Summary of lecture 3:

We left the finite difference method, and took up the "expansion method". In this method one establishes a set of basis functions $\phi_i(x), i = 1, 2, ..N$, and determines the expansion coefficients a_i (previously called c_i) for the unknown function $u(x)$ in the expansion

$$u^{(N)}(x) = \sum_{i=1}^{N} a_i \phi_i(x),\ a \leq x \leq b. \tag{1}$$

The equation to be solved for $u(x)$ is

$$\hat{L}u = f \tag{2}$$

where $\hat{L}$ is a *linear* operator actring on u, and $f(x)$ is a known "driving" function. Two methods were mentioned to solve Eq.(2) for the coefficients a_i.

The Galerkin and Collocation methods are given by $< \phi_j Lu >=< \phi_j f >$, and $< \delta(x - \xi_j) Lu >= f(\xi_j)$, respectively, with $j = 1, 2, ..N$. Here $< | >$ is the integral

$$< \phi_j \psi > = \int_a^b \phi_j(x) \psi(x) \rho(x) dx. \tag{3}$$

Due to the linearity of the operator $\hat{L}$, the equations above lead to matrix equations for the a_i's

$$\sum_{i=1}^{N} L_{ji} a_i = F_j \tag{4}$$

where

$$L_{ij}^{(G)} = < \phi_j \hat{L} \phi_i >,\ F_j^{(G)} =< \phi_j f > \tag{5}$$

$$L_{ij}^{(C)} = [\hat{L}\phi_i]_{\xi_j}, \qquad F_j^{(C)} = f(\xi_j) \tag{6}$$

and where the superscript denotes either Galerkin (G) or Collocation (C). For the Galerkin method the choice of mesh points (also called support points) is not critical.

Both for the Galerkin and Collocation methods a good choice of mesh-points makes the evaluation of the matrix elements $L_{ij}^{(G,C)}$ very convenient, and insures that the inverse of these matrices are available. If the mesh-points

$$\xi_1, \xi_2, ...\xi_N,$$

are of such a type, then the Gauss form of the integral $< \phi_j \psi >$ is given by

$$< \phi_j \psi > = \sum_{k=1}^{N} \phi_j(\xi_k) \psi(\xi_k) w_k \tag{7}$$

to a good approximation, where the weights w_k are given and known for each choice of basis functions $\{\phi\}$.

The Lagrange functions make an excellent basis $\phi_i(x) = \mathcal{L}_i(x)$ for the Galerkin method, since they have the property that they vanish at all mesh-points other than ξ_i . The $\mathcal{L}_i(x)$ are given in Eq. (11) of Lecture 3. In this case $< \mathcal{L}_j \psi > = \psi(\xi_j) w_j$ (no summation involved), and $L_{ij}^{(G)} = [\hat{L}\mathcal{L}_i]_{\xi_j}$, and $F_j^{(G)} = f\left(\xi_j\right)$. In order to salve Eq. (4) for the expansion coefficients a_i the inverse of the matrix L_{ji} is required. At the time of writing, an analytical form of $(L_{ij})^{-1}$ is not known.

However, once the function $u^{(N)}$is obtained, then the relation

$$\sum_{i=1}^{N} a_i \phi_i(x) = u^{(N)}(x) \tag{8}$$

can be written N times, with x replaced by ξ_k, $k = 1, 2, ..N$, and can be expressed through the matrix relationship

$$C\ (a) = (u)$$

where the elements C_{kj} of the matrtix C are given by $\phi_i(\xi_k)$. In view of the discrete orthogonality of the functions ϕ, the inverse of the matrix C can be obtained by writing Eq. (1) repeatedly for x replaced by ξ_k, $k = 1, 2, ..N$, multiplying each of these equations by $c_k \phi_i(\xi_k)$, summing over k and making use of the discrete orthogonality of the functions $\{\phi\}$. One finds

$$(a) = C^{-1}(u)$$

or, more explicitly

$$a_j = \sum_{k=1}^{N} c_k \phi_j(\xi_k) u^{(N)}(\xi_k) \tag{9}$$

which shows that the inverse of the matrix C is given by $c_k \phi_j(\xi_k)$.

This type of Galerkin method, using the Lagrange basis set, is well suited for the calculation of bound eigenstates of a Schroedinger equation. In this case $L = T + V - E$, where $T = -d^2/dx^2$, and one can rewrite Eq. (4) as

$$\sum_{i=1}^{N} (T_{ji} + V_{ji}) a_i = \sum_{i=1}^{N} E_{ji} a_i = E a_j. \tag{10}$$

The last step in Eq. (10) is due to the fact that the matrix E_{ji} is diagonal, and hence the eigenvalues of the matrix $(T_{ji} + V_{ji})$ are the energy eigenvalues E, and the corresponding eigenfunctions are given by Eq. (1). In order to properly implement this scheme, it is important to use as basis functions those that obey the right boundary conditions , i.e., vanish as $x \to \pm\infty$. Laguerre polynomials might be a good choice.

Start of Lecture 4: The collocation method.

To simplify the writing, the following notation will be introduced:

$$(\psi) \equiv \begin{pmatrix} \psi(\xi_1) \\ \psi(\xi_2) \\ \vdots \\ \psi(\xi_N) \end{pmatrix}; \quad (a) \equiv \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix} \tag{11}$$

i.e., a parenthesis around a function ψ means a column vector of the values of ψ at the support points $\psi(\xi_i)$, and a column vector of expansion coefficients a_i is denoted as (a). With a superscript, $\left(a^{\psi}\right)$ denotes that these $a's$ correspond to the expansion of the function ψ. The superscript (C) in Eqs. (6) will also be deleted in the present section (it is reserved for a future notation), and the superscript (N) for the function $u^{(N)}(x)$ will also be dropped. The difference between $u^{(N)}(x)$ and $u(x)$ will be considered in a later chapter.

For the collocation method, Eq. (4) $\sum_{i=1}^{N} \hat{L}\phi_i(\xi_j)a_i = f(\xi_j)$ can be written

$$(\hat{L}u) = (f). \tag{12}$$

where

$$\left(\hat{L}u\right) \equiv \begin{pmatrix} (\hat{L}u)_{\xi_1} \\ (\hat{L}u)_{\xi_2} \\ \vdots \\ (\hat{L}u)_{\xi_N} \end{pmatrix}$$

The equation (9), written as

$$(a^u) = C^{-1}(u), \tag{13}$$

$$(u) = C\ (a^u) \tag{14}$$

where $(C^{-1})_{ij} = w_i\phi_j(\xi_i)$, takes on a specially important rôle. It appears in the work of Curtis and Clenshaw [5]. Because of the discrete orthogonality of the functions $\{\phi\}$, the square matrix C is also known. Equation (13) shows that, in order to obtain the expansion coefficients a_i of a function $u(x)$, instead of using the quadrature relation $\int_a^b \phi_i(x)u(x)\rho(x)dx$, the matrix relationship (13) can be used. The two expressions are not identical, but differ from each other very little.

Armed with the equations above, an equation for the expansion coefficients can now be obtained. Starting from Eq. (12), and replacing (u) by Eq. (14), one finds

$$C^{-1}\hat{L}\ C(a^u) = (a^f). \tag{15}$$

Here L is the operator that acts on each entry of the column function $C(a^u)$, giving rise to a new column function, and the matrix C^{-1} transforms this column function back into an expansion coefficient column. One finally obtains

$$(a^u) = \left[C^{-1}\hat{L}\ C\right]^{-1}(a^f). \tag{16}$$

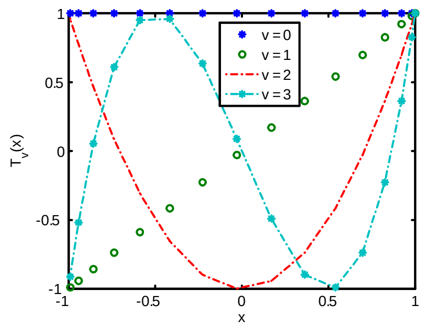

Figure 1: Plots of the Chebyshev polynomials $T_v(x)$. The symbols denote the values at the 14 mesh-points ξ_k, which are the zero's of T_{14}.They are not eqi-spaced.

Chebyshev Polynomials

Chebyshev Polynomials $T_v(x),\ v = 0, 1, 2...$ provide a very useful set of basis functions for expansion purposes. The variable x is contained in the interval $-1 \rightarrow +1$, and is related to an angle θ by $x = \cos\theta$. The last equation shows that the $x's$ are projections on the $x-$axis of the tip of a radius vector of unit length that describes a semi-circle as θ goes from 0 to π. In terms of the $x-$variable the T_n's are given by

$$\begin{aligned} T_0 &= 1 \\ T_1 &= x \\ T_2 &= 2x^2 - 1 \\ T_{n+1} &= 2xT_n - T_{n-1} \end{aligned} \tag{17}$$

In terms of the θ variable they are given by

$$T_n = \cos(n\ \theta); \quad 0 \le \theta \le \pi. \tag{18}$$

It is clear from Eq.(18) that $-1 \le T_n(x) \le 1$, and that the larger the index n, the more zeros these polynomials have, as is shown in Fig 1 The T_n's are orthogonal to each other with the weight function $\rho(x) = (1 - x^2)^{-1/2}$. The integral $\mathcal{I}$

$$\mathcal{I}_{n,m} = \int_{-1}^{+1} T_n(x)\ T_m(x)\ (1 - x^2)^{-1/2}\ dx = \int_0^{\pi} \cos(n\theta)\ \cos(m\theta)\ d\theta \tag{19}$$

has the value 0 if $n \ne m$, and the values $\pi/2$ if $n = m \ne 0$ and π if $n = m = 0$.

They also obey a discrete orthogonality

$$\frac{\pi}{N} \sum_{k=1}^{N} T_n(\xi_k)\ T_m(\xi_k) = \frac{\pi}{2} \delta_{n.m}(1 + \delta_{0n}) \quad n < N,\ m < N \tag{20}$$

where the ξ_k are the zero's of T_N, given by

$$\xi_k = \cos[\frac{\pi}{N}(k - 1/2)], \quad k = 1, 2, ...N. \tag{21}$$

This set of support (or mesh) -points are the ones used by Deloff [2] and also in our own work, because they do not attain the values ± 1, thus avoiding possible singularities in the functions being calculated at these points. By contrast, the support points used by Trefethen [1] are

$$x_k = \cos[\frac{\pi}{N}k], \quad k = 0, 1, 2, ...N. \tag{22}$$

They do include the points ± 1, and are especially useful to construct differentiation matrices for functions that are not periodic, because these functions can be made periodic by extending the angles of the support points (previously defined in $0 \leq \theta \leq \pi$) all the way around the circle from $\pi \leq \theta \leq 2\pi$. Since at the mesh-points the angles are equi-spaced, Fourier series and FTT's can be calculated with this variable, another useful property.

The Chebyshev polynomials can be calculated as a function of x by either using Eq. (18), with $\theta = \arccos(x)$, or by means of the recursion relations

$$T_n(x) = 2x\ T_{n-1}(x) - T_{n-2}(x), \quad n \geq 2 \tag{23}$$

As can be seen from Fig. 1, at the end points their values are

$$T_n(1) = 1, \text{ and } T_n(-1) = (-)^n \text{ for all } n \tag{24}$$

Many additional properties are given in text books [4].

References

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