PHYS 2326
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Spectral Methods for ODEs

Basic Idea

The funtion that solves the ODE is to be expanded in a complete set of convenient functions. The derivatives of that solution function are found by using recursion relations, and the coefficients in the ODE are also found using recursion relations if possible. When this is possible the solution can be found without ever imposing a grid, but working only with the coefficients of the expansions.

Here we will do examples using expansions in Legendre polynomials on the interval [-1,1]. One reason for this is that these are quite familiar; another is that a representation of a function in a Legendre series up to the power x^N gives the best L2 representation, on [-1,1] of any polynomial of order N.

Let $f(x)$ be the function we are looking for on [-1,1], the function that solves our ODE and boundary conditions. We know that f can be written as the infinite Legendre series

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x)\,. \tag{1}$$

We turn this from a theoretical nicety into a useful approach to a numerical solution by truncating the series at some order, call it N:

$$f(x) = \sum_{n=0}^{N} a_n P_n(x)\,. \tag{2}$$

In applied mathematics, the complete set of basis functions, the $P_n(x)$ in our case, is said to be a basis in the space of all functions. By truncating the series as in Eq. (2) we are restricting our search to a subspace of the space of all functions. This general technique of restricting to a subspace is called a "Galerkin" method.

Recursion for Derivatives

We will start by considering the way in which the derivative of a Legendre polynomial can be expressed in terms of undifferentiated Legendre polynomials. It will be useful to have a list of the first few explicit Legendre polynomials in a convenient place:

$$\begin{aligned}
P_0 &= 1\\
P_1 &= x\\
P_2 = &= \frac{1}{2}(3x^2-1)\\
P_3 = &= \frac{1}{2}(5x^3-3x)\\
P_4 = &= \frac{1}{8}(35x^4-30x^2+3)
\end{aligned}$$

We next iteratively use the recursion relationship

$$(2n+1)P_n(x) = \frac{d}{dx}\left[P_{n+1}(x) - P_{n-1}(x)\right] \tag{3}$$

to find

$$\begin{aligned}
&\frac{d}{dx}P_0(x) = 0\\
&\frac{d}{dx}P_1(x) = P_0(x)\\
&\frac{d}{dx}P_2(x) = 3P_1(x)\\
&\frac{d}{dx}P_3(x) = P_0(x) + 5P_2(x)\\
&\frac{d}{dx}P_4(x) = 3P_1(x) + 7P_3(x)\\
&\frac{d}{dx}P_5(x) = 3P_0(x) + 5P_2(x) + 11P_4(x)\\
&\cdots \quad \cdots
\end{aligned} \tag{4}$$

These relationships can be written in the index form

$$\frac{d}{dx}P_n = D_{nk}P_k\,, \tag{5}$$

where it is understood that the index k is summed over the range $0, N$. This relationship can also be written in the matrix form

$$P' = \mathcal{D}P \tag{6}$$

where $\mathcal{D}$ is the matrix (here truncated at order 9:

$$\mathcal{D} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 3 & 0 & 7 & 0 & 0 & 0 & 0 & 0 & 0\\
1 & 0 & 5 & 0 & 9 & 0 & 0 & 0 & 0 & 0\\
0 & 3 & 0 & 7 & 0 & 11 & 0 & 0 & 0 & 0\\
1 & 0 & 5 & 0 & 9 & 0 & 13 & 0 & 0 & 0\\
0 & 3 & 0 & 7 & 0 & 11 & 0 & 15 & 0 & 0\\
1 & 0 & 5 & 0 & 9 & 0 & 13 & 0 & 17 & 0
\end{pmatrix}$$

This is the formalism we use to replace first derivatives in ODEs. What about second derivatives? We simply apply the derivative operator twice, so that

$$P'' = \mathcal{D}\times DP = \mathcal{D}^2P\,. \tag{7}$$

Simple First Order Example

We will illustrate this method applied to the problem

$$f' + f = 1 + x \qquad\qquad f(0) = 1\,. \tag{8}$$

It is easy to check that the exact solution to this problem is

$$f(x) = x + e^{-x} \qquad \text{exact solution} \tag{9}$$

We will solve this by working in a subspace of order $N = 3$, i.e., with 4 unknown coefficients

$$f = \sum_{0}^{3} a_n P_n = a_0 P_0 + a_1 P_1 + a_2 P_2 + a_3 P_3\,. \tag{10}$$

The truncated form of Eq. (8) is

$$\sum_{0}^{3} a_n P_n' + a_n P_n = \sum_n a_n \sum_k \mathcal{D}_{nk} P_k + a_n P_n = \sum_n b_n P_n\,. \tag{11}$$

With a little index renaming this is

$$\sum_n \sum_k \left(\mathcal{D}_{nk} + \mathcal{I}_{nk}\right) a_k P_n = \sum_n b_n P_n\,. \tag{12}$$

By matching coefficients of P_n we get the system of linear equations

$$\left(\mathcal{D}_{kn} + \mathcal{I}_{kn}\right) a_k = b_n \tag{13}$$

where summation over k is implicit. Here $\mathcal{I}_{kn} = \delta_{kn}$.

It is important to note that in this last equation the summation is over the row index of the doubly indexed quantities, not the column index. For that reason the matrix form of the last equation is

$$\left(\mathcal{D}^T + \mathcal{I}^T\right) a = b\,, \tag{14}$$

where the T index indicates transpose of the matrix, and where a means the column vector of coefficients of the solution, and b means the column vector with the coefficients of the Legendre expansion of the right hand side of the ODE. The b column follows simply from the fact that

$$\sum b_n P_n = 1 + x = P_0 + P_1\,, \tag{15}$$

from which we have $b_0 = b_1 = 1$ and $b_2 = b_3 = 0$.

The matrix equation to be solved then becomes

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ 0 & 1 & 3 & 0 \\ 0 & 0 & 1 & 5 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} \tag{16}$$

.

The solution is easily seen to be $a_1 = 1$ and $a_0 = a_2 = a_3 = 0$, in other words the solution is $f = x$. This does solve the ODE, but not the auxiliary condition that $f(0) = 1$. But of course! We never "told" the mathematics about that condition. Lacking that, the math gave us a solution that assumes a sort of best fit to a low order polynomial, in this case the fit is an exact solution that doesn't fit the auxiliary data.

To fix the problem, to get the auxiliary data into the math, we apply the auxiliary condition $f(0) = 1$ to the truncated form of the solution approximation:

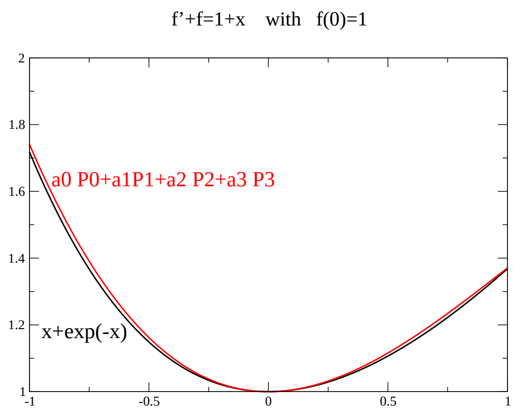
$$f(0) = a_0P_0(0) + a_1P_1(0) + a_2P_2(0) + a_3P_3(0) = a_0 - \frac{1}{2}a_2 = 1. \tag{17}$$

We now use this equation in place of the last row in Eq. (16) so that our matrix equation now becomes

$$\begin{pmatrix} 1 & 1 & 0 & 1 \\ 0 & 1 & 3 & 0 \\ 0 & 0 & 1 & 5 \\ 1 & 0 & -1/2 & 0 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 0 \\ 1 \end{pmatrix} \tag{18}$$

. The solution to *this* matrix equation is

$$a_0 = \frac{32}{27} \qquad a_1 = \frac{-3}{27} \qquad a_2 = \frac{10}{27} \qquad a_3 = \frac{-2}{27} \tag{19}$$



The figure shows that the truncated Legendre series with these coefficients is an excellent approximation to the exact solution $f = x + e^{-x}$.

Simple Second Order ODE Example

We now try the problem

$$f'' - f = 1 + x \qquad f(0) = 1 \qquad f'(0) = 2\,. \tag{20}$$

The exact solution to this equation is

$$f = x + e^x \,. \tag{21}$$

We will solve this using a truncation to $N = 5$, i.e., with 6 unknowns. By a more or less obvious modification of the steps in the last section we get the matrix equation

$$\left(\mathcal{D}^2 - \mathcal{I}\right)^T a = b \,. \tag{22}$$

The matrix realization of this equation is

$$\begin{pmatrix} -1 & 0 & 3 & 0 & 10 & 0 \\ 0 & -1 & 0 & 15 & 0 & 42 \\ 0 & 0 & -1 & 0 & 35 & 0 \\ 0 & 0 & 0 & -1 & 0 & 63 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{23}$$

.

As before this isn't going to work, because we have not given the math the auxiliary conditions. Those conditions are contained in the equations

$$f(0) = a_0 - \frac{1}{2}a_2 + \frac{3}{8}a_4 = 1 \tag{24}$$

and

$$f'(0) = a_1 - \frac{3}{2}a_3 + \frac{15}{8}a_5 = 2 \,. \tag{25}$$

We now insert these in place of the last two equations in (23) to get

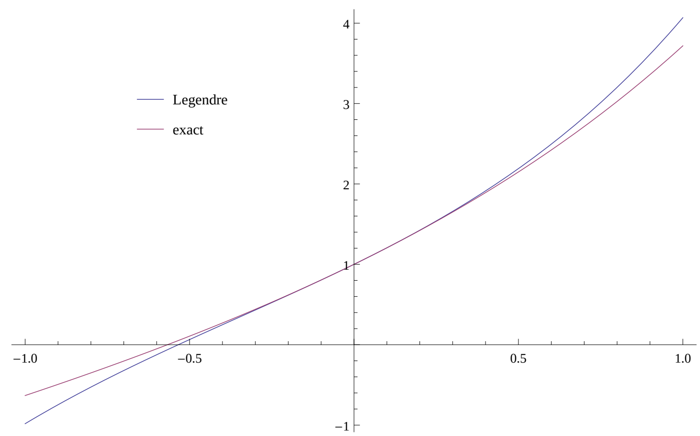
$$\begin{pmatrix} -1 & 0 & 3 & 0 & 10 & 0 \\ 0 & -1 & 0 & 15 & 0 & 42 \\ 0 & 0 & -1 & 0 & 35 & 0 \\ 0 & 0 & 0 & -1 & 0 & 63 \\ 1 & 0 & -1/2 & 0 & 3/8 & 0 \\ 0 & 1 & 0 & -3/2 & 0 & 15/8 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 1 \\ 2 \end{pmatrix} \tag{26}$$

.

The solution to these equation is

$$a_0 = \frac{920}{783} \quad a_1 = \frac{1837}{795} \quad a_2 = \frac{280}{783} \quad a_3 = \frac{1837}{795} \quad a_4 = \frac{56}{265} \quad a_5 = \frac{8}{783} \quad a_6 = \frac{8}{2385} \quad .$$

The comparison of the exact solution and this truncated Legendre solution, shown in the plot below, is very good.



Nonconstant Coefficients

Consider now the problem

$$f' + xf = 1 + x^2 \qquad\qquad f(0) = 0\,. \tag{27}$$

The exact solution is clearly $f = x$, but how can we in principle find this solution using a spectral method wihout a grid? The answer is to use another recursion relation for the Legendres

$$(2n+1)xP_n(x) = nP_{n-1}(x) + (n+1)P_{n+1(x)}\,. \tag{28}$$

From this, and from the explicit forms for the first few Legendres, we get

$$\begin{aligned}
&xP_0 + 0 = P_1\\
&xP_1 = \frac{1}{3}P_0 + \frac{2}{3}P_2\\
&xP_2 = \frac{2}{5}P_1 + \frac{3}{5}P_3\\
&xP_3 = \frac{3}{7}P_2 + \frac{4}{7}P_4\\
&\cdots \quad \cdots
\end{aligned}$$

In matrix form we can write this as

$$xP = \mathcal{X}P, \tag{29}$$

where, to order $N = 3$ the matrix $\mathcal{M}$ is

$$\mathcal{X} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/3 & 0 & 2/3 & 0 \\ 0 & 2/5 & 0 & 3/5 \\ 0 & 0 & 3/7 & 0 \end{pmatrix} \tag{30}$$

The ODE in Eq. (27) can then be written as

$$(\mathcal{X}+\mathcal{I})^T\, a = b\,. \tag{31}$$

The Legendre expansion of the right hand side of our ODE in Eq.!(27) is easily shown to be

$$1+x^2=\frac{4}{3}P_0+\frac{2}{3}P_2\,. \tag{32}$$

To order $N=3$ the explicit form of the matrix equation in (31) is

$$\begin{pmatrix} 0 & 4/3 & 0 & 0 \\ 1 & 0 & 17/5 & 0 \\ 0 & 2/ & 0 & 38/7 \\ 1 & 0 & -1/2 & 0 \end{pmatrix}\begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix}=\begin{pmatrix} 4/3 \\ 0 \\ 2/3 \\ 0 \end{pmatrix}. \tag{33}$$

In a step that should now be familiar, we have replaced the fourth row of the matrix equation with the condition, from (27), that $f(0)=0$, in the form

$$a_0-\frac{1}{2}a_1=0\,. \tag{34}$$

The solution to Eq. (31) is easily seen to be $a_1=1$ and $a_0=a_2=a_3=0$. This means that the solution by our $N=3$ spectral method is $f=x$. We have found the exact solution because it lies in our subspace spanned by $P_0\cdots P_3$.

It is easy to generalize the technique used here to ODEs with coefficients that are polynomials. For example, an ODE with the left hand side

$$xf''+(x^3+x)f\,, \tag{35}$$

but care is needed with the ordering of the matrices. For this example the equation for the coefficients should be viewed as operating with the derivatives first, then with the x operator. This means, for our example, that in the equation for the a coefficients xf'' is represented by the matrix

$$\mathcal{X}^T\mathcal{D}^T\mathcal{D}^T\,. \tag{36}$$

Since the order of matrix multiplicaion is reversed under transposition this means that the the left hand side of the equation for the a coefficents in our example is

$$\left(\mathcal{D}^2\mathcal{X}+\mathcal{X}^3+\mathcal{X}\right)^T a\,. \tag{37}$$

Integration Preconditioning

Often the system of equations to be solved is very large, and special iterative techniques are needed to deal with the matrices. The efficiency of these iterative techniques depends on how well "conditioned" the governing matrix is. A very modern technique is to improve the conditioning by doing the equivalent of integrating a second order differential equation twice.

The basic idea is that we accomplish differentiation with the transpose of $\mathcal{D}$. We can find the approximate inverse of $\mathcal{D}$ by just reversing the use of the recursion relations in Eq. (3) and treating the integration as

$$(2n+1)\int P_n(x)\,dx = P_{n+1}(x) - P_{n-1}(x)\,. \tag{38}$$

From this our integration matrix becomes

$$\mathcal{B} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -\frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 \\ 0 & -\frac{1}{5} & 0 & \frac{1}{5} & 0 & 0 \\ 0 & 0 & -\frac{1}{7} & 0 & \frac{1}{7} & 0 \\ 0 & 0 & 0 & -\frac{1}{9} & 0 & \frac{1}{9} \\ 0 & 0 & 0 & 0 & -\frac{1}{11} & 0 \end{pmatrix} \tag{39}$$

As a demonstration of the action of B we have

$$\mathcal{B}^T\mathcal{D}^T = \begin{pmatrix} 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{40}$$

The use will become clear in the following example. Our differential equation will be

$$f'' + f = 6x + x^3 - 2e^x \equiv \mathrm{rhs}(x)\,, \tag{41}$$

with auxiliary conditions $f(0) = -1$ and $f'(0) = -1$. It is easy to confirm that the exact solution to this problem is $f = x^3 - e^x$. We will find a spectral approximation to this solution in polynomials of order 5 in the form $f \approx \sum_0^5 a_n P_n$.

Following the previous patterns we arrive at the spectral form of the ODE

$$\left(\mathcal{D}^T\mathcal{D}^T + \mathcal{I}\right) a = b\,, \tag{42}$$

where the elements of column vector b are

$$b_n = \frac{2n+1}{2}\int_{-1}^{1} P_n(x)\mathrm{rhs}(x)\,dx \tag{43}$$

The explicit form of the matrix equation for order 5 is

$$\begin{pmatrix} 1 & 0 & 3 & 0 & 10 & 0 \\ 0 & 1 & 0 & 15 & 0 & 42 \\ 0 & 0 & 1 & 0 & 35 & 0 \\ 0 & 0 & 0 & 1 & 0 & 63 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} -2.3504 \\ 4.39272 \\ -0.715629 \\ 0.259089 \\ -0.0199303 \\ -0.00219917 \end{pmatrix} \tag{44}$$

We next multiply this equation, on the left, with $\mathcal{B}^T\mathcal{B}^T$ to get

$$\begin{pmatrix} -\frac{1}{3} & 0 & -\frac{14}{15} & 0 & -1 & 0 \\ 0 & -\frac{2}{5} & 0 & -\frac{209}{35} & 0 & -15 \\ \frac{1}{3} & 0 & \frac{19}{21} & 0 & \frac{1}{63} & 0 \\ 0 & \frac{1}{15} & 0 & \frac{43}{45} & 0 & \frac{1}{99} \\ 0 & 0 & \frac{1}{35} & 0 & \frac{75}{77} & 0 \\ 0 & 0 & 0 & \frac{1}{63} & 0 & \frac{98}{99} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} 0.735759 \\ -1.74969 \\ -0.715629 \\ 0.281311 \\ -0.0199289 \\ 0.00413473 \end{pmatrix} \tag{45}$$

The justification for this multiplication by $\mathcal{B}^T\mathcal{B}^T$ is that the matrix in Eq. (45) is better conditioned (easier to invert) than the matrix in (44). This is not at all obvious in our example because, of necessity, our example must have small dimensionality. If the dimensionality were much higher, and the matrices much larger, we would see that the matrix in Eq. (45) were much more sparse, i.e., had fewer nonzero entries, than the entries in (44).

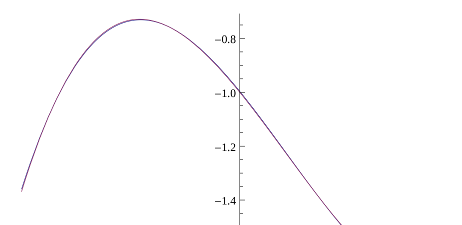
We are, of course, not yet finished with this problem, since we have not yet put in the auxiliary conditions $f(0) = -1$ and $f'(0) = -1$. We do this by simply replacing the first two rows of Eq. (45) with the equivalent restrictions on the a_n coefficients:

$$\begin{pmatrix} 1 & 0 & -\frac{1}{2} & 0 & \frac{3}{8} & 0 \\ 0 & 1 & 0 & -\frac{3}{2} & 0 & \frac{15}{8} \\ \frac{1}{3} & 0 & \frac{19}{21} & 0 & \frac{1}{63} & 0 \\ 0 & \frac{1}{15} & 0 & \frac{43}{45} & 0 & \frac{1}{99} \\ 0 & 0 & \frac{1}{35} & 0 & \frac{75}{77} & 0 \\ 0 & 0 & 0 & \frac{1}{63} & 0 & \frac{98}{99} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \\ -0.715629 \\ 0.281311 \\ -0.0199289 \\ 0.00413473 \end{pmatrix} \tag{46}$$

The solution of this matrix equation gives the polynomial

$$0.823856x^3 - 0.536736x^2 - 0.997924x - 0.996263\,.$$

The plot in the figure below shows that this polynomial and the exact solution,$x^3 - e^x$, are almost indistinguishable. The quantitative statement of this is that the $L2$ error is 2.2×10^{-5}.



Note that this numericalsuccess is not an indication of the usefulness of multiplication by $\mathcal{B}^T\mathcal{B}^T$. Aside from some differences in round off error we would have gotten the same solution by the straightforward approach without multiplication by $\mathcal{B}^T\mathcal{B}^T$. It is only for large problems that the multiplication by $\mathcal{B}^T\mathcal{B}^T$ makes a significant difference.