r) = \frac{r - t_i}{t_{i+k-1} - t_i} B_i^{k-1}(r) + \frac{t_{i+k} - r}{t_{i+k} - t_{i+1}} B_{i+1}^{k-1}(r). \tag{7}$$

B-splines form a partition of unity. The partition of unity is an important property we verify in our code by ensuring that the sum of all B-splines at any collocation point r_i is equal to 1:

$$\sum_i B_i^k(r_i) = 1. \tag{8}$$

2.3 Collocation Method with B-splines

To solve Eq. (5), we represent the unknown function $\varphi(r)$ as a linear combination of B-splines:

$$\varphi(r) = \sum_i c_i B_i^k(r), \tag{9}$$

where c_i are the coefficients we want to obtain.

Taking the second derivative of the basis expansion and evaluating it at a set of collocation points $\{r_i\}$ we find the following linear system:

$$\sum_i c_i \frac{\partial^2 B_i^k(r_i)}{\partial r^2} = -r_i \frac{4\pi\rho(r_i)}{4\pi\varepsilon_0}. \tag{10}$$

We end up with a linear system of equation such as:

$$\mathbb{AC} = \mathbb{B} \tag{11}$$

where $\mathbb{A} = \frac{\partial^2 B_i^k(r_i)}{\partial r^2}$ is the collocation matrix and $\vec{B} = -r_i 4\pi\rho(r_i)$ gives the right hand side of the equation.

2.4 Boundary Conditions

Each row of our collocation matrix corresponds to one equation at a knot point and its columns represent the number of unknown coefficients c_i i.e. number of basis functions. This dimensions do not match. Thus, in order to fix the problem we impose some boundary conditions:

First we note that φ must vanish at the origin so our potential does not go to infinity there:

$$\varphi(r = 0) = 0, \tag{12}$$

and should approach the total charge Q at large r, which we enforce at the last collocation point:

$$\varphi(r = r_{\max}) = Q. \tag{13}$$

To implement these boundary conditions in our code, we first check that only the first B-spline contributes at the first collocation point and only the last B-spline contributes at the last collocation point. This is achieved by choosing appropriate knot multiplicities at the boundaries.

Now, we are able to remove the first column of our collocation matrix and to add a final row where we analyse the B-spline at r_{max}. We also insert a final row into our right hand side $\vec{B}$ that we set equal to Q. Once we have solved Eq. (11) and obtained our coefficient array, we add the value of $c_0 = 0$ at the beginning of the array.

2.5 Charge Distributions and Analytical Solutions

We solve Eq. (5) for three different charge distributions and compare our implementation with the analytical solutions:

1. **Uniform charge distribution inside a sphere with radius R:**

$$\rho(r) = \begin{cases} Q/V, & 0 \leq r \leq R \\ 0, & r > R \end{cases} \tag{14}$$

where $V = \frac{4}{3}\pi R^3$ is the volume of the sphere.

The analytical potential is given by:

$$V(r) = \begin{cases} \dfrac{Q}{4\pi\varepsilon_0 R}\left(\dfrac{3}{2} - \dfrac{r^2}{2R^2}\right), & r \leq R \\ \dfrac{Q}{4\pi\varepsilon_0 r}, & r > R \end{cases} \tag{15}$$

2. **Uniform charge distribution inside a spherical shell:**

$$\rho(r) = \begin{cases} 0, & r < R_1 \\ Q/V_{\text{shell}}, & R_1 \leq r \leq R_2 \\ 0, & r > R_2 \end{cases} \tag{16}$$

where $V_{\text{shell}} = \frac{4\pi}{3}\left(R_2^3 - R_1^3\right)$.

For a constant charge distribution between R_1 and R_2, the analytical potential within the charged region (i.e. for r with $R_1 \leq r \leq R_2$) takes the form:

$$V(r) = \frac{\rho(r)}{4\pi\varepsilon_0}\left[\frac{1}{r}\int_{R_1}^{r} r'^2 dr' + \int_{r}^{R_2} r'\, dr'\right] = \frac{\rho(r)}{4\pi\varepsilon_0}\left[\frac{r^3 - R_1^3}{3r} + \frac{R_2^2 - r^2}{2}\right]. \tag{17}$$

3. **Electron charge density from the hydrogen ground state wave function:**

$$\frac{4\pi\rho(r)}{4\pi\varepsilon_0} = \frac{e}{4\pi\varepsilon_0}\, 4\pi\psi^*(r)\psi(r), \tag{18}$$

where:

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi} a_0^{3/2}} \mathrm{e}^{-r/a_0} \tag{19}$$

and:

$$|\psi_{1s}(r)|^2 = \frac{1}{\pi a_0^3} \mathrm{e}^{-2r/a_0} \tag{20}$$

Here, a_0 is the Bohr radius which we set to 1 as well as $e/(4\pi\varepsilon_0) = 1$. The analytical potential is given by:

$$V(r) = \frac{e}{4\pi\varepsilon_0}\left(\frac{1}{r} - \mathrm{e}^{-2r}\left(\frac{1}{r} + 1\right)\right) \tag{21}$$

3 Results and Discussion

Here we analyse the numerical solution of the Poisson equation for the three different charge distributions using the B-spline collocation method. We describe the spline setup, show the shape of the B-spline basis functions and their second derivatives, and finally compare the analytical and numerical results for each charge distribution.

3.1 Spline Parameters and Knot Construction

We use cubic B-splines, corresponding to splines of degree $p = 3$. The knot sequence is constructed by choosing n_{knots} uniformly spaced points over a domain $[a, b]$. To ensure a clamped spline basis, the first and last knots are repeated p times. Thus, the augmented knot vector has the form:

$$t = \underbrace{a, \ldots, a}_{p \text{ times}}, t_1, t_2, \ldots, t_{n_{\text{knots}}}, \underbrace{b, \ldots, b}_{p \text{ times}}.$$

This results in $n_{\text{basis}} = \text{len}(t) - p - 1$ B-spline basis functions. The collocation points, where the differential equation is enforced, are taken to be the same as the original (non-augmented) knot points.

3.2 B-splines visualization

To validate the construction of our B-splines and their second order derivatives we plot them as shown in Figure 1:

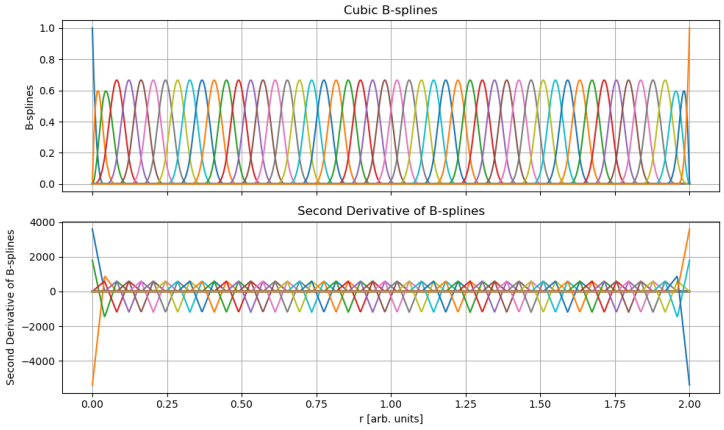

Figure 1: Cubic B-splines and their second order derivatives for $n_{\text{knots}} = 50$ for a domain of $[0, 2]$.

3.3 Uniformly Charged Sphere

For a uniformly charged sphere of radius $R = 1.0$, we first consider the domain $r \in (0, 2]$:

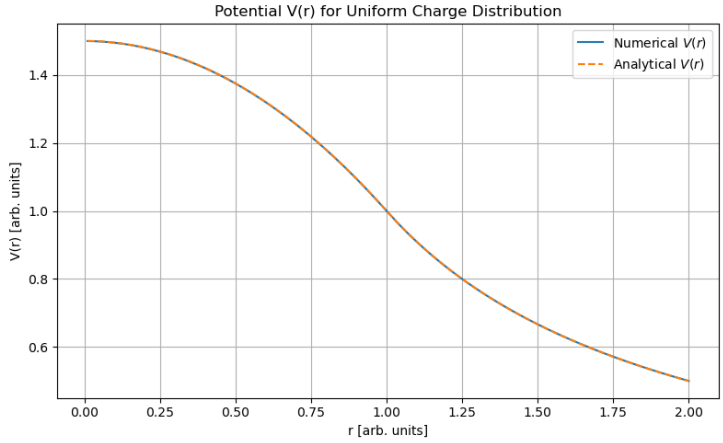

Figure 2: Potential $V(r)$ for uniformly charged sphere where $n_{\text{knots}} = 50$ compared with analytical results.

The results presented in Figure 2 show perfect agreement with the analytical solutions.

Now we repeat the simulation on a domain $r \in (0, 10]$:

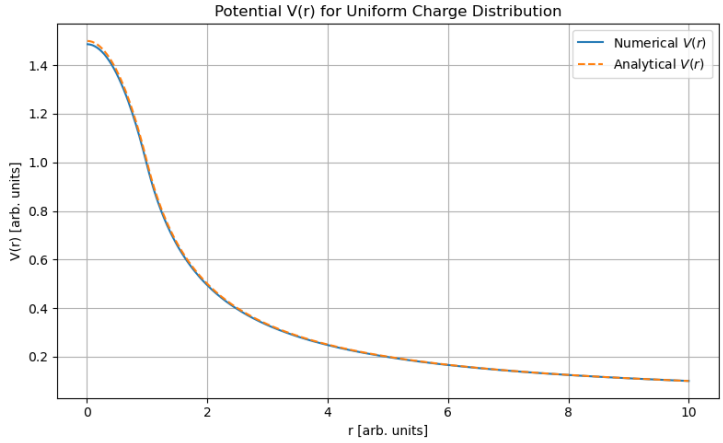

Figure 3: Potential $V(r)$ for uniformly charged sphere where $n_{\text{knots}} = 800$ compared with analytical results.

Figure 3 shows still good agreement between our numerical implementation and the analytical results although we can observe a small deviation

between the two solution at the beginning of our domain. Here we note how we had to increase our number of knots significantly in order for our numerical solution to try and reach analytical accuracy.

3.4 Uniformly Charged Spherical Shell

We now consider a spherical shell with inner radius $R_1 = 0.5$ and outer radius $R_2 = 1.0$ for a domain $r \in (0, 2]$:

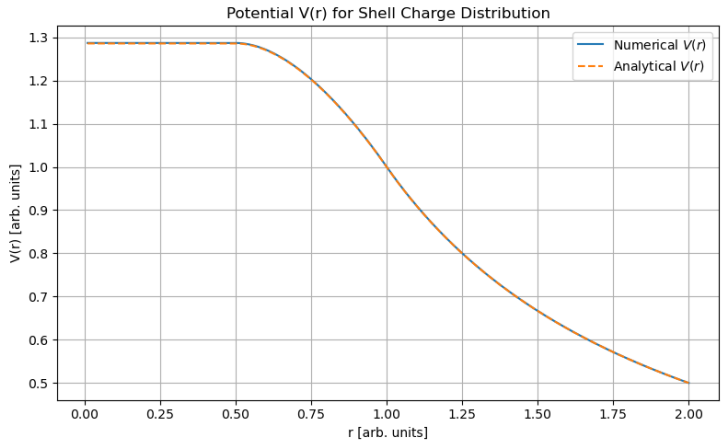

Figure 4: Potential $V(r)$ for uniformly charged spherical shell where $n_{\text{knots}} = 500$ compared with analytical results.

For Figure 4 we again observe a correct agreement between analytical and numerical results. We note how we needed to increase the number of knots significantly to achieve analytical accuracy compared with the first tested case in Figure 2.

Repeating the simulation for $R_1 = 5$ and $R_2 = 10.0$ in a domain $r \in (0, 10]$ we obtain:

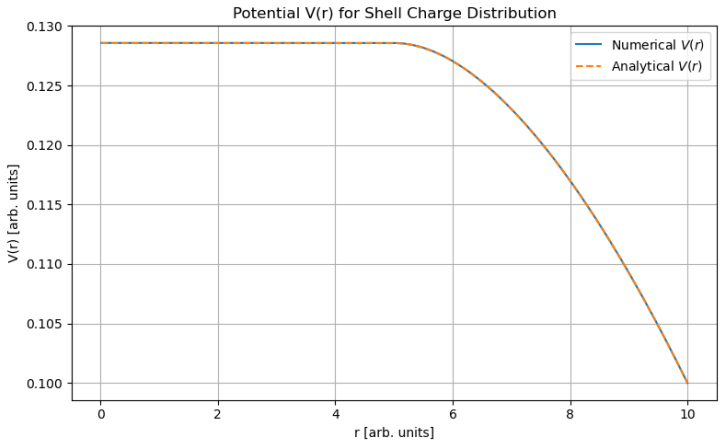

Figure 5: Potential $V(r)$ for uniformly charged spherical shell where $n_{\text{knots}} = 50$ compared with analytical results.

Again, Figure 5 confirms the good agreement between analytical and numerical solutions. We note how only 50 number of knots were needed in order to achieve accurate results.

3.5 Electron charge density from the hydrogen ground state wave function

Finally, we consider the electron charge density from the hydrogen ground state wave function. We compute the solution over the domain $r \in (0, 10]$ and again find great agreement between numerical and analytical results as shown in Figure 6.

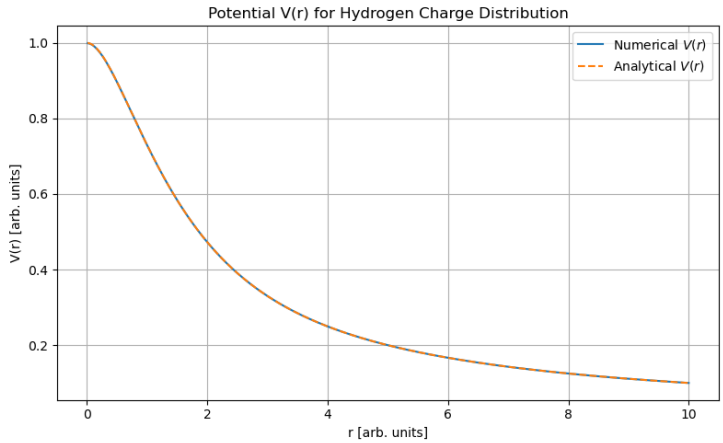

Figure 6: Potential $V(r)$ for electron charge density from the hydrogen ground state wave function where $n_{\text{knots}} = 200$ compared with analytical results.

However, we note that for the hydrogen atom, the choice of domain is important. A small domain (e.g., $r \in (0, 2]$) may introduce numerical errors in our calculations.

4 Limitations and Conclusion

One limitation of the B-spline collocation method is that the accuracy of the method depends on the density and placement of collocation points and knots.

Despite this, our implementation yields accurate numerical solutions that match analytical results for all the three considered cases. This confirms that the B-spline collocation method is a powerful approach for solving the Poisson equation under spherical symmetry for different types of charge distributions.