A THESIS ON
ERROR ESTIMATES OF CERTAIN QUADRATURE AND CUBATURE FORMULAS

By

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CERTIFICATE

This is to certify that the thesis entitled 'Error Estimates of Certain Quadrature and Cubature Formulas' which is being submitted by Miss Raj Verma for the award of Degree of Doctor of Philosophy (Mathematics) to the Indian Institute of Technology, Delhi, is a record of bonafide research work. She has worked for the last three and half years under my guidance and supervision.

The thesis has reached the standard fulfilling the requirements of the regulations relating to the degree. The results obtained in this thesis have not been submitted to any other University or Institute for the award of any degree or diploma.

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S Y N O P S I S

The usual real variable theory estimate for a rule of numerical integration is given in terms of certain high order derivatives of the integrand. In the case of a quadrature rule the error estimate is usually gives in the form $k_n f^n(\xi)$ where k_n is a positive constant depending upon the rule and $f^n(\xi)$ is the nth order derivative evaluated at an intermediate point ξ while for a cubature formula, the error is usually expressed in the form $k'_n f^n(\xi_1)+k''_n f^n(\xi_2)$ where k'_n, $k''_n > 0$ are constants independent of f, and the derivatives of the function appearing are evaluated at certain intermediate points ξ_1 and $\xi_2 \varepsilon I$. Since these estimates are of the mean value type, the exact location ξ is mostly unknown. Instead, sometimes, the error is bounded by $k_n . \max_{x \varepsilon I} |f^n(x)|$. However in many cases it is far from convenient to obtain f^n or the bounds on it even for quite elementary functions.

A method based on Hilbert space technique was proposed by Davis in 1953 for estimating errors of the rules of numerical approximations for analytic functions. This method is essentially an application of the Riesz representation theorem, and Schwarz inequality $|E(f)| < \|E\| \, \|f\|$ is used to obtain bounds for the error E of rules of numerical approximation. Davis and Rabnowitz and a number of other workers have recently used this approach for estimating errors of numerical integration over the Hilbert space $L^2(E_\rho)$.

In this thesis we have investigated the problem of obtaining error estimates for certain rules of numerical integration, for example the Newton-Cotes rules, the Gaussian quadrature formulas, the Romberg integration scheme and Gaussian-Product formulas. In the thesis we have used two different approaches for obtaining these error estimates. In the first the Fourier method is used to express the errors of numerical integration in terms of certain coefficients in the orthonormal expansion of the integrand, and different methods have been proposed for the computation of these Fourier coefficients. In the second approach to estimate errors of quadratures, Davis' method has been used over the Hilbert space $H^2(E_\rho)$ and from the results obtained here, it appears that the Hilbert space $H^2(E_\rho)$ is more appropriate to work with than $L^2(E_\rho)$ which has been used so far. A number of tables giving the error norm and error estimates over $H^2(E_\rho)$ have been given which are useful for practical applications of Davis' method.

The thesis consists of the following five chapters:

Chapter I

In this chapter, estimates involving only the values of the integrand have been obtained for the Gauss-Legendre and the Gauss-Chebyshev cubature formulas. The method consists of expressing the error of a Gaussian product formula in terms of the corresponding Gauss quadrature formulas and estimating the errors of the later in terms of certain coefficients in the Fourier-Chebyshev expansion of the integrands.

The Fourier-Chebyshev coefficients involved in the estimates can be computed by the scheme proposed by Clenshaw (see also chapter II). Thus these estimates can be computed efficiently in terms of functional values without any further analysis of the integrand. Examples given indicate the effectiveness of the estimates even for moderate values of n. In the second part of the chapter a Gaussian-product formula is obtained for the unit circle which is the same except for a rotation as that given by Pierce. Similar techniques are used to estimate the errors of this Gaussian cubature formula for the unit circle.

Chapter II

For the calculation of the Chebyshev coefficients in the expansion of a function the method was proposed by Clenshaw using discrete point orthogonality relations of the Chebyshev polynomials over the abscissas $x_i = \cos \frac{i\pi}{n}$, $i=0,\ldots, n$. First, in this chapter, we show that these orthogonality relations, result from the usual orthogonality over $[-1,1]$ with the weight $(1-x^2)^{-\frac{1}{2}}$ by replacing the integral by the Gauss-Chebyshev quadrature formula of the closed type with fixed abscissas at $x = \pm 1$. Then we have developed two semi-closed Gauss-Chebyshev quadrature formulas corresponding to the fixed abscissa $x = 1$ or $x = -1$. The error analysis of these quadrature formulas is also included. These two semi-closed Gauss quadrature formulas are, then, used to obtain two new orthogonality relations for the Chebyshev polynomials, which lead to two better schemes for the approximate calculation of the Chebyshev coefficients. These schemes are used for the approximate calculation of integrals when the integrand is expressed by a truncated Chebyshev series. Numerical examples indicate that these two schemes give better results.

Chapter III

For estimating the errors of quadratures for functions analytic over $[-1,1]$, Davis has proposed a Hilbert space method using the Hilbert space $L^2(E_\rho)$. Davis and Rabinowitz have produced the table of the error norms over $L^2(E_\rho)$ for the Trapezoidal, Simpson, Weddle, Gauss 2,3,7,10,13, 16-point rules and for different values of the ellipse parameter $\alpha = (\rho+\rho^{-1})/2$, $\rho > 1$. This table was, later, corrected by Lo, Lee and Sun. In the present chapter we have studied numerically Davis' method over the Hilbert space $H^2(E_\rho)$. Error norms over the Hilbert space $H^2(E_\rho)$ have been calculated for the Trapezoidal, Simpson, Gauss-Legendre 2 to 16-point, Gauss-Chebyshev and Lobatto quadrature formulas and for the values $1.0001 < \alpha < 5.0$. It has been observed that the error norms over $H^2(E_\rho)$ are much smaller than those obtained over $L^2(E_\rho)$. In fact we observe that for ρ close to unity (the range of interest when the singularity of the integrand are close to the interval of integration) the line integral norm is much smaller than the double integral norm. For example, for the Trapezoidal rule and for $\alpha = 1.0001$ the double integral norm is nearly a thousand time greater than the corresponding line integral norm. Another interesting observation is that the line integral norm for a quadrature formula with fixed number of points stays smaller than the corresponding double integral norm as α increases till it assumes some value α_0 and this transitional value α_0 goes up as the number of points employed in the quadrature formula increases. Thus, for example, for Gauss five and higher point formulas the line integral norm is less than the double integral norm for all $\alpha > 1$ through 5. Since in practice, one needs the error estimates $\sigma_L(\rho)$ rather than just the norm of the error, we have also tabulated $\sigma_L(\rho)$ along with $\|E\|_L$, and for the sake of comparison the error estimate $\sigma_D(\rho)$ over the Hilbert space $L^2(E_\rho)$ are also given. Again it is observed that $\sigma_L(\rho)$ is consistently smaller than $\sigma_D(\rho)$ for all $\rho > 1$.

Chapter IV

Since for a fixed selection of abscissas z_k and weights $w_k, k = 0,1,\ldots, n$ in a quadrature formula, the usual $(n+1)$-point rule need not yield a minimum value of the corresponding error norm. In the present chapter we have studied the optimization of certain quadrature formulas over the Hilbert space $H^2(E_\rho)$. For each of these quadrature formulas we have found a new set of weights called the optimal weights corresponding to which the line integral error norm is minimized. For the Trapzoidal rule and for the n-point Gauss-Chebyshev quadrature formula we have obtained closed form expressions for the corresponding optimal weights. However, for Simpson, Gauss-Legendre three to eight point and Lobatto four to eight point we have obtained numerically the corresponding optimal weights by solving the corresponding linear norm minimizing equations by an iterative scheme. The corresponding values of the minimal error norms corresponding to these optimal weights have also been tabulated. It is observed that the weights settle down to the classical values, as the ellipse parameter α increases, much faster than the corresponding optimal weights over $L^2(E_\rho)$. Also the resulting optimal quadratures over $H^2(E_\rho)$ give smaller error estimates than the corresponding error estimates over $L^2(E_\rho)$.

Chapter V

In this chapter we have studied the Romberg integration scheme. The error analysis of this method has been attempted by using Peano's theorem by Meinguet and for the case of analytic functions by Davis' method by Meinguet and Stroud using the Hilbert space $L^2(E_\rho)$. Here we have extended the procedure of estimating error by Davis' method of chapter III for the Romberg procedure. We have obtained the error norms and error estimates for the Romberg formula using $N = 2^n+1$ points which have a precision of $2n+1$ over the Hilbert space $H^2(E_\rho)$ and for values of α from 1.4 to 3.0. We observe that the line integral error norms are superior to those obtained over $L^2(E_\rho)$ by Stroud.

C O N T E N T S