Assignment 4: Collocation method with B-splines

deadline Thursday April 21 2022

With the *collocation method* we can solve a boundary value problem

$$\frac{\partial^2 f(x)}{\partial x^2} + p(x)\frac{\partial f(x)}{\partial x} + q(x)f(x) = g(x),\ \ a \leq x \leq b \tag{1}$$

with boundary conditions that can be of different types, for example

$$f(a) = \alpha,\ \ f(b) = \beta. \tag{2}$$

First the solution is expanded in some suitable basis functions. A good choice is to use B-splines

$$f(x) = \sum_n c_n B_{n,k}(x). \tag{3}$$

For a second order differential equation, k has to be larger or equal to 4. The B-splines are then twice differentiable everywhere on the knot sequence and the second order derivative is continues. Second we ask Eq. 1 to be fulfilled in specific points. This is the meaning of *collocation*. For this we can (usually) choose the knot points. Note though that for this problem there is nothing special with the knot points. In principle we could have asked Eq. 1 to be fulfilled in between the knot points, but the knot points are the simplest choice. If we chose to have N knots points and put k knots points in the first and last physical point we will have $N-2\times(k-1)$ distinct physical points and $(N-k)$ B-splines. The equality at the knot points gives thus $N-2\times(k-1)$ equations. Since only $k-1$ B-splines are non-zero at the knot points each equations involves $(k-1)$ B-splines;

$$f(x_i) = \sum_{n=i-k+1}^{i-1} c_n B_{n,k}(x_i), \tag{4}$$

where x_k is the first physical knot point. With $k=4$ we have thus $(N-6)$ equations and $(N-4)$ unknown c_n in Eq. 3. For the last two equations we can use the boundary conditions. These last equations has to be chosen for the particular problem at hand. We have then a system of $N-4$ linear equations

$$\mathbb{A}\mathbb{C} = \mathbb{B}, \tag{5}$$

where $\mathbb{C}$ is the column vector with the coefficients c_i. $\mathbb{A}$ is a banded matrix and $\mathbb{B}$ is the right-hand side. This equation can be solved with standard routines, e.g. the LaPack routines. The collocation method transforms thus a differential equation to a system of linear equations.

The Poisson equation; spherical symmetry. You will solve electro statical equations for two different geometries. We start with a one dimensional spherical symmetric charge distribution. The Poisson equation can then be written,

$$\nabla^2 V(r) = -\frac{4\pi\rho(r)}{4\pi\varepsilon_0}, \tag{6}$$

where

$$\nabla^2 V(r) = \frac{\partial^2 V(r)}{\partial r^2} + \frac{2}{r}\frac{\partial V(r)}{\partial r} \tag{7}$$

If we chose

$$V(r) = \frac{\varphi(r)}{r} \tag{8}$$

we get

$$\nabla^2 V(r) = \frac{1}{r}\frac{\partial^2 \varphi(r)}{\partial r^2} = -\frac{4\pi\rho(r)}{4\pi\varepsilon_0}, \tag{9}$$

i.e.

$$\frac{\partial^2 \varphi(r)}{\partial r^2} = -r\frac{4\pi\rho(r)}{4\pi\varepsilon_0}, \tag{10}$$

The ansatz is now

$$\varphi(r) = \sum_n c_n B_n^k(r). \tag{11}$$

Inserting it into Eq. 10, we get

$$\sum_n c_n \frac{\partial^2 B_n^k(r)}{\partial r^2} = -r\frac{4\pi\rho(r)}{4\pi\varepsilon_0}. \tag{12}$$

Asking that the equation should be fulfilled in the knot points, and choosing $k = 4$, we find:

$$\sum_{n=i-3}^{i-1} c_n \left.\frac{\partial^2 B_n^{k=4}(r)}{\partial r^2}\right|_{r=r_i} = -r_i\frac{4\pi\rho(r_i)}{4\pi\varepsilon_0}. \tag{13}$$

The matrix $\mathbb{A}$ in Eq.5 will thus contain the second derivatives of the B-splines in the knot points and the right-hand side $\mathbb{B}$ is given by the right-hand side of Eq. 13. For one of the two still missing equations you can use that $\varphi(r = 0) = 0$ (otherwise the potential would go to infinity there). This condition is easily implemented - it just means that $c_1 = 0$ since only B_1 is non-zero at the first point. This gives you in fact one unknown less, i.e. we are down to $N - 5$ unknowns, and Eq. 12 gives $N - 6$ equations. The very last equation can be obtained from the fact that when $r \to \infty$, then $V(r) \to Q/\left(4\pi\varepsilon_0 r\right)$ and $\varphi(r) \to Q/\left(4\pi\varepsilon_0\right)$, where Q is the total charge. If you want you can let your program work with $4\pi\varepsilon_0 = 1$.

• Solve Eq. 10 for the following distributions

a) A uniform charge distribution inside a sphere with radius R, i.e.

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

where V is the volume of the sphere.

b) A uniform charge distribution inside a spherical shell, i.e.

$$\begin{aligned} \rho(r) =& 0 & r < R_1 \\ =& Q/V & R_1 \leq r \leq R_2 \\ =& 0 & r > R_2, \end{aligned} \tag{15}$$

and V is the volume of the shell. You can assume that the total charge is unity in both cases.

c) The electron charge density as given from the hydrogen ground state wave function;

$$\frac{4\pi\rho(r)}{4\pi\varepsilon_0} = \frac{e}{4\pi\varepsilon_0}\, 4\pi\, \psi^*(r)\, \psi(r), \tag{16}$$

where ψ is normalized according to;

$$\int 4\pi\, \psi^*(r)\, \psi(r) r^2 dr = 1. \tag{17}$$

You can make the calculation for $e/4\pi\varepsilon_0 = 1$. (If you want you can also try excited states. Only the s-wave functions ($\ell = 0$) are however spherically symmetric). In a later assignment you will reuse the calculation of the potential from the charge distribution as given by the wave functions.

Note that the different distributions just affect the right-hand side. If LU factorization is used for the matrix it is very fast to get the result for a new distribution. In many realistic situations the charge distribution will change (either in time and because one is trying to find better and better approximations), and then this property will be very valuable.

Comments on the Analytical Solution of the Poisson Equation
The analytical solutions to the problems above can be used to check your program. You should do that for at least case a), and b). Here follows some information on how to find the analytical results.

The general solution of the Poisson equation can be written

$$V(\mathbf{r}') = \frac{1}{4\pi\varepsilon_0} \int\int\int \frac{\rho(\mathbf{r})}{\mid \mathbf{r} - \mathbf{r}' \mid} dV, \tag{18}$$

where $\rho(\mathbf{r})$ is the charge density. This expression is a generalization of Coulombs law for the potential from point charges q_i placed at $\mathbf{r_i}$;

$$V(\mathbf{r}') = \frac{1}{4\pi\varepsilon_0} \sum_i \frac{q_i(\mathbf{r_i})}{\mid \mathbf{r_i} - \mathbf{r}' \mid}. \tag{19}$$

Letting

$$q_i(\mathbf{r_i}) \to \rho(\mathbf{r_i})dV \text{ and } \sum_i \to \int\int\int dV \tag{20}$$

we obtain Eq. (14) from Eq. (15). For more details see Jackson chapter 1.7 and Arfken chapter 1.14-1.15.

For a uniformly charged sphere (radius R and volume V) with constant charge density Eq. (14) gives (in spherical coordinates)

$$V(\mathbf{r}') = \frac{1}{4\pi\varepsilon_0} \frac{Q}{V} \int_0^R \int_0^\pi \int_0^{2\pi} \frac{1}{\mid \mathbf{r} - \mathbf{r}' \mid} r^2 dr sin\theta d\theta d\phi. \tag{21}$$

Since the charge density is spherically symmetric we may choose the orientation of the coordinate system such that $\mathbf{r}'$ lies on the z-axis, and thus the angle between the two vectors $\mathbf{r}'$ and $\mathbf{r}$ is θ. This gives

$$\begin{aligned} V(\mathbf{r}') &= \frac{1}{4\pi\varepsilon_0} \frac{Q}{V} \int_0^R \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{r^2 + r'^2 - 2rr'cos\theta}} r^2 dr sin\theta d\theta d\phi \\ V(\mathbf{r}') &= \frac{1}{4\pi\varepsilon_0} \frac{Q}{V} 2\pi \int_0^R \int_{-1}^1 \frac{1}{\sqrt{r^2 + r'^2 - 2rr'z}} r^2 dr dz, \end{aligned} \tag{22}$$

where the last equation is obtained after the variable transformation $z = cos\theta$. This last expression can be used to obtain the potential at a any point $\mathbf{r}'$

$$V(r') = \frac{1}{4\pi\varepsilon_0} \frac{Q}{V} 4\pi \int_0^R \frac{1}{r_>} r^2 dr \text{ where } r_> = r' \text{ if } r' > r,\ r_> = r \text{ if } r' < r \tag{23}$$

and we see that the potential only depends on the radial coordinate r'. Is interesting to note that if $r' > R$ the result is

$$V(r') = \frac{Q}{4\pi\varepsilon_0} \frac{1}{r'}, \tag{24}$$

and the results is independent of the radius R. If we now let $R \to 0$, Coulomb's law for a point charge in the origin is recovered.

Some information on B-Splines

B-Splines are piecewise polynomial functions defined on a given interval that contains a certain number of points, t_i, referred to as a *knot sequence*, where $t_i \leq t_{i+1}$. The B-Splines of order k (polynomial order $k-1$) are recursively defined as

$$B_{i,k=1} = 1 \text{ if } t_i \leq x < t_{i+1},\ \ B_{i,k=1} = 0 \text{ else} \tag{25}$$

and for $k > 1$:

$$B_{i,k}(x) = \frac{x - t_i}{t_{i+k-1} - t_i} B_{i,k-1}(x) + \frac{t_{i+k} - x}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(x), \tag{26}$$

where the knotpoint numbering *includes* any extra *ghost* points placed in the first and last points. The B-splines will be non-zero only in a limited region of space. If the numbering is such that t_1 is the first knot point and $B_{1,k}$ is the first B-splines, then a B-spline $B_{i,k}$ is non-zero only between t_i and t_{i+k}. The B-splines form a complete set on the knot sequence and one manifestation of this is that

$$\sum_i B_{i,k}(x_i) = 1 \tag{27}$$

everywhere from t_1 to t_{last}. If the first and last knot is multiple, such that k knots are placed in the same physical point, the B-splines will be confined to the the region $t_1 \leq x \leq t_{last}$. This is a common approach. A consequence of this choice is that only the first B-spline is non-zero in the first point, and only the last in the last point. This makes it especially simple to implement a boundary condition which requires that the function is zero on the boundary.

The derivative of a B-spline is obtained as

$$\frac{\partial}{\partial x} B_{i,k}(x) = (k-1) \left(\frac{B_{i,k-1}(x)}{t_{i+k-1} - t_i} - \frac{B_{i+1,k-1}(x)}{t_{i+k} - t_{i+1}} \right) \tag{28}$$

and the second derivative

$$\frac{\partial^2 B_{i,k}(x)}{\partial x^2} = \frac{(k-1)(k-2) B_{i,k-2}(x)}{(t_{i+k-1} - t_i)(t_{i+k-2} - t_i)} - \frac{(k-1)(k-2) B_{i+1,k-2}(x)}{(t_{i+k-1} - t_i)(t_{i+k-1} - t_{i+1})} \tag{29}$$

$$- \frac{(k-1)(k-2) B_{i+1,k-2}(x)}{(t_{i+k} - t_{i+1})(t_{i+k-1} - t_{i+1})} + \frac{(k-1)(k-2) B_{i+2,k-2}(x)}{(t_{i+k} - t_{i+1})(t_{i+k} - t_{i+2})} \tag{30}$$

In Athena (under Assignment 4) there is a link to a well commented Fortran routine (f77) for the generation of B-splines. The routine is from the book, "A practical Guide to Splines", by Carl de Boor. See more information at Athena. For your convenience you can also use the routines; (bget) to obtain a specific B-spline in a given point , or (bder) the derivative of a specific B-spline in a given point, or (bder2) the second derivative of a specific B-spline in a given point, all available at the home page. There is also a MatLab- and a C-routine to get the B-splines and their derivatives on a predefined grid. You can use these as starting routines for your programs (you will have to change the knot sequence to adopt to your problem etc.). Python has routines for generating splines, see the Athena page. You will find that most of the documentation is intended for those who want to use cubic splines (that is $k = 4$) for interpolation, but it should still be possible for you to extract the information necessary for this assignment.