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LETTER TO THE EDITOR

A new set of orthogonal polynomials for use in neutron transport theory

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Abstract. The proper set of orthogonal polynomials to use in approximation work depends on the weight function of the problem. Here, we introduce a new set of polynomials orthogonal with respect to a simple closed-form approximate representation of the weight function of Case's half-range neutron transport theory. The accuracy of this approximate weight function is shown to be very good, and the construction procedure of the new set of orthogonal polynomials, $\{C_i(\mu), c \leq \mu \leq 1\}$, is demonstrated.

The choice of the proper set of orthogonal polynomials for construction of approximate solutions of problems in mathematical physics is of central importance if the approximation is to yield reliable results with a reasonable number of terms. Among the equations in physics, the one-speed neutron transport equation is especially interesting, because the complete set of relevant eigenfunctions contain, besides regular functions, singular distributions in the form of the Cauchy principal value and Dirac delta distributions. These eigenfunction(al)s are complete in $L_2[0, 1]$ with respect to the weight function

$$w(\mu)=\frac{c\mu}{2(1-c)}\frac{1}{(\nu_0+\mu)X(-\mu)} \tag{1}$$

where

$$X(-\mu)=\frac{1}{\alpha+\mu}\Omega(-\mu) \tag{2}$$

$$\Omega(-\mu)=1-\frac{c\nu_0^2}{2}\mu\int_0^1\frac{1-t^2x^2(0)}{(\nu_0^2-t^2)(\mu+t)\Omega(-t)}\,dt \tag{3}$$

and

$$\alpha=X(0)^{-1}=\nu_0(1-c)^{1/2}$$

$$\frac{c\nu_0}{2}\ln\frac{1+\nu_0}{1-\nu_0}=1.$$

We note that the weight function $w(\mu)$ is expressed in terms of the function $\Omega(-\mu)$ which satisfies a non-linear integral equation (3).

For obtaining approximate solutions of the neutron transport equation, it is usual to use the classical orthogonal polynomials of Legendre or Chebyshev, as the fundamental basis functions. It is the purpose of this letter to point out that the use of the

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classical orthogonal polynomials, though convenient, is not the best possible method in transport theory, because the actual set consists of the Case eigenfunction(al)s with respect to the weight function $w(\mu)$. Hence it is more appropriate to seek polynomials that are orthogonal in (0, 1) with respect to the given weight function $w(\mu)$, and to use this new set for transport theory work.

This, of course, would have been a straightforward programme had it not been for the transcendental nature of the weight function as given by equations (1)-(3). We have, however, constructed [1] a very simple and accurate approximation of the weight function given by

$$w^{(0)}(\mu)=\frac{c}{2\Omega^{(0)}(1-c)}\,\frac{\mu(\alpha+\mu)}{\nu_0+\mu} \tag{4}$$

where

$$\Omega^{(0)}=\tfrac{1}{2}(\Omega_++\Omega_-)$$

with

$$\Omega_+=-\frac{c(\alpha D_1+D_2)}{2(1-c)X(\nu_0)} \qquad \Omega_-=\frac{c(\alpha E_1+E_2)}{2(1-c)X(-\nu_0)}$$

and

$$X(-\nu_0)=\left(\frac{|a_{0+}|(1-\alpha^2)}{2\alpha^2(\nu_0^2-1)}\right)^{1/2} \qquad X(\nu_0)=X(-\nu_0)/a_{0+}$$

$$a_{0+}=-\exp(-2z_0/\nu_0)$$

z_0 being the extrapolated end point, and

$$D_1=\frac{1}{2\nu_0(\nu_0-1)}-\frac{1}{2c\nu_0^2} \qquad D_2=\frac{1}{2(\nu_0-1)}+\frac{1}{2c\nu_0}-\ln\frac{\nu_0}{\nu_0-1}$$

$$E_1=\frac{1}{2c\nu_0^2}-\frac{1}{2\nu_0(\nu_0+1)} \qquad E_2=\frac{1}{2\nu_0(\nu_0+1)}-\frac{3}{2c\nu_0}+\ln\frac{\nu_0}{\nu_0+1}.$$

The above approximation is obtained from the orthogonality integrals

$$(\phi_{0+},\phi_{0\pm})_{\omega^{(0)}}=\mp(\tfrac{1}{2}c\nu_0)^2X(\pm\nu_0)$$

(see [1] for details). Thus equations (2) and (3) are approximated as

$$X^{(i)}(-\mu)=\frac{1}{\alpha+\mu}\,\Omega^{(i)}(-\mu)$$

$$\Omega^{(i+1)}(-\mu)=1-\frac{c\nu_0^2}{2}\,\mu\int_0^1\frac{1-t^2X^2(0)}{(\nu_0^2-t^2)(\mu+t)\Omega^{(i)}(-t)}\,\mathrm{d}t \qquad i=0,1,2,\ldots.$$

Specifically, we have

$$\Omega^{(1)}(-\mu)=1-\tfrac{1}{2}c\nu_0^2\mu(S^{(0)}/\Omega^{(0)})$$

where

$$S^{(0)}=\alpha_1\ln\frac{1+\nu_0}{\nu_0}+\alpha_2\ln\frac{v_0-1}{\nu_0}+\alpha_3\ln\frac{1+\mu}{\mu}$$

$$\alpha_1 = c[2\nu_0(\nu_0 - \mu)(1-c)]^{-1} \qquad \alpha_2 = c[2\nu_0(\nu_0 + \mu)(1-c)]^{-1}$$

$$\alpha_3 = X^2(0) - c[(1-c)(\nu_0^2 - \mu^2)]^{-1}.$$

The fractional *per cent* errors of $X^{(0)}(-\mu)$ and $X^{(1)}(-\mu)$ as given by

$$E_X^{(i)}(-\mu) = \frac{X(-\mu) - X^{(i)}(-\mu)}{X(-\mu)} \times 100$$

where $X(-\mu)$ are tabulated in [2], are typically of the order of 10^{-1} and 10^{-2} respectively, for all values of μ and c. A representative display of the approximate values of the various quantities of interest is shown in table 1.

Table 1. Approximate values of various quantities of interest for different μ and c.

c	0.1			0.5			0.99		
μ	0.1	0.5	1.0	0.1	0.5	1.0	0.1	0.5	1.0
Ω_+	0.9899	0.9899	0.9899	0.9597	0.9597	0.9597	0.9336	0.9336	0.9336
Ω_-	0.9912	0.9912	0.9912	0.9594	0.9594	0.9594	0.9334	0.9334	0.9334
$\Omega^{(0)}$	0.9905	0.9905	0.9905	0.9595	0.9595	0.9595	0.9335	0.9335	0.9335
$\Omega^{(1)}(-\mu)$	0.9926	0.9894	0.9906	0.9660	0.9546	0.9610	0.9401	0.9269	0.9394
$X^{(0)}(-\mu)$	0.9446	0.6838	0.5083	1.1444	0.7748	0.5519	1.3734	0.8646	0.5909
$X^{(1)}(-\mu)$	0.9465	0.6830	0.5083	1.1520	0.7708	0.5528	1.3832	0.8585	0.5947
$\lvert E_X^{(0)}(-\mu)\rvert$	0.2104	0.1139	0.0037	0.6954	0.4925	0.1636	0.8024	0.6385	0.6842
$\lvert E_X^{(1)}(-\mu)\rvert$	0.0015	0.0012	0.0004	0.0303	0.0231·	0.0162	0.0938	0.0723	0.0513

The relative accuracy of $w^{(0)}$ as compared to w was checked by evaluating

$$(\phi_{0+}, \phi_\nu)_{w^{(0)}} = \frac{c^2\nu_0}{4\Omega^{(0)}(1-c)(\nu_0^2 - \nu^2)} \times \left[\nu\lambda(\nu)(\alpha+\nu) + \frac{c\nu}{2}\left(\frac{A_1}{2}\ln\frac{\nu_0^2}{\nu_0^2 - 1} + \frac{A_2}{c\nu_0^2} + A_3 \ln\frac{\nu}{1-\nu}\right)\right]$$

where

$$A_1 = -\nu_0[\nu_0 + \nu(1-c)^{1/2}] \qquad A_2 = -\nu_0^2(\nu+\alpha) \qquad A_3 = \nu(\nu+\alpha)$$

and comparing it with the exact result obtained from the orthogonality relation $(\phi_{0+}, \phi_\nu)_w = 0$. Some illustrative results for $\nu = 0.1$, 0.5 and 0.9 are: $c = 0.1$, $(\phi_{0+}, \phi_\nu)_{w^{(0)}} = 6.457(-7)$, $-2.843(-6)$, $-6.361(-6)$; $c = 0.5$, $(\phi_{0+}, \phi_\nu)_{w^{(0)}} = 8.796(-5)$, $-3.758(-4)$, $-8.088(-4)$; $c = 0.99$, $(\phi_{0+}, \phi_\nu)_{w^{(0)}} = 3.384(-3)$, $-1.633(-2)$, $-3.291(-2)$ respectively, where $a(-b) \equiv a \times 10^{-10}$. This, together with the simpler example given in [1], provides the confidence necessary in using the very simple expression for $w^{(0)}(\mu)$, as given by equation (4), in place of the transcendental, non-linear exact $w(\mu)$ of equations (1)-(3).

Having been assured of the utility of $w^{(0)}(\mu)$, we orthogonalise $\{1, \mu, \mu^2, \ldots\}$ in the interval $0 \leq \mu \leq 1$, following the simple prescription of Golub and Welsch [3]. Thus, let us define the moments of $w^{(0)}$ by

$$m_{ij} = \int_0^1 w^{(0)}(\mu)\mu^{i+j-2}\,d\mu \qquad i, j = 1, 2, \ldots, N+1$$

and let

$$r_{ij}=r_{ii}^{-1}\left(m_{ij}-\sum_{k=1}^{i-1} r_{ki}r_{kj}\right) \qquad i<j$$

where

$$r_{ii}=\left(m_{ii}-\sum_{k=1}^{i-1} r_{ki}^2\right)^{1/2}.$$

Now construct

$$\delta_i=\frac{r_{i,i+1}}{r_{ii}}-\frac{r_{i-1,i}}{r_{i-1,i-1}} \qquad \rho_i=\frac{r_{i+1,i+1}}{r_{ii}} \qquad i=1,2,\ldots,N$$

where

$$r_{00}=1 \qquad r_{01}=0.$$

Then with $C_0=1$, $C_{-1}=0$, the set $\{C_i(\mu)\}_{i=0}^{N}$ obtained from the three-term recurrence relation

$$\rho_i C_i(\mu)=(\mu-\delta_i)C_{i-1}(\mu)-\rho_{i-1}C_{i-2} \qquad i=1,2,\ldots,N \tag{5}$$

form a complete orthonormal system in (0, 1) with respect to $w^{(0)}(\mu)$. In the present case, we have

$$m_{ij}=\frac{c}{2\Omega^{(0)}(1-c)}\int_0^1 \frac{\alpha+\mu}{\nu_0+\mu}\,\mu^{i+j-1}\,\mathrm{d}\mu$$

which may be conveniently expressed in terms of

$$I_n=\int_0^1 \frac{\mu^n}{\nu_0+\mu}\,\mathrm{d}\mu=\frac{1}{n}(1-\nu_0 n I_{n-1})$$

where

$$I_0=\ln\frac{\nu_0+1}{\nu_0}$$

as

$$m_{ij}=\frac{c}{2\Omega^{(0)}(1-c)}(\alpha I_{i+j-1}+I_{i-j}).$$

The above m_{ij} can be evaluated recursively; hence r_{ii}, δ_i, ρ_i and finally $C_i(\mu)$ is obtained from equation (5). The set $\{C_i\}$ constitutes the orthonormal set we wished to obtain. The new set of polynomials, which depend on the properties of the medium through c and ν_0, is now being used by us, together with a rational function approximation of Case's singular eigenfunction [4], to obtain a discretised spectral representation of the solution of the one-speed neutron transport equation. This solution, which will be reported in a forthcoming publication, replaces the Case transient integral by an infinite sum, involving only regular functions, having the property that this sum tends to the integral, as an approximation parameter in the former tends to zero.

References

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