

NASA Contractor Report 181934
ICASE Report No. 89-72

ICASE

COMPUTATIONAL ASPECTS OF PSEUDOSPECTRAL LAGUERRE APPROXIMATIONS

Daniele Funaro

Contract No. NAS1-18605
October 1989

Institute for Computer Applications in Science and Engineering
NASA Langley Research Center
Hampton, Virginia 23665-5225

Operated by the Universities Space Research Association

(NASA-CR-181934) COMPUTATIONAL ASPECTS OF
PSEUDOSPECTRAL LAGUERRE APPROXIMATIONS Final
Report (ICASE) 16 p CSCL 12A

N90-14038

Unclass

G3/84 0252154



National Aeronautics and
Space Administration

Langley Research Center
Hampton, Virginia 23665-5225

COMPUTATIONAL ASPECTS OF PSEUDOSPECTRAL LAGUERRE APPROXIMATIONS

Daniele Funaro¹
Dipartimento di Matematica
Università de Pavia
Streda Nuova 65, 27100 Pavia ITALY

ABSTRACT

Pseudospectral approximations in unbounded domains by Laguerre polynomials lead to ill-conditioned algorithms. We introduce a scaling function and appropriate numerical procedures in order to limit these unpleasant phenomena.

¹This research was supported in part by the National Aeronautics and Space Administration under NASA Contract No. NAS1-18605 while the author was in residence at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA 23665.

1. Introduction

Recently, spectral methods have been successfully applied in the approximation of differential boundary value problems defined in unbounded domains. At the present, different solution techniques are available. Among these, an approach consists in using the collocation method based on the nodes of Gauss formulas related to unbounded intervals. This involves computations with orthogonal polynomials, such as Laguerre or Hermite polynomials. For details about theory and numerical experiments we refer for instance to [2], [5], [6], where, for certain classes of problems, a spectral type convergence behavior is shown. In this paper we are concerned with the implementation of these methods. In fact, computations with Laguerre or Hermite polynomials lead to ill-conditioned algorithms and undesired round-off errors instabilities, even when the degree is low. After recalling some basic properties of such polynomials, our aim is to give suggestions in order to improve the performances in practical applications.

2. Preliminary Properties and Remarks

We review some basic properties of Laguerre polynomials. Let $\alpha > -1$ be a real parameter and let $L_n^{(\alpha)}$ denote the n -degree Laguerre polynomial. For any $n \in \mathbb{N}$, $L_n^{(\alpha)}$ is solution to the following Sturm-Liouville problem (see [8]):

$$x \frac{d^2}{dx^2} L_n^{(\alpha)}(x) + (\alpha + 1 - x) \frac{d}{dx} L_n^{(\alpha)}(x) + n L_n^{(\alpha)}(x) = 0, \forall x \in]0, +\infty[, \quad (2.1)$$

with the normalizing condition:

$$L_n^{(\alpha)}(0) = \binom{n + \alpha}{n} = \frac{\Gamma(n + \alpha + 1)}{\Gamma(\alpha + 1)n!}. \quad (2.2)$$

The determination of $L_n^{(\alpha)}$ at a given point x can be performed via the recurrence formula:

$$\begin{cases} L_0^{(\alpha)}(x) = 1 \\ L_1^{(\alpha)}(x) = 1 + \alpha - x \\ L_n^{(\alpha)}(x) = \frac{1}{n} [(2n + \alpha - 1 - x) L_{n-1}^{(\alpha)}(x) - (n + \alpha - 1) L_{n-2}^{(\alpha)}(x)], \quad n \geq 2. \end{cases} \quad (2.3)$$

This procedure has a cost proportional to n . Of course, the evaluation of $\frac{d}{dx} L_n^{(\alpha)}$ at a point

x , is given by the recurrence formula obtained by differentiating (2.3), i.e:

$$\begin{cases} \frac{d}{dx} L_0^{(\alpha)}(x) = 0 \\ \frac{d}{dx} L_1^{(\alpha)}(x) = -1 \\ \frac{d}{dx} L_n^{(\alpha)}(x) = -\frac{1}{n} L_{n-1}^{(\alpha)}(x) + \frac{2n + \alpha - 1 - x}{n} \frac{d}{dx} L_{n-1}^{(\alpha)}(x) - \frac{n + \alpha - 1}{n} \frac{d}{dx} L_{n-2}^{(\alpha)}(x), \quad n \geq 2. \end{cases} \quad (2.4)$$

Moreover, after defining the weight function $w^{(\alpha)}(x) = x^\alpha e^{-x}$, $x \in]0, +\infty[$, $\alpha > -1$, we have the orthogonality relation:

$$\int_0^{+\infty} L_n^{(\alpha)} L_m^{(\alpha)} w^{(\alpha)} dx = \delta_{nm} \frac{\Gamma(n + \alpha + 1)}{n!}, \quad n, m \in \mathbb{N}. \quad (2.5)$$

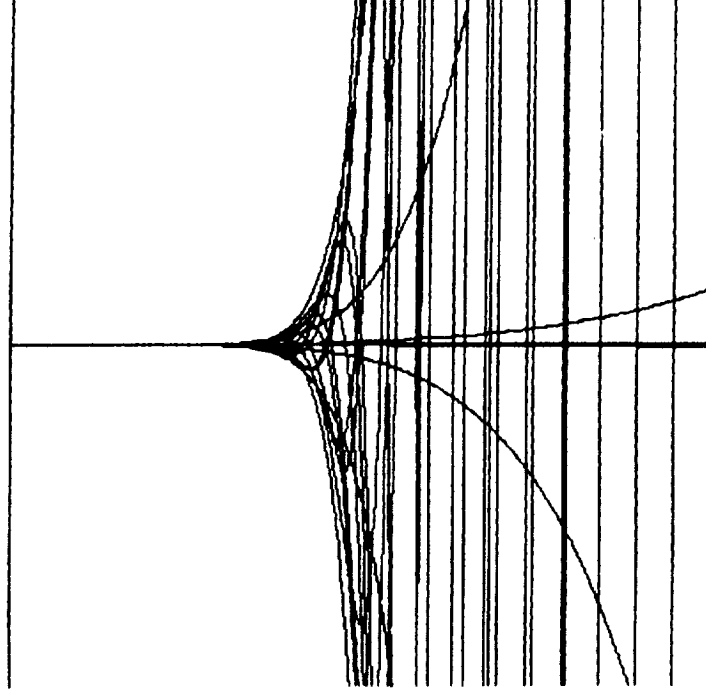


Figure 2.1 - Plot of $L_n^{(0)}$, for $n = 1, 20$.

As we shall see in the next, the expressions (2.3) and (2.4) are those mainly used in practical applications. Unfortunately, due to the particular structure of Laguerre polynomials, (2.3) and (2.4) are sources of numerical instabilities. A look to the plot of the first twenty polynomials (see Figure 2.1) gives an idea of the troubles one can expect. In Figure 2.1, we have $\alpha = 0$ and the plots are contained in the rectangle $[0, 70] \times [-5000000, 5000000]$. Even for small values of the degree n , it is impossible to get a reasonable picture. Relatively

small values in the first part of the abscissas interval have to be compared with very sharp oscillations in the second part. From the theoretical point of view, we can give the following asymptotic results (see [8]).

Proposition 2.1 - For any $\alpha > -1$ and $n \geq 2$ the values of the relative maxima of $e^{-x/2}x^{(\alpha+1)/2}|L_n^{(\alpha)}(x)|$ form an increasing sequence when $x > x_0$ where:

$$x_0 = 0 \text{ if } \alpha^2 \leq 1, \quad x_0 = \frac{\alpha^2 - 1}{2n + \alpha + 1} \text{ if } \alpha > 1.$$

Proposition 2.2 - For any $\alpha > -1$ and $x_0 > 0$, we can find a constant $C > 0$ such that:

$$\max_{x \in [x_0, +\infty[} |e^{-x/2}x^{(\alpha+1)/2}L_n^{(2)}(x)| \approx Cn^{1/6}n^{\alpha/2}. \quad (2.6)$$

From the previous statements one concludes that, even when multiplied by a decaying exponential, Laguerre polynomials are not easy to keep under control. We will analyze in the next section more about this subject.

Similar properties to those presented above are satisfied by the family of Hermite polynomials. According to [8], the n^{th} degree Hermite polynomial H_n is defined to be a solution of the differential equation:

$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0, \quad \forall x \in \mathbf{R}, \quad (2.7)$$

with the conditions:

$$H_n(0) = (-1)^{n/2} \frac{n!}{(n/2)!} \quad \text{if } n \text{ is even}, \quad (2.8)$$

$$H_n'(0) = (-1)^{(n-1)/2} \frac{(n+1)!}{((n+1)/2)!} \quad \text{if } n \text{ is odd}. \quad (2.9)$$

Again we have a recurrence formula, namely:

$$\begin{cases} H_0(x) &= 1 \\ H_1(x) &= 2x \\ H_n(x) &= 2xH_{n-1}(x) - 2(n-1)H_{n-2}(x), \quad n \geq 2. \end{cases} \quad (2.10)$$

Orthogonality is also achieved in view of the next expression:

$$\int_{-\infty}^{\infty} H_n(x)H_m(x)e^{-x^2}dx = \delta_{nm}\sqrt{\pi}2^n n!, \quad n, m \in \mathbf{N}. \quad (2.11)$$

Considerations similar to those previously discussed, concerning the implementation of formula (2.10), also hold. Actually, the two families are closely related by the following equalities:

$$H_n(x) = (-1)^{n/2}2^n(n/2)!L_{n/2}^{(-1/2)}(x^2), \quad \text{if } n \text{ is even}, \quad (2.12)$$

$$H_n(x) = (-1)^{(n-1)/2} 2^n ((n-1)/2)! L_{(n-1)/2}^{(1/2)}(x^2), \quad \text{if } n \text{ is odd.} \quad (2.13)$$

3. Scaled Laguerre Functions

As we noticed in Section 2, the determination of $L_n^{(\alpha)}(x)$ for a given x , brings to an ill-conditioned algorithm. According to Propositions 2.1 and 2.2, we can try a first experiment. Instead of computing $L_n^{(\alpha)}(x)$, we could evaluate $\tilde{L}_n^{(\alpha)}(x) = e^{-x/2} L_n^{(\alpha)}(x)$. This can be done by just modifying the first two terms of (2.3) by setting $\tilde{L}_0^{(\alpha)}(x) = e^{-x/2}$ and $\tilde{L}_1^{(\alpha)}(x) = (1 + \alpha - x)e^{-x/2}$. In this way, when x is large we can avoid overflow errors. The plots of $\tilde{L}_n^{(\alpha)}$ for $\alpha = 0$ and $n = 1, 20$ are given in Figure 3.1. This time they are all included in the rectangle $[0, 70] \times [-1, 1]$.

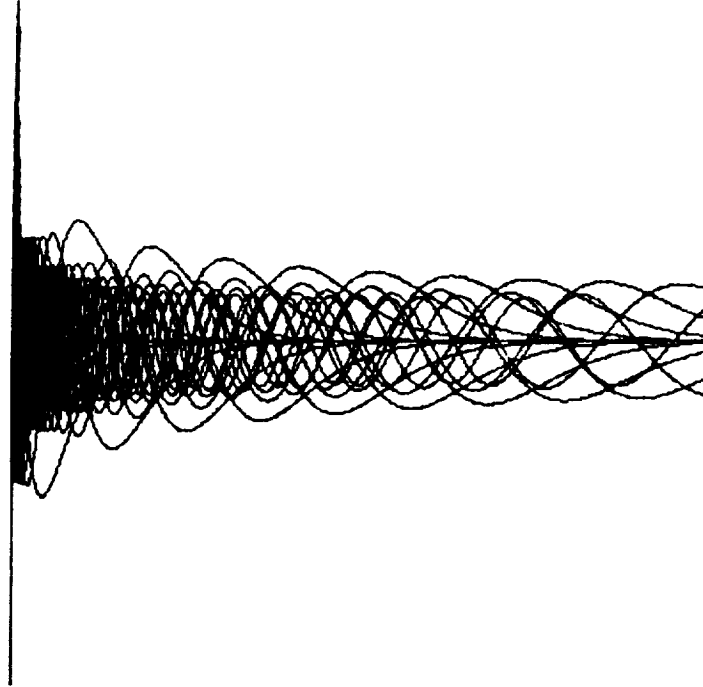


Figure 3.1 - Plot of $\tilde{L}_n^{(0)}$, for $n = 1, 20$.

Nevertheless, the new recurrence formula is still ill-conditioned. In fact, when x is large, the determination of $\tilde{L}_0^{(\alpha)}(x)$ gives rise to underflow problems. Our goal is to find a more suitable scaling function. In order to be really effective, this function, denoted by $S_n(x)$, has to actually depend on both x and n . Then, we would like to define:

$$\hat{L}_n^{(\alpha)}(x) = S_n(x) L_n^{(\alpha)}(x), \quad n \in \mathbb{N}, x \in [0, +\infty[. \quad (3.1)$$

We can try first by setting: $S_n(x) = \left(1 + \frac{x}{2n}\right)^{-n}$, $n \geq 1$. In this way, for any fixed n , S_n^{-1} behaves like a polynomial and, for any fixed x , we have $\lim_{n \rightarrow \infty} S_n(x) = e^{-x/2}$. After such a scaling, computations seem to be more flexible. An appropriate recursive formula can be written for $\hat{L}_n^{(\alpha)}$. Unfortunately, one can check that, with this choice of S_n , the cost for implementing the formula is proportional to n^2 .

Therefore we suggest another scaling function, i.e.

$$S_n(x) = \left[\binom{n+\alpha}{n} \prod_{k=1}^n \left(1 + \frac{x}{4k}\right) \right]^{-1}, \quad n \geq 1, \quad (3.2)$$

and we take $S_0(x) = 1$. Thus we obtain the following formula:

$$\begin{cases} \hat{L}_0^{(\alpha)}(x) = 1 \\ \hat{L}_1^{(\alpha)}(x) = \frac{4(\alpha+1-x)}{(\alpha+1)(x+4)} \\ \hat{L}_n^{(\alpha)}(x) = \frac{4n}{(n+\alpha)(4n+x)} \left[(2n+\alpha-1-x) \hat{L}_{n-1}^{(\alpha)}(x) - \frac{4(n-1)^2}{4n+x-4} \hat{L}_{n-2}^{(\alpha)}(x) \right], n \geq 2. \end{cases} \quad (3.3)$$

From (3.3) we can obtain the value of $\hat{L}_n^{(\alpha)}(x)$ at a given x , with a cost proportional to n . In the next, we shall refer to $\hat{L}_n^{(\alpha)}$, obtained by (3.1) with the help of (3.2), as *scaled Laguerre functions*.

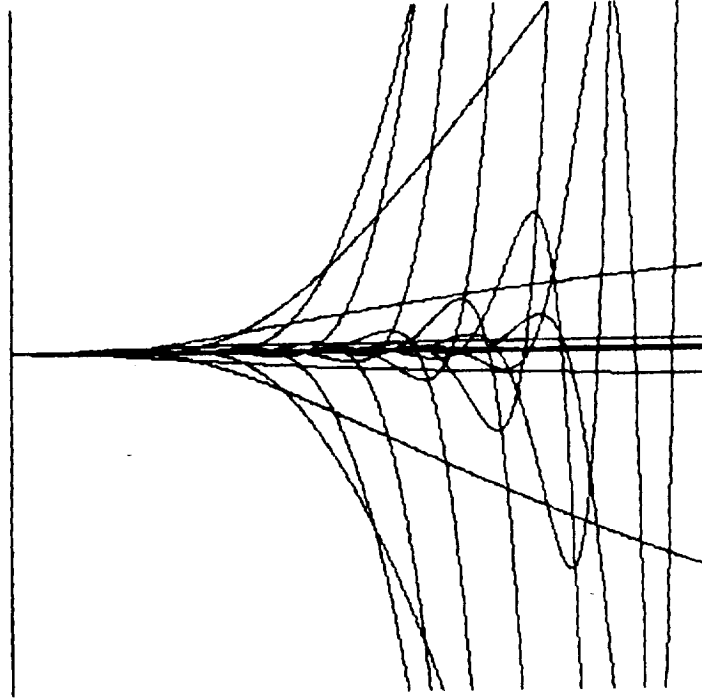


Figure 3.2 - Plot of $\hat{L}_n^{(0)}$, for $n = 1, 20$.

It is clear that these are not polynomials. Their structure is more appealing for numerical tests. The plot of the first twenty scaled Laguerre functions (with $\alpha = 0$) is given in Figure 3.2. Now all the plots are included in the rectangle $[0, 70] \times [-500, 500]$. The computational range is reduced. We make clear this fact by a numerical experiment. In the first column of Table 3.1 we give the values of $|L_2^{(0)}(x)/L_{40}^{(0)}(x)|$ for various x . There is a difference of 13 digits between the highest and the lowest value. In the second column of Table 3.2, we report $|\hat{L}_2^{(0)}(x)/\hat{L}_{40}^{(0)}(x)|$. Now the width is reduced to 5 digits.

x	Column 1	Column 2
10	7.273E-00	3.129E + 03
20	1.779E-00	1.035E + 05
30	1.607E-03	6.215E + 03
40	2.405E-05	3.743E + 03
50	1.954E-07	8.379E + 02
60	1.786E-09	1.554E + 02
70	1.638E-11	2.285E + 01
80	2.187E-13	4.015E + 00

Table 3.1 - *Comparison between Laguerre polynomials and scaled Laguerre functions.*

We remark that $\hat{L}_n^{(\alpha)}(0) = 1, \forall n \in \mathbb{N}$. For convenience we also give the formula to compute the derivatives, i.e.:

$$\left\{ \begin{array}{l} \frac{d}{dx} \hat{L}_0^{(\alpha)}(x) = 0 \\ \frac{d}{dx} \hat{L}_1^{(\alpha)}(x) = -\frac{4}{(x+4)^2} \frac{\alpha+5}{\alpha+1} \\ \frac{d}{dx} \hat{L}_n^{(\alpha)}(x) = \frac{4n}{(n+\alpha)(4n+x)} \left[(2n + \alpha - 1 - x) \frac{d}{dx} \hat{L}_{n-1}^{(\alpha)}(x) - \frac{6n+\alpha-1}{4n+x} \hat{L}_{n-1}^{(\alpha)}(x) + \right. \\ \left. + \frac{4(n-1)^2}{4n+x-4} \left(\frac{2(4n+x-2)}{(4n+x)(4n+x-4)} \hat{L}_{n-2}^{(\alpha)}(x) - \frac{d}{dx} \hat{L}_{n-2}^{(\alpha)}(x) \right) \right], \quad n \geq 2. \end{array} \right. \quad (3.4)$$

We will see in the next section how to apply the scaled functions to pseudospectral computations.

4. Numerical Integration

Let $N \geq 1$ be an integer. Let us define $\eta_{k,N}^{(\alpha)}, k = 1, \dots, N$ to be zeroes of $L_N^{(\alpha)}, \alpha > -1$. It can be shown that $\eta_{k,N}^{(\alpha)} > 0, k = 1, \dots, N$. Then define the weights:

$$w_{k,n}^{(\alpha)} = \frac{\Gamma(N + \alpha + 1)\eta_{k,n}^{(\alpha)}}{(N + 1)![(N + 1)L_{N+1}^{(\alpha)}(\eta_{k,N}^{(\alpha)})]^2}, k = 1, \dots, N. \quad (4.1)$$

The following quadrature formula is known (see for instance [8]):

$$\int_0^{+\infty} f w^{(\alpha)} dx = \sum_{k=1}^N f(\eta_{k,N}^{(\alpha)}) w_{k,N}^{(\alpha)} + \frac{\Gamma(N + \alpha + 1)}{N!(2N)!} f^{(2N)}(\xi), \quad (4.2)$$

where $0 < \xi < +\infty$. In particular, the second term on the right hand side vanishes when f is a polynomial of degree at most $2N - 1$. For convenience, we shall set $\eta_k = \eta_{k,N}^{(\alpha)}$ and $w_k = w_{k,N}^{(\alpha)}$. We are concerned with the numerical evaluation of η_k and $w_k, k = 1, \dots, N$. An approximation of the zeroes of $L_N^{(\alpha)}$ can be obtained by the following procedure (see [7] and [8]). We first define $y_k, k = 1, \dots, N$ to be solutions of the equations.

$$y_k - \sin y_k = 2\pi \frac{N - k + 3/4}{2N + \alpha + 1}, \quad k = 1, \dots, N. \quad (4.3)$$

Afterwards we set $z_k = [\cos(\frac{1}{2}y_k)]^2, k = 1, \dots, N$, and finally we get:

$$\eta_k \approx 2(2N + \alpha + 1)z_k + -\frac{1}{6(2N + \alpha + 1)} \left[\frac{5}{4(1 - z_k)^2} - \frac{1}{1 - z_k} - 1 + 3\alpha^2 \right]. \quad (4.4)$$

Starting from this approximated value for η_k , we can refine it by very few iterations of the Newton method. The computed zeroes are in general very accurate. However, evaluating $L_N^{(\alpha)}(\eta_{k,N}^{(\alpha)})$ and $\frac{d}{dx} L_N^{(\alpha)}(\eta_{k,N}^{(\alpha)}), k = 1, \dots, N$, in order to use the Newton method, may give problems when performed by (2.3) and (2.4). Nevertheless, since the zeroes of $L_N^{(\alpha)}$ are the same than the zeroes of $\hat{L}_N^{(\alpha)}$, we can use (3.3) and (3.4). This allows the determination of the zeroes for larger values of N . Concerning the weights, they are decreasing and converging to zero very fast. It is convenient to define other weights as follows (recall (3.2)):

$$\begin{aligned} \hat{w}_{k,N}^{(\alpha)} &= \hat{w}_k = \frac{w_k}{[S_N(\eta_k)]^2} = \\ &= \frac{\Gamma(N + \alpha + 1)\eta_k}{(N + 1)!\Gamma^2(\alpha + 1)} \left[\frac{4(N + 1)}{(N + \alpha + 1)(4N + 4 + \eta_k)\hat{L}_{N+1}^{(\alpha)}(\eta_k)} \right]^2. \end{aligned} \quad (4.5)$$

The new weights are in the machine range for larger values of N . Of course, one has to write:

$$\frac{\Gamma(N + \alpha + 1)}{(N + 1)!} = \frac{N + \alpha}{N + 1} \left(\frac{N + \alpha - 1}{N} \left(\dots \left(\frac{\alpha + 1}{2} \right) \dots \right) \right) \Gamma(\alpha + 1), \quad (4.6)$$

obtaining a more reliable algorithm.

If p is a polynomial of degree at most $2N - 1$, from (4.2) and (4.5) we obtain:

$$\int_0^{+\infty} p w^{(\alpha)} dx = \sum_{k=1}^N [p(\eta_k) S_N^2(\eta_k)] \hat{w}_k. \quad (4.7)$$

Moreover, if u_N is a polynomial of degree at most N , we have:

$$\int_0^{+\infty} u_N^2 w^{(\alpha)} dx \approx \sum_{k=1}^N [(u_N S_N)(\eta_k)]^2 \hat{w}_k. \quad (4.8)$$

This suggests to work with $u_N S_N$ instead than u_N when approximating the solution of a differential equation by the collocation method based on Laguerre polynomials. We analyze in the next section in which way this can be actually done.

5. Pseudospectral Laguerre Approximations

Let us focus our attention on a very simple equation, namely:

$$\begin{cases} -U_{xx} + \lambda U &= f \text{ in }]0 + \infty[, \lambda > 0, \\ U(0) &= \gamma \in \mathbf{R}, \\ \lim_{x \rightarrow +\infty} U(x) &= 0. \end{cases} \quad (5.1)$$

Under suitable assumptions on f and λ , one can prove that there exists a unique solution of (5.1) (see [2]). For approximations with Laguerre polynomials we require for U an exponential decay at infinity. By setting $V = U e^x$, problem (5.1) becomes:

$$\begin{cases} -V_{xx} + 2V_x + (\lambda - 1)V = g \text{ in }]0, +\infty[, \\ V(0) = \gamma, \end{cases} \quad (5.2)$$

where $g = f e^x$.

Keeping the same notations of the previous section, let $\eta_k, k = 1, \dots, N$ be the zeroes of $L_N^{(\alpha)}$. Then the solution of (5.2) is approximated by a polynomial v_N of degree less or equal N satisfying the collocation problem:

$$\begin{cases} -v_{N,xx}(\eta_k) + 2v_{N,x}(\eta_k) + (\lambda - 1)v_N(\eta_k) = g(\eta_k), & k = 1, \dots, N, \\ v_N(0) = \gamma. \end{cases} \quad (5.3)$$

As usual (see [1] and [4]), (5.3) is equivalent to an appropriate linear system whose unknowns are $v_N(\eta_k), k = 1, \dots, N$. When N tends to infinity, v_N converges to V in a suitable weighted Sobolev space (see [2]).

The basic tool for computations is the derivative operator D_N in the space of polynomials of degree N . With the aim of getting the entries $d_{ij}, i, j = 0, \dots, N$ of D_N , we consider the Lagrange polynomials with respect to the nodes $\eta_k, k = 0, \dots, N$ where we defined $\eta_0 = 0$. These are given by:

$$l_j(x) = \frac{x L_N^{(\alpha)}(x)}{\eta_j [\frac{d}{dx} L_N^{(\alpha)}(\eta_j)]} \frac{1}{x - \eta_j}, \quad j = 1, \dots, N, \quad (5.4)$$

$$l_0(x) = \frac{L_N^{(\alpha)}(x)}{L_N^{(\alpha)}(0)}. \quad (5.5)$$

The l_j 's are polynomials of degree N . Then we have

$$d_{ij} = l_j'(\eta_i) \quad i, j = 0, \dots, N. \quad (5.6)$$

Moreover for any polynomial p of degree at most N , one gets:

$$\sum_{j=0}^N d_{ij} p(\eta_j) = p'(\eta_i), \quad i = 0, \dots, N. \quad (5.7)$$

The following useful relations can be recovered from (2.1):

$$\frac{d^2}{dx^2} L_N^{(\alpha)}(\eta_j) = \frac{\eta_j - \alpha - 1}{\eta_j} \frac{d}{dx} L_N^{(\alpha)}(\eta_j), \quad j = 1, \dots, N, \quad (5.8)$$

$$\frac{d}{dx} L_N^{(\alpha)}(0) = -\frac{N}{\alpha + 1} L_N^{(\alpha)}(0), \quad (5.9)$$

$$\frac{d^2}{dx^2} L_N^{(\alpha)}(0) = \frac{N(N-1)}{(\alpha+1)(\alpha+2)} L_N^{(\alpha)}(0), \quad (5.10)$$

$$\frac{d^3}{dx^3} L_N^{(\alpha)}(\eta_j) = \left[\frac{(\eta_j - \alpha - 2)(\eta_j - \alpha + 1)}{\eta_j^2} - \frac{N-1}{\eta_j} \right] \frac{d}{dx} L_N^{(\alpha)}(\eta_j), \quad j = 1, \dots, N. \quad (5.11)$$

Thus, with the help of (5.8) - (5.11), one gets:

$$d_{ij} = \begin{cases} \frac{\eta_i \frac{d}{dx} L_N^{(\alpha)}(\eta_i)}{\eta_j \frac{d}{dx} L_N^{(\alpha)}(\eta_j)} \frac{1}{\eta_i - \eta_j} & i, j = 1, \dots, N, i \neq j, \\ \frac{1 - \alpha + \eta_i}{2\eta_i} & i = j = 1, \dots, N, \\ \frac{\frac{d}{dx} L_N^{(\alpha)}(\eta_i)}{L_N^{(\alpha)}(0)} & i = 1, \dots, N, j = 0, \\ -\frac{L_N^{(\alpha)}(0)}{\eta_j^2 \frac{d}{dx} L_N^{(\alpha)}(\eta_j)} & j = 1, \dots, N, i = 0, \\ -\frac{N}{\alpha + 1} & i = j = 0. \end{cases} \quad (5.12)$$

The second derivative operator is obtained either by squaring D_N either by evaluating $l_j'''(\eta_i)$. In the last case, recalling (5.8) - (5.11), we have:

$$l_j'''(\zeta_i) = \begin{cases} \frac{\frac{d}{dx} L_N^{(\alpha)}(\eta_i)}{\eta_j \frac{d}{dx} L_N^{(\alpha)}(\eta_j)} \frac{(1 - \alpha + \eta_i)(\eta_i - \eta_j) - 2\eta_i}{(\eta_i - \eta_j)^2} & i, j = 1, \dots, N, i \neq j, \\ \frac{(\eta_i - \alpha)^2}{3\eta_i^2} - \frac{N - 1}{3\eta_i} & i = j = 1, \dots, N, \\ -\frac{\alpha + 1 - \eta_i}{\eta_i} \frac{\frac{d}{dx} L_N^{(\alpha)}(\eta_i)}{L_N^{(\alpha)}(0)} & i = 1, \dots, N, j = 0, \\ -\frac{2(N + \alpha + 1)}{\eta_j^3(\alpha + 1)} \frac{L_N^{(\alpha)}(0)}{\frac{d}{dx} L_N^{(\alpha)}(\eta_j)} & j = 1, \dots, N, i = 0, \\ \frac{N(N - 1)}{(\alpha + 1)(\alpha + 2)} & i = j = 0. \end{cases} \quad (5.13)$$

After taking into account the boundary conditions, we end up with the matrix corresponding to the linear system (5.3).

As pointed out in the previous section, Laguerre polynomials are not suitable for computations. However we can use scaled Laguerre functions. Therefore, we define $\hat{v}_k = v_N(\eta_k) S_N(\eta_k)$, $k = 0, \dots, N$. The \hat{v}_k 's will be the new unknowns. Besides, we define a new matrix $\hat{D}_N = \{\hat{d}_{ij}\}$ as follows:

$$\hat{d}_{ij} = d_{ij} \frac{S_N(\eta_i)}{S_N(\eta_j)}, \quad i, j = 0, \dots, N. \quad (5.14)$$

Due to (5.7) we have:

$$S_N(\eta_i)v'_N(\eta_i) = S_N(\eta_i) \sum_{j=0}^N d_{ij}v_N(\eta_j) = \sum_{j=0}^N \hat{d}_{ij}\hat{v}_j, \quad i = 0, \dots, N. \quad (5.15)$$

Similar relations hold for higher order derivatives. Thus, by multiplying the equations in (5.3) by $S_N(\eta_k)$, $k = 0, \dots, N$ we can easily obtain a new linear system in the unknowns \hat{v}_j , $j = 0, \dots, N$, involving the knowledge of the coefficients \hat{d}_{ij} instead than d_{ij} . The \hat{d}_{ij} 's are less affected by ill-conditioning problems, since they are related to scaled Laguerre functions. In fact, we observe that:

$$S_N \frac{d}{dx} L_N^{(\alpha)} = \frac{d}{dx} \hat{L}_N^{(\alpha)} + \hat{L}_N^{(\alpha)} S_N \frac{d}{dx} (S_N^{-1}). \quad (5.16)$$

Moreover:

$$\left[S_N \frac{d}{dx} (S_N^{-1}) \right] (x) = \sum_{k=1}^N \frac{1}{4k+x}. \quad (5.17)$$

Finally, we define:

$$Q_i = \frac{d}{dx} \hat{L}_N^{(\alpha)}(\eta_i) + \hat{L}_N^{(\alpha)}(\eta_i) \sum_{k=1}^N \frac{1}{4k+\zeta_i}, \quad i = 0, \dots, N. \quad (5.18)$$

Therefore, by substituting in (5.12), one gets:

$$\hat{d}_{ij} = \begin{cases} \frac{\eta_i Q_i}{\eta_j Q_j} \frac{1}{\eta_i - \eta_j} & i, j = 1, \dots, N, i \neq j, \\ \frac{1 - \alpha + \eta_i}{2\eta_i} & i = j = 1, \dots, N, \\ Q_i & i = 1, \dots, N, j = 0, \\ \frac{-1}{\eta_j^2 Q_j} & j = 1, \dots, N, i = 0, \\ \frac{-N}{\alpha + 1} & i = j = 0. \end{cases} \quad (5.19)$$

We can argue similarly for the second derivative matrix. After solving the new preconditioned system we obtain \hat{v}_j , $j = 1, \dots, N$. After this, one can recover the values $v_N(\eta_j)$, $j = 1, \dots, N$, which are in general very large, when j is close to N . On the other hand, these values are associated to the weight w_j that is negligible when j is close to N . Nevertheless, we remark that in order to evaluate the weighted norm of v_N , one does not need to know its values at the collocation nodes. Actually, recalling (4.8) we have:

$$\int_0^{+\infty} v_N^2 w^{(\alpha)} dx \approx \sum_{j=1}^N \hat{v}_j^2 \hat{w}_j. \quad (5.20)$$

The right-hand side of (5.19) is now more suitable for computations. The procedure here described can be clearly generalized to other kinds of problems.

6. Hermite Approximations

All we developed above for Laguerre polynomials can be extended to cover the case of Hermite polynomials. In analogy with (2.12) and (2.13), it is convenient to define the *scaled Hermite functions* as follows:

$$\hat{H}_n(x) = \hat{L}_{n/2}^{(-1/2)}(x^2), \quad \text{if } n \text{ is even,} \quad (6.1)$$

$$\hat{H}_n(x) = x \hat{L}_{(n-1)/2}^{(1/2)}(x^2), \quad \text{if } n \text{ is odd.} \quad (6.2)$$

In particular, we obtain:

$$\hat{H}_n(0) = 1, \quad \text{if } n \text{ is even,} \quad (6.3)$$

$$\hat{H}'_n(0) = 1, \quad \text{if } n \text{ is odd.} \quad (6.4)$$

The derivative matrices for the Hermite case have been presented in [3]. These matrices can be suitably preconditioned when using scaled Hermite functions. As before, the scaling procedure we adopt, is only to be considered as a trick to perform computations in a better way. Theoretical analysis and convergence estimates remain the same, since the collocation scheme is not actually modified. Of course, improvements could be expected when adopting other functions S_n in place of (3.2).

References

- [1] C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang, *Spectral Methods in Fluid Dynamics*, Springer Series in Computational Physics, Springer-Verlag, New York (1989).
- [2] O. Coulaud, D. Funaro, and O. Kavian, Laguerre Spectral Approximation of Elliptic Problems in Exterior Domains, Preprint No. 690, IAN-CNR, Pavia, Italy. Also to appear in Proceedings of the ICOSAHOM, Como, Italy, June, 1989.
- [3] D. Funaro and O. Kavian, Approximation of Some Diffusion Evolution Equations in Unbounded Domains by Hermite Functions," to appear in Math. Comp.
- [4] D. Gottlieb and S. A. Orszag, *Numerical Analysis of Spectral Methods: Theory and Applications*, CBMS Regional Conference Series in Applied Mathematics, SIAM (1977).
- [5] Y. Maday, B. Pernaud-Thomas, and H. Vandeven, Une Réhabilitation des Méthodes de Type Laguerre, La Recherche Aéronautique, No. 6 (1985), pp. 353-375.
- [6] C. Mavriplis, Laguerre Polynomials for Infinite-Domain Spectral Elements, to appear in J. Comput. Phys.
- [7] L. Gatteschi, Proprietà Asintotiche di una Funzione Associata ai Polinomi di Laguerre e loro Utilizzazione al Calcolo Numerico degli Zeri dei Polinomi Stessi, Atti della Accademia delle Scienze di Torino, Vol. 98 (1963-64).
- [8] G. Szegő, *Orthogonal Polynomials*, AMS New York (1939).



Report Documentation Page

1. Report No. NASA CR-181934 ICASE Report No. 89-72		2. Government Accession No.		3. Recipient's Catalog No.	
4. Title and Subtitle COMPUTATIONAL ASPECTS OF PSEUDOSPECTRAL LAGUERRE APPROXIMATIONS				5. Report Date October 1989	
				6. Performing Organization Code	
7. Author(s) Daniele Funaro				8. Performing Organization Report No. 89-72	
				10. Work Unit No. 505-90-21-01	
9. Performing Organization Name and Address Institute for Computer Applications in Science and Engineering Mail Stop 132C, NASA Langley Research Center Hampton, VA 23665-5225				11. Contract or Grant No. NAS1-18605	
				13. Type of Report and Period Covered Contractor Report	
12. Sponsoring Agency Name and Address National Aeronautics and Space Administration Langley Research Center Hampton, VA 23665-5225				14. Sponsoring Agency Code	
15. Supplementary Notes Langley Technical Monitor: Richard W. Barnwell Final Report Applied Mathematics Computations					
16. Abstract Pseudospectral approximations in unbounded domains by Laguerre polynomials lead to ill-conditioned algorithms. We introduce a scaling function and appropriate numerical procedures in order to limit these unpleasant phenomena.					
17. Key Words (Suggested by Author(s)) Laguerre Polynomials, Pseudospectral Approximations, Numerical Algorithms			18. Distribution Statement 64 - Numerical Analysis Unclassified - Unlimited		
19. Security Classif. (of this report) Unclassified		20. Security Classif. (of this page) Unclassified		21. No. of pages 15	22. Price A03