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The Method of Splitting for Multidimensional Integration with Singularities

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Introduction

Numerical integration of functions with one or more singularities always poses some problems. For simple, one-dimensional integration, however, the method of transformation of variables has been shown to be satisfactory for most cases. In multidimensional integration, the same technique does not help much unless the domain of integration is a sphere (or infinite as a special case) and the singular point is situated at its center. When the boundary is rectangular, for example, no simple transformation can be found that eliminate the singularity or map it to infinity and still retain a simple form of the boundary.

One conventional approach that can be imagined is to divide the domain to a sphere and the remaining part (i.e. a rectangular body with a spherical hole). Then the integral for the spherical part can be easily evaluated using polar coordinate, but the integration over the remaining domain will be intractable owing to its awkward shape.

Lyness[1] has proposed a method to be used for such problems.

It is essentially the method of extrapolation like the well-known Romberg method. From the knowledge of the type of the singularity one can find out the general form of the asymptotic expansion of the quadrature error as function of mesh size. Then one can determine the unknown coefficients of the expansion, together with the true value of the integral, by solving a system of simultaneous equations obtained from the results of numerical quadrature for several different mesh sizes. His method has been shown to give satisfactory results for a number of test problems. However, one drawback of the method is the loss of significant figures due to the ill condition of the equation, as is often encountered in curve fitting using a family of more or less monotone basis functions.

The method I am going to present is much more straightforward and elementary. It somewhat resembles the method of the division of the domain. But, instead of dividing the domain into disjoint parts separated by a sharp boundary, we try to split the integrand into two parts, so that one part is a function regular over the entire domain and the other part is virtually zero outside a spherical region lying in the domain. In some sense, this may be regarded as an effective division of the domain, but the boundary is "blurred" by use of continuous weighting functions.

With this "splitting", the first part is easily evaluated using any known method of dealing with multiple integrals. Since the domain of integration for the second part is actually a sphere,it can be integrated using polar coordinate.

Weighting Functions

To make the argument more specific,we assume with Lyness that the integrand has a form

$$f(\mathbf{r}) = r^{\alpha} g(\mathbf{r}) \tag{1}$$

where $g(\mathbf{r})$ is a polynomial or otherwise a regular function of the cartesian coordinates $x_1, x_2, \ldots, x_n$, which means that it has a convergent power series expansion around the origin. The above-mentioned splitting can then be realised by splitting the "singular part" r^{α} as

$$r^{\alpha} = \phi_1(r) + \phi_2(r) \tag{2}$$

so that

1) $\phi_1(r)$ is a regular, even function of r, and

2) $\phi_2(r)$ tends to zero rapidly as r tends to infinity, so $\phi_2(r)$ is negligible for $r > r_0$.

Then we have the integral as a sum of two integrals I_1 and I_2, each defined by

$$I_1 = \int \phi_1(r) g(\mathbf{r}) d\mathbf{r} \tag{3.1}$$

$$I_2 = \int \phi_2(r) g(\mathbf{r}) d\mathbf{r} \tag{3.2}$$

respectively.

The first integral I_1 can be evaluated in ordinary way, i.e. using the product form Newton-Cotes formula of any order on a regular mesh points. It should however be born in mind that, although $\phi_1(r)$ is a regular function, it can have a rather sharp peak around the origin, so that, even when $g(\mathbf{r})$ is a fairly smooth function, the resulting integrand may require a considerable number of mesh points in order to secure a reasonable precision.

To evaluate the second integral I_2 we use the polar coordinate $(r, \theta_1, \theta_2, \ldots, \theta_{n-1})$, and write

$$(4) \qquad I_2 = \int \phi_2(r)\, g_0(r)\, r^{n-1}\, dr$$

with

$$(5) \qquad \int g(\theta_1, \ldots, \theta_{n-1})\, \omega(\theta_1, \ldots, \theta_{n-1})\, d\theta_1 \cdots d\theta_{n-1} = g_0(r)$$

where $\omega(\theta_1, \ldots, \theta_{n-1})$ is the metric factor such that $r^{n-1} \cdot \omega(\theta_1, \ldots, \theta_{n-1})\, d\theta_1 \ldots d\theta_{n-1}$ is the volume element of the hyperspherical shell having a radius r.

The integral (5) in angle variables may be evaluated using conventional method. The integrand in (4), on the other hand, has a singularity at $r = 0$, but it is most conveniently integrated using a variable transformation $r = e^{\rho}$, so that

$$(6) \qquad \int_0^{\infty} \phi_2(r)\, g_0(r)\, r^{n-1}\, dr = \int_{-\infty}^{\infty} \phi_2(e^{\rho})\, g_0(e^{\rho})\, e^{n\rho}\, d\rho$$

In integrating (6), one should use the trapezoidal formula[2] (not the Newton-Cotes or other more sophisticated formula).

The Incomplete Gamma Function as the Splitting Function

To find a good splitting function having the properties (1) and (2), we observe that

$$\int_0^{\infty} u^{k-1} e^{-ur^2}\, du = \Gamma(k)\, r^{-2k}$$

This leads us at once to the following splitting functions:

$$(7.1) \qquad \phi_1(r) = \frac{1}{\Gamma(k)} \int_0^c u^{k-1} e^{-ur^2} du$$

$$(7.2) \qquad \phi_2(r) = \frac{1}{\Gamma(k)} \int_c^\infty u^{k-1} e^{-ur^2} du$$

Evidently,

$$(8) \qquad \phi_1(r) + \phi_2(r) = r^{-2k}$$

so that, if $\alpha<0$, we may put $k=-\alpha/2$. If $\alpha>0$ we can always find a positive integer m so that

$$(9) \qquad \alpha = 2m - 2k, \quad 0 < k < 2$$

and we may put

$$(10) \qquad f(\mathbf{r}) = r^\alpha g(\mathbf{r}) = r^{-2k} \cdot r^{2m} g(\mathbf{r}) = r^{-2k} \bar{g}(\mathbf{r})$$

It is indeed possible to take as m any integer larger than the one given by (9), but use of unnecessarily large m, and hence of large k, is undesirable. **A** large value of k results in a sharper peak of $\phi_1(r)$ and hence leads to the necessity of a finer mesh in evaluating I_1 to secure a prescribed precision.

It is easy to see that these functions satisfy the requirements (1) and (2) above. The condition for $\phi_1(r)$ is satisfied since it results from a convergent superposition of regular functions e^{-ur^2} with a bounded parameter u. The condition for $\phi_2(r)$ follows from the following estimation. Take r_1 so that $0<r_1<r_0$. Then

$$\phi_2(r) = \frac{1}{\Gamma(k)} \int_c^\infty u^{k-1} e^{-u(r^2-r_1^2)} \cdot e^{-ur_1^2} du$$

$$< \frac{1}{\Gamma(k)} e^{-c(r^2-r_1^2)} \int_c^\infty u^{k-1} e^{-ur_1^2} du = O(e^{-cr^2})$$

The functions $\phi_1(r)$ and $\phi_2(r)$ can be written as

$$(11.1)\qquad \phi_1(r) = \gamma(k, cr^2)/\Gamma(k)$$

$$(11.2)\qquad \phi_2(r) = \Gamma(k, cr^2)/\Gamma(k)$$

where $\gamma(k, x)$ and $\Gamma(k, x)$ are the incomplete gamma functions defined by

$$\gamma(k, x) = \int_0^x t^{k-1} e^{-t} dt$$

$$\Gamma(k, x) = \int_x^\infty t^{k-1} e^{-t} dt$$

There are tables of these functions, but they are also easily calculated using power series or continued fractions.

For smaller x, the most convenient way is to use the power series

$$x^{-k}\gamma(k, x) = e^{-x}\left(\frac{1}{k} + \frac{x}{k(k+1)} + \frac{x^2}{k(k+1)(k+2)} + \cdots\right)$$

$$= e^{-x}\sum_{n=0}^{\infty}\frac{\Gamma(k)}{\Gamma(k+n+1)} x^n$$

For larger x ($x > 3$, say) the following continued fraction for $\Gamma(k, x)$ is recommended:

$$x^{-k}\Gamma(k, x)$$

$$= e^{-x}\left(\frac{1}{x+}\,\frac{1-k}{1+}\,\frac{1}{x+}\,\frac{2-k}{1+}\,\frac{2}{x+}\cdots\frac{n-k}{1+}\,\frac{n}{x+}\cdots\right)$$

Practical Considerations

In applying the method, the first thing to do is to choose the parameters. It is apparent that r_0, the radius of the sphere, should be made largest possible subject to the condition that the sphere lie wholly inside the integration domain. Then the cutoff point c is determined in accordance with the precision required. It should be taken just large enough to keep the error due to the neglect of the integral outside the sphere below the tolerance. Making c larger would result in a sharper central peak of $\phi_1(r)$ and a finer mesh as a consequence, increasing the computing cost.

Numerical Examples

The accompanying figures show the results of the method applied to a few examples which are similar to those used by Lyness. They are:

$f(\mathbf{r}) = r^{\alpha} \cdot \exp(-2x^2-y^2)$, $\alpha=-3/2,-1/2,1/2$;

$f(\mathbf{r}) = r^{\alpha} \cdot x$ $\qquad \alpha=-1/2,\ 1.$

The figures show the dependence of the error on the number of mesh points used. The errors for I_1 and I_2 are also shown. Lyness' method was also tested and its results are shown for comparison.

So far as one can see from these figures, our method does not compare favorably to Lyness' method. However, it must be stressed that our method gives results which are correct almost to the working accuracy, as contrasted to Lyness' method.

It will be seen from the figures that most of the computing cost concerns the first pare I_1. It should also be noticed that contribution of the second part I_2 to the result strongly depends on the exponent in the singularity. When $\alpha=-3/2$, I_2 is comparable in magnitude to I_1, but it is two orders of magnitude below I_1 when $\alpha=1/2$.

To summarise, it will be said that the method of splitting offers an alternative way to evalute the special type of multiple integrals as dealt with by Lyness, which is at least as efficient as his method as to the amount of computation.

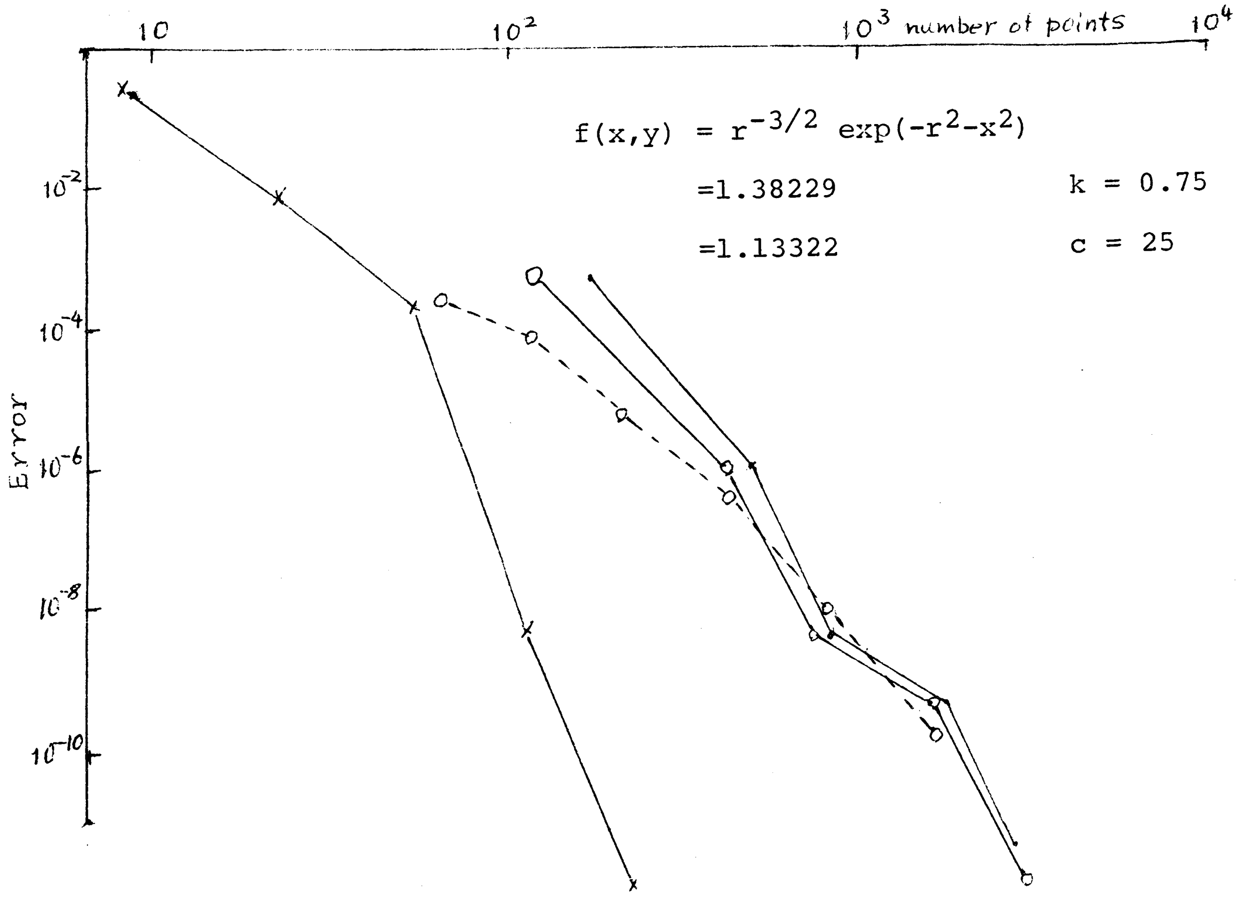
Finally, the author would like to thank Mr. Akio Saito for numerical works, which was done as a part of his work for preparing the Master's Thesis.

References

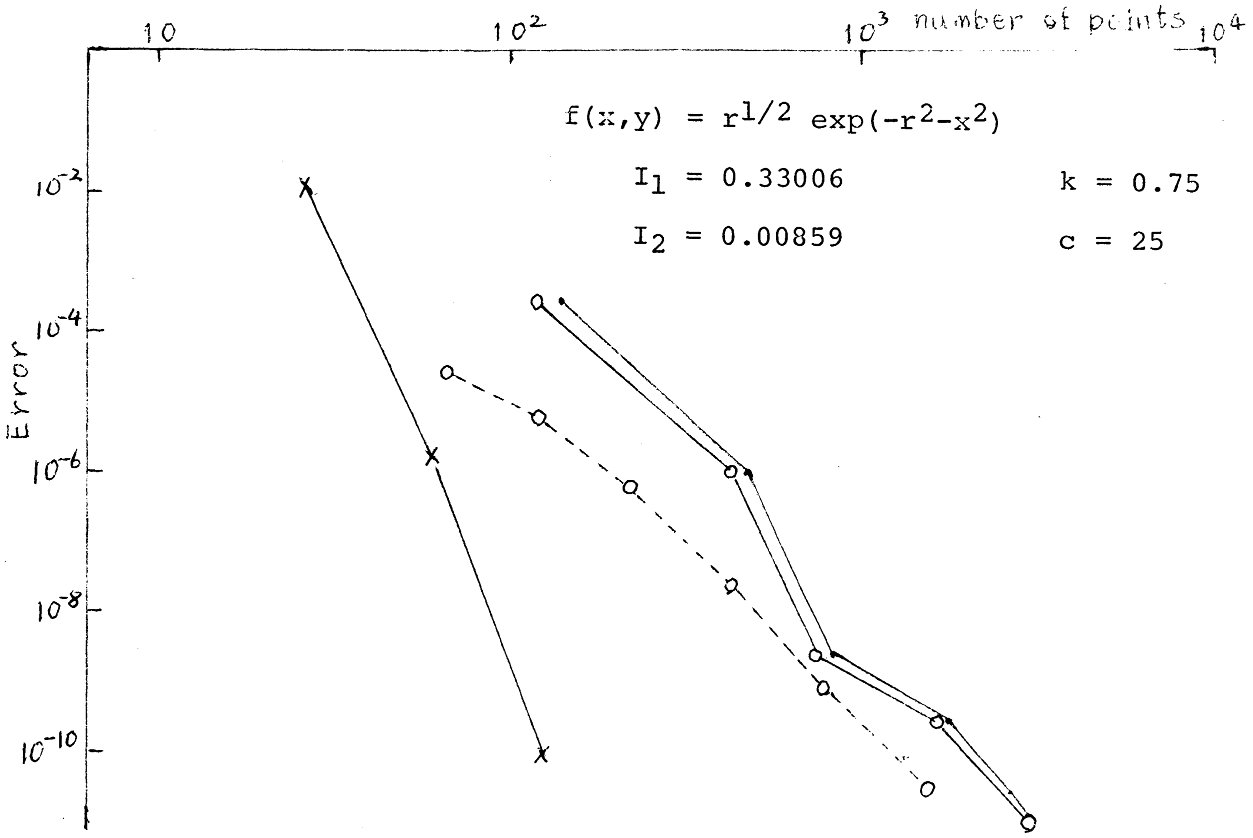
1) J. N. Lyness, "Applications of extrapolation techniques to multidimensional quadrature of some integrand functions with a singularity," J. Comp. Physics, 20 (1976), 346-364.

2) H.Takahasi and M. Mori, "Quadrature formulas obtained by variable transformation," Num. Math. 21 (1973), 206-219.

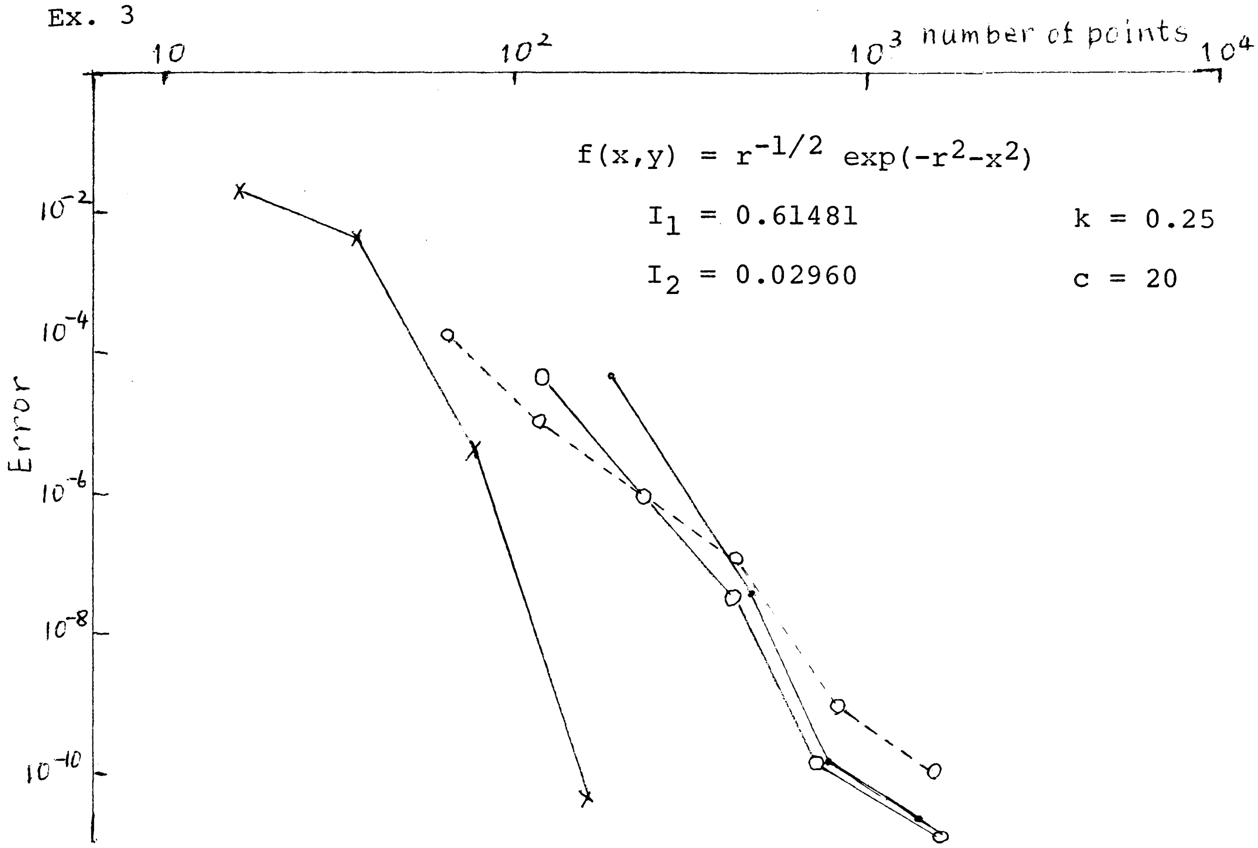
Ex. 1

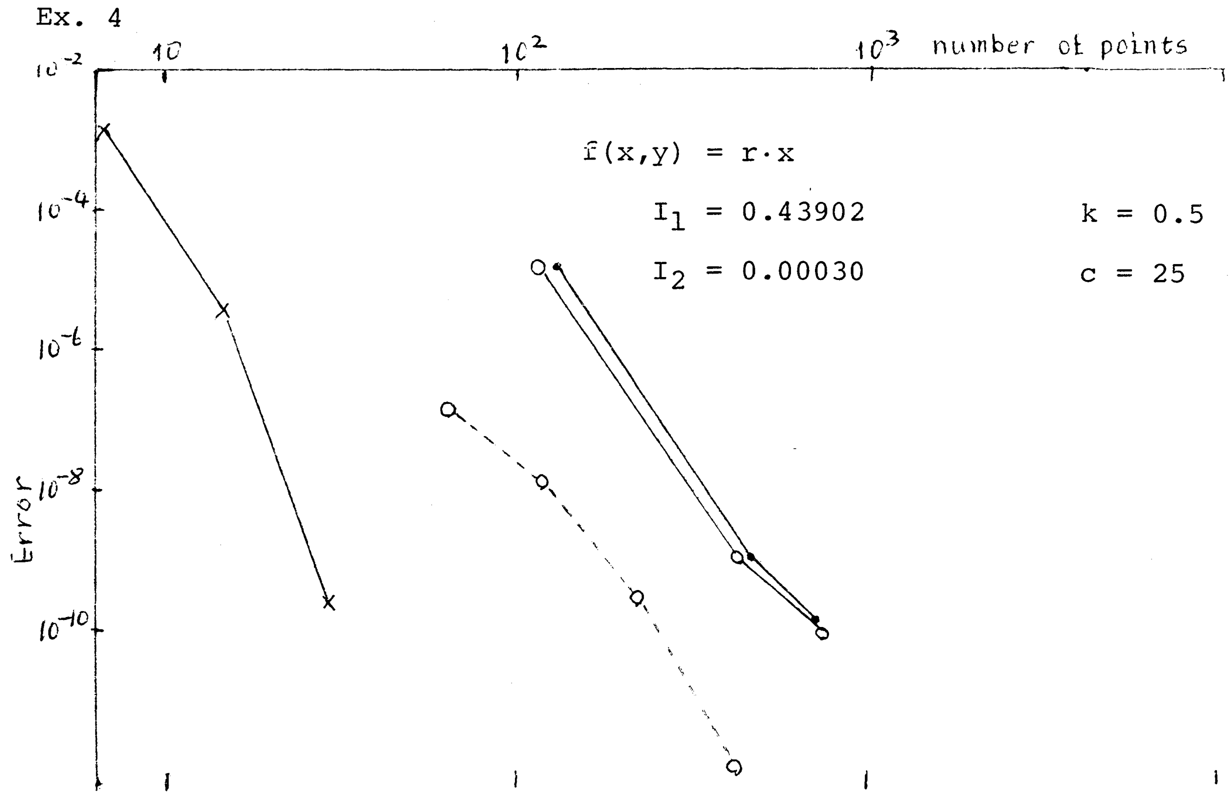

10
10^2
10^3 number of points
10^4
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
Error
$f(x,y) = r^{-3/2} \exp(-r^2-x^2)$
=1.38229
=1.13322
k = 0.75
c = 25

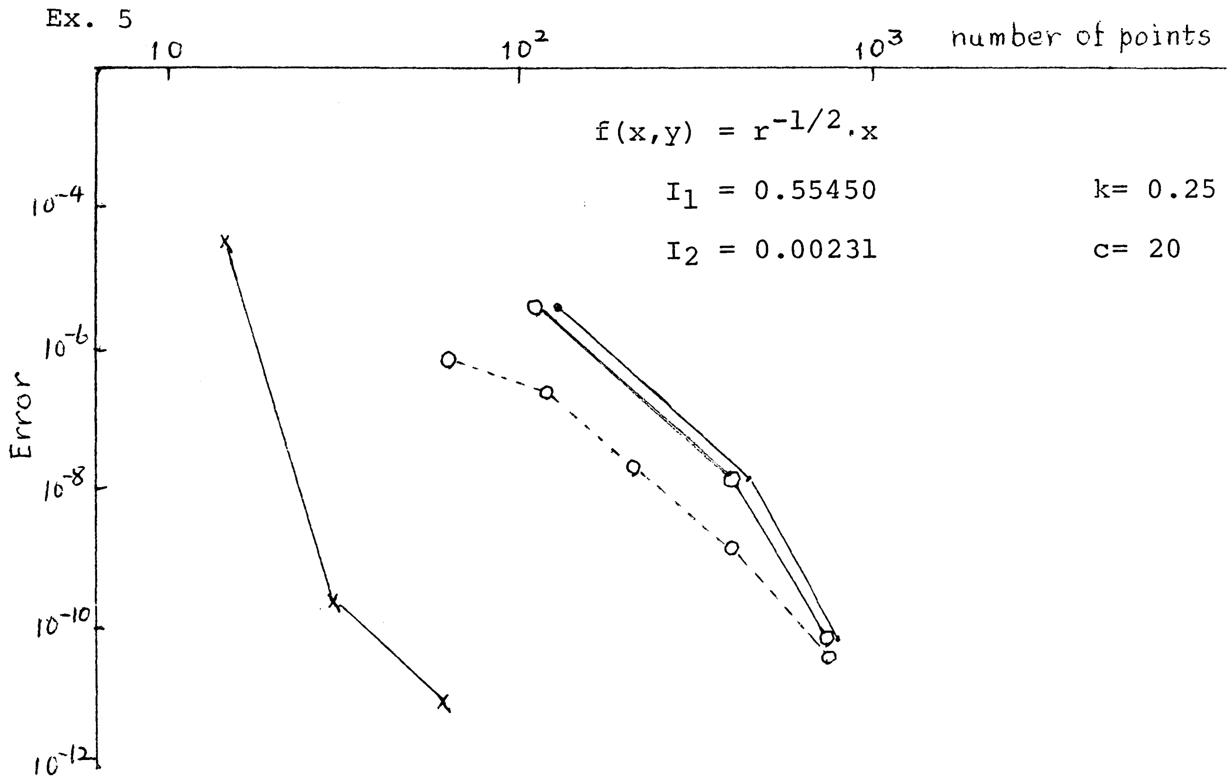
Ex. 2


10
10^2
10^3 number of points
10^4
$f(x,y) = r^{1/2} \exp(-r^2-x^2)$
$I_1 = 0.33006$
$I_2 = 0.00859$
$k = 0.75$
$c = 25$
Error
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}

Ex. 3


10
10^2
10^3 number of points
10^4
$f(x,y) = r^{-1/2} \exp(-r^2-x^2)$
$I_1 = 0.61481$
$I_2 = 0.02960$
$k = 0.25$
$c = 20$
Error
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}


Ex. 4
10
10²
10³
number of points
10⁻²
10⁻⁴
10⁻⁶
10⁻⁸
10⁻¹⁰
Error
f(x,y) = r·x
I1 = 0.43902
I2 = 0.00030
k = 0.5
c = 25


Ex. 5
10
10²
10³
number of points
10⁻⁴
10⁻⁶
10⁻⁸
10⁻¹⁰
10⁻¹²
Error
f(x,y) = r^-1/2·x
I1 = 0.55450
I2 = 0.00231
k= 0.25
c= 20