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Studies on the Method of Orthogonal Collocation IV. Laguerre and Hermite Orthogonal Collocation Method

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Abstract. Differential equations for which the zeros of Laguerre and Hermite polynomials are suitable collocation points are identified. It is shown that the equations representing tubular reactors with axial dispersion can be solved efficiently using the zeros of Laguerre polynomials to obtain the inlet concentration.

Nomenclature

c	Constant
Da	Damkohler number
$H_n(y)$	Hermite polynomial of nth order
$L_n(y)$	Laguerre polynomials of nth order
Pe	Peclet number
R(u)	Dimensionless rate of reaction
x	Dimensionless distance or independent variable
y	Dimensionless distance or independent variable (y = Pe x)
u	Dimensionless concentration or dependent variable
v	Dependent variable

Introduction

The choice of collocation points for the solution of boundary value problems by the collocation method is very crucial if it is desirable to solve the problem using a low order polynomial. The zeros of orthogonal polynomials generally give better results than equally distributed collocation points. Villadsen and Michelsen [1] give the proper Jacobi polynomial for certain boundary value problems representing diffusion with chemical reaction in a slab, cylinder and sphere. Although, the zeros of Laguerre polynomials and Hermite polynomials are suitable for use in collocation methods for semi-finite and infinite domain differential equations [2] no attempt has been made to identify the type of equations for which this choice is optimal.

Reference [3] indicated the type of equations for which Jacobi polynomials are suitable for their solution by the orthogonal collocation method. Here we give the type of equations that can be solved efficiently by Laguerre and Hermite polynomials. It is shown in this paper that tubular reactor equations are a special case of this general form of equations solvable by Laguerre polynomials.

Orthogonal polynomials

Two classes of orthogonal polynomials will be of interest in this paper. The first class is Laguerre polynomials $L_n(y)$ which satisfy the orthogonality condition,

$$\int_0^\infty e^{-y} y^\alpha L_n(y) L_m(y) dy = 0, \qquad m \neq n$$
$$\neq 0 \quad ; \qquad m = n$$
$$y \in [\,0, \infty) \tag{1}$$
$$\alpha > -1$$
$$m = 1, 2, \ldots, n$$

The second class is Hermite polynomials $H_n(y)$ which satisfy the orthogonality condition

$$\int_{-\infty}^\infty e^{-y^2} H_n(y) H_m(y) dy = 0, \qquad m \neq n$$
$$\neq 0 \quad ; \qquad m = n$$
$$y \in (-\infty, \infty) \tag{2}$$
$$m = 1, 2, \ldots, n$$

Laguerre orthogonal collocation method

In this section we give the general form of equation for which Laguerre polynomials are most suitable. In addition we give formula for interpolation, first order derivative, second order derivative and Laguerre quadrature weights for one and two points collocation method. Laguerre polynomials satisfy the differential equation

$$\frac{e^{y}}{y^{\alpha}}\frac{d}{dy}\left[e^{-y}y^{\alpha+1}\frac{dv}{dy}\right]+nv=0\ ,\quad \alpha>-1 \tag{3}$$

or

$$y\frac{d^{2}v}{dy^{2}}+(\alpha+1-y)\frac{dv}{dy}+nv=0 \tag{4}$$

where $v = L_n(y)$.

Define

$$u=uo+y\sum_{i=0}^{N}a_{i}L_{i}(y) \tag{5}$$

and construct the differential equation

$$y\frac{d^{2}\left(\frac{u-u_{o}}{y}\right)}{dy^{2}}+(\alpha+1-y)\frac{d\left(\frac{u-u_{o}}{y}\right)}{dy}+\frac{c(u-u_{o})}{y}=\phi^{2}u \tag{6}$$

or

$$\frac{d^{2}u}{dy^{2}}+(\frac{\alpha-1-y}{y})\frac{du}{dy}+(u-u_{o})\frac{(cy+1-\alpha+y)}{y^{2}}=\phi^{2}u \tag{7}$$

where $u(0) = u_o$

This is the general form that can be solved efficiently using the collocation method where the N collocation points are the zeros of Laguerre polynomials $L_N(y)$. This is due to the fact that the solution at the collocation points makes the left hand side and the right hand side of the equation independent of a_N when we substitute the polynomial solution u(y) (equation (5)) on both sides. In addition the following integral

$$I=\int_{0}^{\infty}e^{-y}y^{\alpha-1}u(y)dy \tag{8}$$

evaluated at the zeros of Laguerre polynomial $L_N(y)$ will not depend on a_N. Thus we expect that this Laguerre quadrature will be accurate for u(y) given by equation (5).

We give here the Lagrange interpolation formulae, first order and second order weights and Laguerre quadrature weights for one and two points collocation method.

(i) One point collocation method

$$L_1(y) = (\alpha + 1) - y \tag{9}$$

$$y_1 = 1 + \alpha \qquad \text{(zero of } L_1(y)) \tag{10}$$

$$u(y) = \frac{-(y - y_1)u_o + yu_1}{1+\alpha} \tag{11}$$

$$\left.\frac{du}{dy}\right|_{y=y_1} = \frac{u_1 - u_o}{1+\alpha} \tag{12}$$

$$\left.\frac{d^2u}{dy^2}\right|_{y=y_1} = 0 \tag{13}$$

$$\int_o^\infty e^{-y} y^{\alpha-1} dy = \frac{(u_o + \alpha u_1)\Gamma(\alpha)}{1+\alpha} \tag{14}$$

(ii) Two points collocation method

Let
$$b = 2 + \alpha \tag{15}$$

$$L_2(y) = y^2 - 2by + b(b-1) \tag{16}$$

$$\left.\begin{aligned} y_1 &= b - \sqrt{b} \\ y_2 &= b + \sqrt{b} \end{aligned}\right) \qquad \text{(zeros of } L_2(y)\text{)} \tag{17}$$

$$u(y) = \frac{(y-y_1)(y-y_2)}{b(b-1)}u_o - \frac{(1+\sqrt{b})y(y-y_2)u_1}{2b(b-1)} - \frac{(1-\sqrt{b})y(y-y_1)u_2}{2b(b-1)} \tag{18}$$

$$\left.\frac{du}{dy}\right|_{y=y_1} = \frac{[2b+(3-b)\sqrt{b}]}{2b(b-1)}(u_1-u_o)+\frac{[(1+b)\sqrt{b}-2b]}{2b(b-1)}(u_2-u_o) \tag{19}$$

$$\left.\frac{du}{dy}\right|_{y=y_2} = \frac{[2b+(1+b)\sqrt{b}]}{2b(b-1)}(u_1-u_o)+\frac{[2b-(3-b)\sqrt{b}]}{2b(b-1)}(u_2-u_o) \tag{20}$$

$$\left.\frac{d^2u}{dy^2}\right|_{y=y_1} = \left.\frac{d^2u}{dy^2}\right|_{y=y_2} = \frac{-(1+\sqrt{b})(u_1-u_o)}{b(b-1)}+\frac{(\sqrt{b}-1)}{b(b-1)}(u_2-u_o) \tag{21}$$

$$\int_o^\infty y^{\alpha-1}e^{-y}\,u\,dy = \left[\frac{2}{b(b-1)}u_o+\frac{(b-2)(1+b+2\sqrt{b})}{2b(b-1)}u_1 + \frac{(b-2)(1+b-2\sqrt{b})}{2b(b-1)}u_2\right]\Gamma(\alpha) \tag{22}$$

Programs are available for calculating zeros of Laguerre polynomials, derivative weights and quadrature weights, see for example reference [4].

Another form of equation for which Laguerre polynomials are most suitable can be obtained if we have the following boundary conditions,

$$u|_{y=o} = u(o), \quad u \to 0 \quad \text{as } y \to \infty \tag{23}$$

We replace u(y) by e^y u(y) in Eq. (7) to obtain

$$\frac{d^2u}{dy^2}+\left(\frac{\alpha-1+y}{y}\right)\frac{du}{dy}+\frac{\alpha-1}{y}u+(u-u(0)e^{-y})\frac{(cy+1-\alpha+y)}{y^2}=\phi^2 u \tag{24}$$

with u(y) given by

$$u(y) = u_o\,e^{-y} + y\,e^{-y}\;\Sigma\; a_i\,L_i(y) \tag{25}$$

The following integral

$$I = \int_0^\infty y^{\alpha-1} u(y) dy \tag{26}$$

can be integrated accurately using Laguerre quadrature.

Hermite orthogonal collocation method

Hermite polynomials $H_n(y)$ satisfy the differential equation

$$e^{y^2} \frac{d}{dy}\left[e^{-y^2} \frac{dv}{dy}\right] + 2nv = 0 \tag{27}$$

or

$$\frac{d^2v}{dy^2} - 2y\frac{dv}{dy} + 2nv = 0 \tag{28}$$

where

$$v = H_n(y) \tag{29}$$

Define

$$u = u_o + y \sum_{i=0}^{N} a_i H_i(y) \tag{30}$$

and construct the differential equation;

$$\frac{d^2(\frac{u-u_o}{y})}{dy^2} - 2y \frac{d(\frac{u-u_o}{y})}{dy} + c\,(\frac{u-u_o}{y}) = \phi^2 u \tag{31}$$

or

$$\frac{1}{y}\frac{d^2u}{dy^2} - \frac{2}{y^2}(1+y^2)\frac{du}{dy} + \frac{2(u-u_o)(1+y^2)}{y^3} + c\frac{(u-u_o)}{y} = \phi^2 u \tag{32}$$

This is the general form for equations that can be solved efficiently using Hermite polynomials.

The following integral will be evaluated by Hermite quadrature,

$$I = \int_{-\infty}^{\infty} e^{-y2} u(y)dy \ . \qquad (33)$$

Since the zeros of odd order Hermite polynomial include y = 0, we need to obtain the limit of equation (32) as $y \rightarrow 0$. This is

$$\frac{1}{3}\frac{d^3u}{dy^3} + c\frac{du}{dy} = \phi^2 u \qquad (34)$$

If in addition to the condition that

$$u(0) = u_o \qquad (35)$$

we have

$$u \rightarrow 0 \text{ as } y \rightarrow \pm\infty \qquad (36)$$

we can replace u by $e^{y^2}u$ in Eq. (28) to obtain

$$\frac{1}{y}\frac{d^2y}{dy^2} + \frac{2(y^2-1)du}{y^2 \ dy} - \frac{2}{y}u + \frac{(2+(c+2)y^2)}{y^3}(u - e^{-y^2}u(0)) = \phi^2 u \qquad (37)$$

with u given by

$$u = e^{-y^2}\left[u_o + y\sum_{i=0}^{N} a_i H_i(y)\right] \qquad (38)$$

and as $y \rightarrow 0$, the differential Eq. (37) becomes

$$\frac{1}{3}\frac{d^3u}{dy3} + (c+2)\frac{du}{dy} = \phi^2 u \qquad (39)$$

The following integral will be integrated using Hermite quadrature

$$I = \int_{-\infty}^{\infty} u \, dy \qquad (40)$$

The use of one point and two points collocation method for problems that will be solved at the zeros of Hermite polynomials require the evaluation of the following weights for derivatives and quadrature.

(i) **One point collocation method**

$$H_1(y) = y \tag{41}$$

$$y_1 = 0 \quad (\text{ zero of } H_1(y)) \tag{42}$$

$$u(y) = u_o + ay \qquad \text{(a is a constant)} \tag{43}$$

$$\left.\frac{du}{dy}\right|_{y=y_1} = a, \left.\frac{d^2u}{dy^2}\right|_{y=y_1} = 0 \tag{44}$$

$$\int_{-\infty}^{\infty} e^{-y^2} u(y)dy = \sqrt{\pi}u_o \qquad \text{(independent of a)}$$

(ii) **Two points collocation method**

$$H_2(y) = 4y^2 - 2 \tag{45}$$

$$y_1 = \frac{\sqrt{2}}{2} \tag{46}$$

$$y_2 = \frac{-\sqrt{2}}{2} \tag{47}$$

$$u(y) = (1 - 2y^2)u_o + y(y - y_2)u_1 + y(y - y_1)u_2 \tag{48}$$

$$\left.\frac{du}{dy}\right|_{y=y_1} = \frac{\sqrt{2}}{2}(3u_1 + u_2 - 4u_o) \tag{49}$$

$$\left.\frac{du}{dy}\right|_{y=y_2} = -\frac{\sqrt{2}}{2}(3u_2 + u_1 - 4u_o) \tag{50}$$

$$\left.\frac{d^2u}{dy^2}\right|_{y=y_1} = \left.\frac{d^2u}{dy^2}\right|_{y=y_2} = 2(u_1 + u_2 - 2u_o) \tag{51}$$

$$\int_{-\infty}^{\infty} e^{-y^2} u(y)dy = \frac{\sqrt{\pi}}{2}(u_1 + u_2) \tag{52}$$

Applications

In this section we give two examples for the application of the method developed in this paper. In the first one, we show how Laguerre orthogonal collocation method can be used to obtain the inlet concentration of tubular reactor with large axial dispersion accurately. In the second example we apply Hermite orthogonal collocation method.

Example 1: Tubular reaction with axial dispersion:

The describing equations for an isothermal tubular reactors with axial dispersion is given by;

$$\frac{1}{Pe}\frac{d^2u}{dx^2} - \frac{du}{dx} = Da\ R(u) \tag{53}$$

with the boundary conditions;

$$\left.\frac{1}{Pe}\frac{du}{dx}\right|_{x=0} = u(o) - 1 \tag{54}$$

and

$$\left.\frac{du}{dx}\right|_{x=1} = 0 \tag{55}$$

We are mainly interested here for the case of large Pe ($Pe \to \infty$). We use the transformation

$$y = Pe\ x \tag{56}$$

Substituting Eq. (56) into Eqs. (53-55), we obtain

$$\frac{d^2u}{dy^2}-\frac{du}{dy}=\frac{Da}{Pe}R(u) \tag{57}$$

with

$$\left.\frac{du}{dy}\right|_{y=0}=u(o)-1=\frac{Da}{Pe}\int_o^\infty e^{-y}R(u)dy \qquad (Pe\to\infty). \tag{58}$$

and u is finite as $y\to\infty$.
If we substitute $\alpha=1, c=-1$ in Eq. (7) we obtain

$$\frac{d^2u}{dy^2}-\frac{du}{dy}=\phi^2u \tag{59}$$

which is the equation of a tubular reactor with a first order reaction.

Equation (57) is a non-linear version of Eq. (59) and thus we expect that Laguerre quadrature will accurately determine the integral in Eq. (58) where u is obtained by the solution of Eq. (57) using the zeros of Laguerre polynomials as collocation points.

Applying the one-point collocation method for the linear case $(R(u)=u)$ we will have from Eq. (57)

$$u_1=\frac{u_o}{1+2DP} \tag{60}$$

where

$$DP=\frac{Da}{Pe} \tag{61}$$

$$I=\int_o^\infty e^{-y}u\,dy=\frac{(u_o+u_1)}{2}=\frac{(1+DP)u_o}{(1+2DP)} \tag{62}$$

From Eq. (58) we have

$$u_o-1=-\frac{DP(1+DP)u_o}{(1+2DP)} \tag{63}$$

Therefore

$$u_o = \frac{(1+2DP)}{(1+3DP+DP^2)} \tag{64}$$

For the case of $Da = 2$, $Pe = 100$, $u_o = 0.9808$.

This is the exact analytical result for four significant figures. The exit concentration (at y = Pe) is negative. We can however improve on the exit concentration if we use y = Pe as extra collocation point or if we increase the number of collocation points. It was shown in reference [5] that if we use the zeros of the proper orthogonal polynomials as collocation points an extra collocation point at any position will not affect the solution at the other collocation points.

In Table 1, we give a comparison between the results of the exact analytical solution, the two points standard collocation method using Legendre polynomials and the two point Laguerre collocation method with the exit point as extra collocation point. The zeros of Legendre polynomials are symmetric around the center of the reactor whereas the zeros of Laguerre polynomials are close to the entrance of the reactor. Thus we notice high accuracy of the concentration near the entrance of the reactor with Laguerre method whereas the concentration is more accurately calculated with the Legendre method near the reactor exit.

Table 1. Concentration profile (u) with different methods

x	Analytical solution u	Legendre collocation u	Laguerre collocation u
0.0	0.9808	0.9833	0.9808
0.1	0.8061	0.8245	0.8063
0.2	0.6626	0.6825	0.6646
0.3	0.5444	0.5571	0.5513
0.4	0.4476	0.4485	0.4622
0.5	0.3677	0.3565	0.3927
0.6	0.3023	0.2813	0.3387
0.7	0.2484	0.2228	0.2957
0.8	0.2042	0.1811	0.2594
0.9	0.1679	0.1560	0.2254
1.0	0.1406	0.1476	0.1893

For the non-linear case $R(u) = u^2$, also one point collocation gives accurate result for $u_o(0.9814)$.

Example 2.
We apply the one and two points collocation on Eq. (32) to obtain:

One point collocation

$$u(y) = u_o \left(1+\frac{\phi^2}{c} y\right) \qquad (c \neq 0) \qquad (65)$$

$$I = \int_{-\infty}^{\infty} e^{-y^2} u dy = \sqrt{\pi} u_o \qquad (66)$$

Two points collocation

$$u(y) = u_o \left[1+\left(\frac{\frac{\phi^2}{c} y+\frac{b\phi^4 y^2}{3}}{(1-\frac{b\phi^4}{6})}\right)\right]$$

$$b = \frac{3}{c(c-2)} \qquad (c \neq 0, c \neq 2) \qquad (67)$$

$$I = \frac{\sqrt{\pi} u_o}{1-\frac{b\phi^4}{6}} \qquad (68)$$

Due to the possibility of the the denominator becoming zero in value of the the integral I in Eq. (68), it is probable that the Hermite method is more efficiently applied to Eq. (32) with the value of c = 1. In this case b = -3 and denominator will not be zero.

Conclusions

In this paper the differential equations that can be solved efficiently using a collocation method where the collocation points are zeros of Laguerre and Hermite polynomials are identified. Two examples were worked out to show the application of the method.

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دراسات على طريقة التنظيم المتعامد – ٤. طرق التنظيم المتعامد للاجور وهيرمت

مصطفى على سليمان
قسم الهندسة الكيميائية، كلية الهندسة، جامعة الملك سعود، ص.ب ٨٠٠،
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ملخص البحث. تم تحديد المعادلات التفاضلية التي يمكن حلها بكفاءة باستخدام جذور كثيرات الحدود للاجور وهيرمت. كما تم حل المعادلات التي توصف التفاعلات في المفاعلات الأنبوبية ذات الانتشار المحوري بكفاءة باستخدام جذور كثيرة الحدود للاجور للحصول على تركيز المواد عند مدخل المفاعل .