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Error Bounds for Multidimensional Laplace Approximation*

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A numerical estimate is obtained for the error associated with the Laplace approximation of the double integral $I(\lambda) = \iint_D g(x,y) e^{-\lambda f(x,y)} dx dy$, where D is a domain in \mathbb{R}^2 , λ is a large positive parameter, f(x, y) and g(x, y) are real-valued and sufficiently smooth, and f(x, y) has an absolute minimum in D. The use of the estimate is illustrated by applying it to two realistic examples. The method used here applies also to higher dimensional integrals.

1. INTRODUCTION

Let D be a domain in \mathbb{R}^2 , not necessarily bounded, and let f(x, y) and g(x, y) be real-valued functions defined in D. In this paper we are concerned with double integrals of the form

$$I(\lambda) = \iint_D g(x, y) e^{-\lambda f(x, y)} dx dy, \qquad (1.1)$$

where λ is a large positive parameter. Assume that (i) the integral $I(\lambda)$ is absolutely convergent for all large values of λ , (ii) f(x, y) has continuous second-order partial derivatives in D, (iii) f(x, y) has an absolute minimum value at and only at an interior point (x_0, y_0) of D so that $f_x(x_0, y_0) = f_y(x_0, y_0) = 0$ and

$$\mathbf{H} \equiv f_{xx}(x_0, y_0) f_{yy}(x_0, y_0) - f_{xy}^2(x_0, y_0) > 0, \qquad (1.2)$$

and (iv) g(x, y) is continuous at (x_0, y_0) and $g(x_0, y_0) \neq 0$. Under these assumptions, it is well-known that as $\lambda \to \infty$,

$$I(\lambda) \sim e^{-\lambda f(x_0, y_0)} g(x_0, y_0) (2\pi/\lambda \mathbf{H}^{1/2}), \qquad (1.3)$$

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Copyright © 1983 by Academic Press, Inc. All rights of reproduction in any form reserved. where **H** is the *Hessian* of f at (x_0, y_0) as given in (1.2). Equation (1.3) was first derived by Hsu [7] in 1948 as a two-dimensional generalization of the Laplace approximation

$$\int_{a}^{b} g(x) e^{-\lambda f(x)} dx \sim e^{-\lambda f(\xi)} g(\xi) \left(\frac{2\pi}{\lambda f''(\xi)}\right)^{1/2}, \qquad (1.4)$$

where $a < \xi < b$, $f'(\xi) = 0$, $f''(\xi) > 0$, and $g(\xi) \neq 0$. Asymptotic formulas such as (1.3) and (1.4) for higher dimensional integrals are also available in the literature; see, e.g., [2, 5, 6]. In fact, infinite asymptotic expansions of these integrals can be found in [2].

In 1968, Olver [12] gave for the first time explicit error bounds for the asymptotic expansion of the integral in (1.4), and thus, in particular, supplied explicit bounds for the error in approximation (1.4). Our objective here is to obtain similar results for approximation (1.3). Although our method is susceptible of generalization to integrals of higher dimensions, for simplicity of exposition we shall work only with the double integral $I(\lambda)$ in (1.1). Also, although our analysis can be extended to give bounds for the error terms associated with the asymptotic expansion of the integral $I(\lambda)$, in view of the overwhelming complexity that will occur, we shall be only concerned with the construction of the error bounds for approximation (1.3).

The idea of Olver is to first subdivide the range of integration in (1.4) so that f'(x) does not change sign in each of the subintervals, next make a change of variable $f(x) = \pm u$ so that each of the integrals becomes a Laplace-type integral, and finally apply the Lagrange inversion formula to obtain x in terms of u. An analogue of this approach is to search for a transformation $T: (x, y) \rightarrow (u, v)$ so that f(x, y) = u + v and then look for regions in which the Jacobian of T, denoted by J(T), does not vanish. Such a transformation T can easily be obtained, but the exact regions in which $J(T) \neq 0$ are difficult to determine. For this reason, we shall abandon this approach and proceed in an entirely different manner. Our analysis is based on a formal (but ingenious) argument of Jones and Kline [9], which has recently been made rigorous in [14]. As illustrations, we shall apply our results to two double integrals whose asymptotic behavior have already been studied in the literature.

2. Assumptions and Preliminaries

Throughout our discussion we shall assume that D is a domain containing the origin. By simple change of variables we may assume without loss of generality that the absolute minimum of f is zero and occurs at the origin, i.e., f(0,0) = 0 and f(x, y) > 0 for all $(x, y) \neq (0, 0)$. Functions satisfying these conditions are said to be *positive definite* in D; see [11]. Conditions $(A_1)-(A_3)$ are also assumed to hold.

(A₁) The function f(x, y) has continuous fourth-order partial derivatives in D, $(\nabla f)(0, 0) = (0, 0)$, and $(\nabla f)(x, y) \neq (0, 0)$ for $(x, y) \neq (0, 0)$, where $\nabla f = (f_x, f_y)$. Furthermore, the Taylor expansion for f(x, y) at (0, 0) takes the form

$$f(x, y) = x^{2} + y^{2} + \sum_{i+j=3}^{2} f_{ij} x^{i} y^{j} + \cdots .$$
 (2.1)

 (A_2) There exists a positive number δ such that

$$xf_x + yf_y \ge 2\delta(x^2 + y^2) \tag{2.2}$$

for all $(x, y) \in D$.

 (A_3) The function g(x, y) has continuous second-order partial derivatives in D, and

$$N_{ij} \equiv \sup_{D} |g_{i,j}(x, y)| < \infty$$
(2.3)

for i + j = 0, 1, 2, where $g_{i,i}(x, y)$ denotes the partial derivative $\partial^{i+j}g/\partial x^i \partial y^j$.

Remark (i). The first part of condition (A_1) is a precise statement that f(x, y) has one and only one minimum value in D, which occurs at the origin. This minimum value was assumed to be zero at the beginning of this section. If $f(0, 0) \neq 0$, then it simply contributes a factor of $e^{-\lambda f(0,0)}$ outside the integral $I(\lambda)$. The cross product term xy in the Taylor expansion of f(x, y) can always be eliminated by using a linear transformation. This procedure is adopted in all derivations of formula (1.3); see [3, pp. 393–394; 2, p. 326]. Also, by rescaling, the coefficients of x^2 and y^2 can always be assume to be 1. Thus the second part of condition (A_1) is not really a restriction.

Remark (ii). The left-hand side of inequality (2.2) is almost the directional derivative of f(x, y) along the direction of the line segment joining (0, 0) to (x, y). Thus, (2.2) compares it with the directional derivative of the function $x^2 + y^2$. In a sense, (2.2) represents a two-dimensional analogue of the condition $f'(x) \ge \delta > 0$ in the one-dimensional case (cf. [12, Eq. (2.2)]).

Now let ∂D denote the boundary of D, and put

$$c = \inf\{f(x, y): (x, y) \in \partial D\}$$
(2.4)

and

$$\Gamma_c = \{ (x, y) \in D : f(x, y) = c \}.$$
(2.5)

Note that c might be infinite, in which case we take $\Gamma_c = \partial D$. If D_c denotes the region bounded by Γ_c , then clearly

$$I(\lambda) = \iint_{D_c} + \iint_{D \setminus D_c} \equiv I_1(\lambda) + I_2(\lambda).$$
(2.6)

An explicit bound for $I_2(\lambda)$ can easily be obtained as follows: Let λ_0 be the constant such that $I(\lambda)$ converges absolutely for all $\lambda \ge \lambda_0$; cf. condition (i) in Section 1. Put

$$K = \iint_{D} |g(x, y)| e^{-\lambda_0 f(x, y)} dx dy.$$
 (2.7)

From (A_1) and (A_2) , we have

$$|I_2(\lambda)| \leqslant K e^{-(\lambda - \lambda_0)c} \qquad (\lambda \geqslant \lambda_0).$$
(2.8)

Note that this estimate is exponentially small in comparison with the Laplace approximation given in (1.3), and hence its contribution is usually negligible. Our problem is thus reduced to that of finding an error bound for the Laplace approximation of $I_1(\lambda)$.

To conclude this section, we also introduce the following notations. Let t_0 be a fixed positive number such that the closed disk

$$\Delta(t_0) = \{(x, y): x^2 + y^2 \leq t_0\}$$
(2.9)

is contained in D_c and write

$$f(x, y) = x^{2} + y^{2} + f_{1}(x, y).$$
(2.10)

By using the Taylor theorem with remainder, it can easily be seen that there are constants $M_{ij}^{(1)}$, i + j = 0, 1, 2, such that

$$\left| \frac{\partial^{i+j}}{\partial x^i \, \partial y^j} f_1(x, y) \right| \leq M_{ij}^{(1)} (x^2 + y^2)^{(3-i-j)/2}$$
(2.11)

for all $(x, y) \in \Delta(t_0)$. Although these constants can be expressed explicitly in terms of the third-order partial derivatives of f(x, y), it is more advantageous to derive the above inequalities directly, the reason being that it is often possible to obtain smaller values for the constants $M_{ij}^{(1)}$ in this manner; see Examples 2 and 3 below. Similarly, if

$$f_1(x, y) = \sum_{i+j=3}^{\infty} f_{ij} x^i y^j + f_2(x, y), \qquad (2.12)$$

then there are constants $M_{ii}^{(2)}$, i + j = 1, such that

$$\left|\frac{\partial^{i+j}}{\partial x^i \partial y^j} f_2(x, y)\right| \leqslant M_{ij}^{(2)} (x^2 + y^2)^{(4-i-j)/2}$$
(2.13)

for all $(x, y) \in \Delta(t_0)$.

The constants $M_{ij}^{(1)}$ and $M_{ij}^{(2)}$ play an important role in the construction of the final error bound. They in general depend on the number t_0 and may tend to infinity as t_0 increases so that the closed disk $\Delta(t_0)$ approaches ∂D . For convenience of presentation, we shall supress the dependence of these constants on t_0 .

3. REDUCTION TO A SINGLE INTEGRAL

The double integral $I_1(\lambda)$ in (2.6) can be calculated as follows: In view of conditions (A₁) and (A₂), the region D_c can be covered by the family of simple closed C^1 curves

$$\Gamma_t = \{(x, y): f(x, y) = t\}, \qquad 0 < t < c.$$
(3.1)

Each Γ_t separates \mathbb{R}^2 into two components, one of which, denoted by D_t , contains (0, 0). Furthermore, if $0 < t_1 < t_2 < c$, then $\Gamma_{t_1} \subset D_{t_2}$, and if $(x, y) \in D_t$, then f(x, y) < t. These are the so-called *nesting properties* for positive definite functions. They are in fact valid without condition (A₂); for a proof of this stronger result, see [1] and [10]. By subdividing the region D_c into infinitesimal curvilinear rectangles determined by the curves Γ_t and their orthogonal trajectories, we can reduce the double integral $I_1(\lambda)$ to the single integral

$$I_1(\lambda) = \int_0^c h(t) e^{-\lambda t} dt, \qquad (3.2)$$

where

$$h(t) = \int_{\Gamma_t} \frac{g(x, y)}{|\nabla f|} \, d\sigma, \qquad (3.3)$$

 σ being the arc length of the curve Γ_t . A detailed discussion of this method of resolving double integrals is given in [4, pp. 445–455].

To obtain a more workable expression for the function h(t) in (3.3), we make the change of variables

$$x = \xi^{1/2} \cos \eta, \qquad y = \xi^{1/2} \sin \eta.$$
 (3.4)

Clearly

$$\boldsymbol{\xi} = \boldsymbol{x}^2 + \boldsymbol{y}^2 \tag{3.5}$$

and

$$\partial(x, y)/\partial(\xi, \eta) = \frac{1}{2}.$$
 (3.6)

Equation (2.1) suggests that we write

$$f(x, y) = \xi + F(\xi, \eta).$$
 (3.7)

Put

$$\Phi(\xi,\eta) = \frac{1}{2}g(x,y).$$
(3.8)

The integral h(t) now becomes

$$h(t) = \int_{\xi+F=t} \frac{\Phi(\xi,\eta)}{|\nabla(\xi+F)|} \, d\sigma', \qquad (3.9)$$

where σ' denotes the length of the curve $t = \xi + F(\xi, \eta)$ and the gradient ∇ is taken with respect to ξ and η . For a proof of the last identity, we refer to [14, Sects. 2 and 3].

From (3.7) we have, by condition (A_2) ,

$$1 + F_{\xi}(\xi, \eta) \ge \delta > 0. \tag{3.10}$$

Thus, for each fixed $\eta \in [0, 2\pi]$, there exists a unique solution $\xi_t = \xi_t(\eta)$ to the equation

$$t = \xi + F(\xi, \eta), \tag{3.11}$$

and furthermore we have explicitly

$$d\sigma' = \sqrt{1 + (\partial \xi/\partial \eta)^2} \, d\eta = \frac{|\nabla(\xi + F)|}{1 + F_{\ell}(\xi_{\ell}, \eta)} \, d\eta. \tag{3.12}$$

Inserting (3.12) in (3.9) gives

$$h(t) = \int_0^{2\pi} \frac{\Phi(\xi_t, \eta)}{1 + F_{\xi}(\xi_t, \eta)} \, d\eta.$$
(3.13)

Here we have used the fact that for each $t \in (0, c)$, the solution $\xi_t(\eta)$ to Eq. (3.11) is a simple closed C^1 curve, which stays entirely within D_c for all η in $[0, 2\pi]$; see the nesting property stated above.

EXAMPLE 1. As a simple application of the above result, we consider the double integral

$$S_n = \iint_{D'} \left[\cos u \cos v \cos(u+v) \right]^n du \, dv, \qquad (3.14)$$

where D' is the hexagonal region given by

$$D' = \{(u, v): |u| < \pi/2, |v| < \pi/2, |u + v| < \pi/2\}.$$
 (3.15)

This integral arose in the asymptotic evaluation of the sum

$$S(3,n) = \sum_{k=0}^{n} {\binom{n}{k}}^{3}; \qquad (3.16)$$

see [6, p. 413]. The integrand can be written in the form $\exp\{-nh(u, v)\}$ with

$$h(u, u) = -\log \cos u - \log \cos v - \log \cos(u + v)$$

= $u^2 + uv + v^2 + \cdots$ (3.17)

In order to eliminate the cross product uv (see Remark (i) in Section 2), we make the change of variables

$$u = x - (1/\sqrt{3}) y, \quad v = (2/\sqrt{3}) y.$$
 (3.18)

The region D' is then transformed into

$$D = \{(x, y): |x \pm (1/\sqrt{3}) y| < \pi/2, |(2/\sqrt{3}) y| < \pi/2\},$$
(3.19)

and the integral becomes

$$S_n = \frac{2}{\sqrt{3}} \iint_D e^{-nf(x,y)} \, dx \, dy, \qquad (3.20)$$

where

$$f(x, y) = -\log \cos \left(x - \frac{1}{\sqrt{3}}y\right) - \log \cos \left(\frac{2}{\sqrt{3}}y\right) - \log \cos \left(x + \frac{1}{\sqrt{3}}y\right).$$
(3.21)

The result developed in this section is now immediately applicable. In the present case, the constant c in (2.4) is $+\infty$, and hence I_2 in (2.6) is absent. From (3.2) and (3.13), it follows that

$$S_n = \frac{2}{\sqrt{3}} \int_0^\infty h(t) \, e^{-nt} \, dt, \qquad (3.22)$$

where

$$h(t) = \frac{1}{2} \int_0^{2\pi} \frac{1}{1 + F_{\ell}(\xi_t, \eta)} \, d\eta.$$
 (3.23)

Let us rewrite h(t) in the form

$$h(t) = \pi - h_1(t) \tag{3.24}$$

with

$$h_1(t) = \frac{1}{2} \int_0^{2\pi} \frac{F_{\ell}(\xi_t, \eta)}{1 + F_{\ell}(\xi_t, \eta)} \, d\eta.$$
(3.25)

By using the inequality $\theta \tan \theta \ge \theta^2$ for all $\theta \in (-\pi/2, \pi/2)$ and the identity

$$(x - (1/\sqrt{3})y)^2 + ((2/\sqrt{3})y)^2 + (x + (1/\sqrt{3})y) = 2(x^2 + y^2), (3.26)$$

the constant δ in (2.2) can easily be shown to be 1. Thus we have

$$1 + F_{\ell}(\xi_t, \eta) \ge 1. \tag{3.27}$$

Furthermore, since each term on the right-hand side of Eq. (3.21) is positive for all (x, y) lying inside the hexagon given in (3.19), from the equation $t = \xi + F(\xi, \eta) = f(x, y)$ it follows that the reciprocals of the quantities $\cos(x - (1/\sqrt{3})y)$, $\cos(2/\sqrt{3})y)$, and $\cos(x + (1/\sqrt{3})y)$ are all bounded by e^t . Therefore

$$x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} \leq 2(x^2 + y^2)e^t, \qquad (3.28)$$

and

$$1 + F_{\ell}(\xi_{\ell}, \eta) \leqslant e^{\ell}. \tag{3.29}$$

Since $F_{\xi} \ge 0$ by (3.27), we also have

$$0 \leqslant F_{\ell}(\xi_t, \eta) \leqslant e^t - 1 \leqslant te^t.$$
(3.30)

Applying this and (3.27) to (3.25) gives

$$|h_1(t)| \le \pi t e^t. \tag{3.31}$$

From (3.22) and (3.24), we obtain

$$S_n = (2/3)[(\pi/n) + \delta_1(n)], \qquad (3.32)$$

where

$$|\delta_1(n)| \le \pi/(n-1)^2.$$
 (3.33)

The success of this result depends heavily on the inequalities in (3.30). In general, these types of inequalities are just not available. In the following section, we shall derive a result which is subject only to the conditions imposed in Section 2.

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4. Error Bounds

Let t_0 be chosen as in (2.9), and put $\varepsilon = \min(1, \delta)$ and $g_{00} = g(0, 0)$. In this section we shall construct an explicit constant C, which depends on t_0 but is independent of t, such that

$$|h(t) - \pi g_{00}| \leqslant Ct, \qquad t \in (0, \varepsilon t_0). \tag{4.1}$$

From this an error bound can easily be derived for the Laplace approximation of $I_1(\lambda)$.

To prove (4.1), let us first make the following observations: From (2.10) and (3.7), it follows that

$$F(\xi, \eta) = f_1(x, y),$$
 (4.2)

$$F_{\xi}(\xi,\eta) = \frac{1}{2\xi} \left(x \frac{\partial f_1}{\partial x} + y \frac{\partial f_1}{\partial y} \right), \tag{4.3}$$

$$F_{\xi\xi}(\xi,\eta) = \frac{1}{4\xi^2} \left(x^2 \frac{\partial^2 f_1}{\partial x^2} + 2xy \frac{\partial^2 f_1}{\partial x \partial y} + y^2 \frac{\partial^2 f_1}{\partial y^2} - x \frac{\partial f_1}{\partial x} - y \frac{\partial f_1}{\partial y} \right).$$
(4.4)

Hence, by (2.11), we have

$$|F(\xi,\eta)| \leqslant M_{00}^{(1)} \xi^{3/2}, \tag{4.5}$$

$$|F_{\xi}(\xi,\eta)| \leq \frac{1}{2}K_{1}(\eta)\,\xi^{1/2},\tag{4.6}$$

$$|F_{\xi\xi}(\xi,\eta)| \leq \frac{1}{4}K_2(\eta)\,\xi^{-1/2},\tag{4.7}$$

where

$$K_1(\eta) = M_{10}^{(1)} |\cos \eta| + M_{01}^{(1)} |\sin \eta|$$
(4.8)

$$K_{2}(\eta) = K_{1}(\eta) + \sum_{i+j=2} {\binom{2}{i}} M_{ij}^{(1)} |\cos^{i} \eta \sin^{j} \eta|.$$
(4.9)

Also, from (2.12) and (2.13), we have

$$|F_{\xi}(\xi,\eta) - \frac{3}{2}c_{3}(\eta)\,\xi^{1/2}| \leqslant \frac{1}{2}K_{3}(\eta)\xi,\tag{4.10}$$

where

$$c_3(\eta)\,\xi^{3/2} = f_{30}x^3 + \dots + f_{03}y^3 \tag{4.11}$$

and

$$K_{3}(\eta) = M_{10}^{(2)} |\cos \eta| + M_{01}^{(2)} |\sin \eta|.$$
(4.12)

In a similar manner, it follows from (3.8) that

$$|\Phi_{\xi}(\xi,\eta)| \leq \frac{1}{4}L_{1}(\eta)\,\xi^{-1/2},\tag{4.13}$$

where

$$L_{1}(\eta) = N_{10} |\cos \eta| + N_{01} |\sin \eta|.$$
(4.14)

LEMMA. Let t_0 be chosen as in (2.9), and put $\varepsilon = \min(1, \delta)$. Then, for every t in $0 < t < \varepsilon t_0$, we have

$$t/K \leqslant \xi_t \leqslant t/\delta, \tag{4.15}$$

where

$$K = 1 + \frac{1}{2}\sqrt{t_0} \left(M_{10}^{(1)} + M_{01}^{(1)} \right).$$
(4.16)

Furthermore,

$$|\xi_t - t| \le M_{00}^{(1)}(t/\delta)^{3/2}.$$
(4.17)

Proof. First, by the mean value theorem, it follows from (3.11) that

$$t = (1 + F_{\ell}(\bar{\xi}_{\ell}, \eta))\xi_{\ell}$$
(4.18)

for some $\bar{\xi}_t$ in $(0, \xi_t)$. In view of (3.10), we immediately obtain $t \ge \delta \xi_t$, thus proving the second inequality in (4.15). Next we observe that (4.18) and (4.6) together imply that

$$t \leq (1 + \frac{1}{2}K_1(\eta)\,\bar{\xi}_t^{1/2})\xi_t. \tag{4.19}$$

Thus, for $t < \varepsilon t_0$ and hence $\xi_t \leq t/\delta \leq t_0$, we have $t \leq K\xi_t$, which proves the first inequality in (4.15). (Note that the use of estimate (4.6) also requires $\xi_t \leq t_0$; see (2.11)). Finally, a combination of (3.11) and (4.5) gives result (4.17).

We now return to Eq. (3.13). The following result is given in [14, Lemma 2, see also Eq. (4.6)]:

$$h(t) = \int_0^{2\pi} \Phi(t,\eta) \, d\eta - \int_0^{2\pi} \left(\Phi_{\xi} F + \Phi F_{\xi} \right)(t,\eta) \, d\eta + \int_0^{2\pi} r_2(t,\eta) \, d\eta, (4.20)$$

where

$$r_{2}(t,\eta) = \frac{\boldsymbol{\Phi}(\boldsymbol{\xi}_{t},\eta) F_{\boldsymbol{\xi}}^{2}(\boldsymbol{\xi}_{t},\eta)}{1+F_{\boldsymbol{\xi}}(\boldsymbol{\xi}_{t},\eta)} - \int_{t}^{t_{t}} \frac{\partial^{2}}{\partial\mu^{2}} (\boldsymbol{\Phi}F)(\mu,\eta) d\eta + \int_{t}^{t_{t}} (t-\mu) \frac{\partial^{2}}{\partial\mu^{2}} \boldsymbol{\Phi}(\mu,\eta) d\eta.$$
(4.21)

Upon making some simplifications and cancellations, we have

$$h(t) = \int_0^{2\pi} \Phi(t,\eta) \, d\eta - \int_0^{2\pi} \Phi(t,\eta) \, F_{\ell}(t,\eta) \, d\eta + \int_0^{2\pi} \rho(t,\eta) \, d\eta, \quad (4.22)$$

where

$$\rho(t,\eta) = \frac{\Phi(\xi_t,\eta) F_t^2(\xi_t,\eta)}{1 + F_t(\xi_t,\eta)} + [\Phi(\xi_t,\eta) - \Phi(t,\eta)] + [(\Phi F_t)(t,\eta) - (\Phi F_t)(\xi_t,\eta)].$$
(4.23)

Let us denote the three terms on the right-hand side of (4.23) by $\rho_1(t, \eta)$, $\rho_2(t, \eta)$, and $\rho_3(t, \eta)$ in succession. From (3.27), (4.6), and (3.8) it is easy to see that

$$|\rho_1(t,\eta)| \leq (1/8\delta^2) N_{00} K_1^2(\eta) t.$$
(4.24)

From (4.17), (4.13), and (4.15) we have by the mean value theorem,

$$|\rho_2(t,\eta)| \le (K^{1/2}/4\delta^{3/2}) M_{00}^{(1)} L_1(\eta)t.$$
(4.25)

In like manner, it follows that for $0 < t < \varepsilon t_0$

$$|\rho_{3}(t,\eta)| \leq \frac{1}{8} M_{00}^{(1)} [(\sqrt{t_{0}}/\delta) L_{1}(\eta) K_{1}(\eta) + N_{00}(\sqrt{K}/\delta^{3/2}) K_{2}(\eta)] t. \quad (4.26)$$

For envenience let us introduce the following notations:

$$\alpha_1 = \int_0^{2\pi} K_1^2(\eta) \, d\eta, \qquad (4.27)$$

$$\alpha_2 = \int_0^{2\pi} L_1(\eta) \, d\eta, \tag{4.28}$$

$$\alpha_3 = \int_0^{2\pi} L_1(\eta) K_1(\eta) \, d\eta, \qquad (4.29)$$

$$\alpha_4 = \int_0^{2\pi} K_2(\eta) \, d\eta. \tag{4.30}$$

Then a combination of the last three estimates gives

$$\left| \int_{0}^{2\pi} \rho(t,\eta) \, d\eta \right| \leq C_3 t, \tag{4.31}$$

where

$$C_{3} = \frac{N_{00}}{8\delta^{2}}\alpha_{1} + \frac{\sqrt{t_{0}}}{8\delta}M_{00}^{(1)}\alpha_{3} + \frac{\sqrt{K}}{8\delta^{3/2}}M_{00}^{(1)}(2\alpha_{2} + N_{00}\alpha_{4}).$$
(4.32)

To estimate the second integral on the right-hand side of (4.22), we note that

$$\Phi(t,\eta) = \frac{1}{2}g_{00} + \Phi_1(t,\eta)$$
(4.33)

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and

$$F_{\xi}(t,\eta) = \frac{3}{2}c_{3}(\eta)t^{1/2} + F_{1}(t,\eta), \qquad (4.34)$$

where

$$|\Phi_1(t,\eta)| \le \frac{1}{2}L_1(\eta)t^{1/2} \tag{4.35}$$

and

$$|F_1(t,\eta)| \leq \frac{1}{2}K_3(\eta)t;$$
 (4.36)

cf. Eqs. (4.14) and (4.10). Since the integral of $c_3(\eta)$ over $(0, 2\pi)$ is zero, it follows that

$$\int_{0}^{2\pi} \Phi(t,\eta) F_{\xi}(t,\eta) d\eta = \frac{1}{2} g_{00} \int_{0}^{2\pi} F_{1}(t,\eta) d\eta + \int_{0}^{2\pi} \Phi_{1}(t,\eta) F_{\xi}(t,\eta) d\eta. \quad (4.37)$$

Put

$$\alpha_{5} = \int_{0}^{2\pi} K_{3}(\eta) \, d\eta. \tag{4.38}$$

Then, in view of the bounds (4.6), (4.35), and (4.36), we obtain

$$\left|\int_{0}^{2\pi} \Phi(t,\eta) F_{\xi}(t,\eta) \, d\eta \right| \leq C_{2} t, \tag{4.39}$$

where

$$C_2 = \frac{1}{4}(\alpha_3 + |g_{00}| \alpha_5). \tag{4.40}$$

By a similar argument, we can also approximate the first integral on the right-hand side of (4.22). Indeed, since

$$g(x, y) = g_{00} + g_{10}x + g_{01}y + \frac{1}{2}[g_{xx}(\bar{x}, \bar{y})x^{2} + 2g_{xy}(\bar{x}, \bar{y})xy + g_{yy}(\bar{x}, \bar{y})y^{2}], \qquad (4.41)$$

by letting

$$L_2(\eta) = \sum_{i+j=2} {\binom{2}{i}} N_{ij} |\cos^i \eta \sin^j \eta|, \qquad (4.42)$$

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we have

$$\left|\int_{0}^{2\pi} \Phi(t,\eta) \, d\eta - \pi g_{00}\right| \leqslant C_1 t, \tag{4.43}$$

where

$$C_1 = \frac{1}{4} \int_0^{2\pi} L_2(\eta) \, d\eta. \tag{4.44}$$

A combination of the results (4.22), (4.31), (4.39), and (4.43) then gives the desired estimate (4.1) with

$$C = C_1 + C_2 + C_3. \tag{4.45}$$

By explicitly evaluating the trigonometric integrals in C_i , i = 1, 2, 3, we obtain

$$C_1 = N_{11} + (\pi/4)(N_{20} + N_{02}), \tag{4.46}$$

$$C_{2} = |g_{00}| \left(M_{10}^{(2)} + M_{01}^{(2)} \right) + \frac{1}{4} \left[M_{10}^{(1)} (\pi N_{10} + 2N_{01}) + M_{01}^{(1)} (\pi N_{01} + 2N_{10}) \right],$$
(4.47)

and

$$C_{3} = \frac{N_{00}}{8\delta^{2}} \left[\pi \left((M_{10}^{(1)})^{2} + (M_{01}^{(1)})^{2} \right) + 4M_{10}^{(1)}M_{01}^{(1)} \right] + \frac{\sqrt{K}}{\delta^{3/2}} M_{00}^{(1)} \left[N_{10} + N_{01} \right] \\ + \frac{\sqrt{t_{0}}}{8\delta} M_{00}^{(1)} \left[\pi (N_{10}M_{10}^{(1)} + M_{01}^{(1)}N_{01}) + 2(M_{10}^{(1)}N_{01} + M_{01}^{(1)}N_{10}) \right] \\ + \frac{\sqrt{K}}{8\delta^{3/2}} M_{00}^{(1)} N_{00} \left[4(M_{10}^{(1)} + M_{11}^{(1)} + M_{01}^{(1)}) + \pi (M_{20}^{(1)} + M_{02}^{(1)}) \right].$$
(4.48)

The constant C given in (4.45) is undoubtly complicated. It involves bounds for the fourth-order partial derivatives of f(x, y) and bounds for the second-order partial derivatives of g(x, y). This is inevitable, however, since even the coefficient b_1 in the expansion

$$h(t) \sim \pi g_{00} + b_1 t + \dots + b_n t^n + \dots$$
 as $t \to 0^+$, (4.49)

has the complicated expression

$$b_{1} = (\pi/2)[(g_{20} + g_{02}) - \frac{1}{2}g_{00}(3f_{40} + f_{22} + 3f_{04}) - \frac{1}{2}(3g_{10}f_{30} + g_{10}f_{12} + g_{01}f_{21} + 3g_{01}f_{03}) + \frac{15}{32}g_{00}(5f_{30}^{2} + 2f_{30}f_{12} + f_{12}^{2} + f_{21}^{2} + 2f_{21}f_{03} + 5f_{03}^{2})], \quad (4.50)$$

where f_{ij} and g_{ij} are the coefficients of $x^i y^j$ in the Taylor expansions of f(x, y) and g(x, y), respectively. The last formula can be obtained from [14, Eq. (4.6)]; cf. [2, p. 338, Eq. (8.3.53); 3, p. 382; 8].

Let us now return to the integral $I_1(\lambda)$ given in (3.2). On the interval $(\varepsilon t_0, c)$, it is easy to see from (3.13) that this integral is dominated by

$$(\pi/\delta\lambda) N_{00} e^{-\varepsilon t_0\lambda}$$

In view of (4.1), we also know that the integral over $(0, \varepsilon t_0)$ can be approximated by $\pi g_{00}/\lambda$ plus the error $E_1^*(\lambda) - E_2^*(\lambda)$, where $|E_1^*(\lambda)| \leq C/\lambda^2$ and $E_2^*(\lambda)$ is equal to

$$(\pi/\lambda) g_{00} e^{-\epsilon t_0 \lambda}$$

Thus a combination of these two results gives

$$I_{1}(\lambda) = (\pi/\lambda) g_{00} + E_{1}(\lambda) + E_{2}(\lambda), \qquad (4.51)$$

where

$$|E_1(\lambda)| \leqslant \frac{C}{\lambda^2} \tag{4.52}$$

and

$$|E_2(\lambda)| \leq \frac{\pi}{\lambda} \left(|g_{00}| + \frac{N_{00}}{\delta} \right) e^{-\varepsilon t_0 \lambda};$$
(4.53)

compare with the one-dimensional approximation given in [13, p. 90, Eq. (9.08) with n = 1].

5. EXAMPLES

EXAMPLE 2. As a simple example of the calculation of error bonds, we consider the double integral S_n given in Example 1. Here we have $c = +\infty$, $\varepsilon = \delta = 1$ and $N_{00} = g_{00} = 1$. To derive the bounds $M_{ij}^{(1)}$ and $M_{ij}^{(2)}$ in (2.11) and (2.13), we take $t_0 = \pi^2/48$ and observe that for any $0 < t < t_0$, the circle $x^2 + y^2 = t$ is circumscribed by the hexagon

$$|x \pm (1/\sqrt{3})y| = 2\sqrt{t/3}, \qquad |(2/\sqrt{3})y| = 2\sqrt{t/3}.$$
 (5.1)

Hence, for every point (x, y) in the disk $x^2 + y^2 \le \pi^2/48$, we have

$$|x \pm (1/\sqrt{3}) y| \le \pi/6, \qquad |(2/\sqrt{3}) y| \le \pi/6.$$
 (5.2)

Also we note, in addition to (3.26), the identity

$$(x - (1/\sqrt{3})y)^4 + ((2/\sqrt{3})y)^4 + (x + (1/\sqrt{3})y)^4 = 2(x^2 + y^2)^2.$$
(5.3)

Thus, considering each term on the right-hand side of (3.21) as a function of one variable and expanding it into a Maclaurin series, we obtain

$$f(x, y) = (x^{2} + y^{2}) + \frac{1}{6}(x^{2} + y^{2})^{2} + \cdots$$
 (5.4)

Since the cubic terms all vanish, it follows from (2.12) that the functions $f_1(x, y)$ and $f_2(x, y)$ are equal, and hence

$$M_{ij}^{(1)} = M_{ij}^{(2)} \qquad \text{for all relevant } i \text{ and } j. \tag{5.5}$$

By applying the one-variable Taylor theorem with remainder to the function $h(\omega) = \log \cos \omega$, we have

$$f_{1}(x, y) = (1/4!)[(x - (1/\sqrt{3})y)^{4}(4 \sec^{2} \tan^{2} + 2 \sec^{4})(\xi_{1}) + ((2/\sqrt{3})y)^{4}(4 \sec^{2} \tan^{2} + 2 \sec^{4})(\xi_{2}) + (x + (1/\sqrt{3})y)^{4}(4 \sec^{2} \tan^{2} + 2 \sec^{4})(\xi_{3})]$$
(5.6)

for some ξ_1, ξ_2 , and ξ_3 in the interval $(-\pi/6, \pi/6)$. Hence

$$|f_1(x, y)| \leq \frac{4}{9}(x^2 + y^2)^2 \leq (\pi/9\sqrt{3})(x^2 + y^2)^{3/2}$$
(5.7)

for all (x, y) in $x^2 + y^2 \le \pi^2/48$. Therefore we choose

$$M_{00}^{(1)} = \pi/9\sqrt{3} = 0.2015.$$
 (5.8)

By the same technique, we have

$$\left|\frac{\partial f_1}{\partial x}\right| \leqslant \frac{8}{9} \left(\left| x - \frac{1}{\sqrt{3}} y \right|^3 + \left| x + \frac{1}{\sqrt{3}} y \right|^3 \right).$$
 (5.9)

If the two quantities inside the absolute value signs have the same sign, then it is easy to see that the right-hand side of (5.9) is dominated by $(4\pi/9\sqrt{3})(x^2 + y^2)$ as long as $(x^2 + y^2) \le \pi^2/48$. On the other hand, if they have opposite signs, then the sum of their absolute values is dominated by $|y(2\sqrt{3}x^2 + (2/3\sqrt{3})y^2)|$. Since in regions where this occurs we have $x^2 \le \frac{1}{3}y^2$ and hence $x^2 \le \frac{1}{4}(x^2 + y^2)$, the quantity inside the bracket in (5.9) is bounded by $|y((\sqrt{3}/2) + (2/3\sqrt{3}), (x^2 + y^2)|$. Consequently, the righthand side of (5.9) is bounded by $\frac{13}{81}\pi(x^2 + y^2)$ for all (x, y) in $x^2 + y^2 \le \frac{\pi^2}{48}$. In either case, we have

$$\left|\frac{\partial f_1}{\partial x}\right| \leqslant \frac{4\pi}{9\sqrt{3}} (x^2 + y^2), \tag{5.10}$$

which suggests that we should take

$$M_{10}^{(1)} = 4\pi/9\sqrt{3} = 0.8061.$$
 (5.11)

Analogous to (5.9), we have

$$\left|\frac{\partial f_1}{\partial y}\right| \leqslant \frac{8}{9\sqrt{3}} \left[\left| x - \frac{1}{\sqrt{3}} y \right|^3 + 2 \left| \frac{2}{\sqrt{3}} y \right|^3 + \left| x + \frac{1}{\sqrt{3}} y \right|^3 \right].$$
(5.12)

Now we divide the disk $x^2 + y^2 \leq t$ into six regions according to the signs of each of the three terms on the right-hand side of (5.12). In each of these regions, we can show that the quantity Q(x, y) inside the square bracket in (5.12) is less than $2\sqrt{3} t^{3/2}$ for all $x^2 + y^2 \leq t$. As an illustration, we consider the case in which all three terms are positive, and hence

$$Q(x, y) = 2x^3 + 2xy^2 + (16/3\sqrt{3})y^3.$$

In this region, the function Q(x, y) clearly does not have a relative maximum; furthermore, it is obvious that its maximum does not occur on the two straight-line boundaries. Hence we may restrict our attention to that portion of the circle $x^2 + y^2 = t$ determined by $0 \le y \le \frac{1}{2}\sqrt{3t}$ and $\frac{1}{2}\sqrt{t} \le x \le \sqrt{t}$. A simple calculation then shows that the maximum must occur at $x = \frac{1}{2}\sqrt{t}$, $y = \frac{1}{2}\sqrt{3t}$. Thus, $Q(x, y) \le 3t^{3/2} \le 2\sqrt{3}t^{3/2}$ for all $x^2 + y^2 \le t$. Inserting this bound into (5.12) gives

$$\left|\frac{\partial f_1}{\partial y}\right| \leqslant \frac{4\pi}{9\sqrt{3}} \left(x^2 + y^2\right) \tag{5.13}$$

which suggests that we should take

$$M_{01}^{(1)} = 4\pi/9\sqrt{3} = 0.8061.$$
 (5.14)

In like manner, we obtain

$$M_{11}^{(1)} = .8639, \qquad M_{20}^{(1)} = M_{02}^{(1)} = \frac{4\pi}{3\sqrt{3}} = 2.4184.$$
 (5.15)

The constant K in (4.16) is hence given by

$$K = 1 + (\pi/8\sqrt{3})((4\pi/9\sqrt{3}) + (4\pi/9\sqrt{3})) = 1.3655.$$
 (5.16)

It is now an easy task to compute the values of C_i , i = 1, 2, 3. Equations (4.46), (4.47), and (4.48) give, respectively, $C_1 = 0$, $C_2 = 1.6122$, and $C_3 = 1.5470$. Hence, we have C = 3.1862. From (3.22) and (4.51), it now follows that

$$S_n = (2/\sqrt{3})[(\pi/n) + E_1(n) + E_2(n)], \qquad (5.17)$$

where

$$|E_1(n)| \le 3.1862/n^2, \tag{5.18}$$

$$|E_2(n)| \le (2\pi/n) \, e^{-n\pi^2/48}. \tag{5.19}$$

Note that the term $E_2(n)$ is exponentially small for large values of n, and hence that the major error comes from $E_1(n)$. The estimate in (5.18) is of course not best possible; but, comparing with (3.33), it appears to be quite realistic.

EXAMPLE 3. An integral which is closely related to S_n is given by

$$T_{n} = \iint_{D'} \left[\cos u \cos v \sin(u+v) \right]^{2n} du \, dv, \tag{5.20}$$

where D' is the triangular region

$$D' = \{(u, v): |u| < \pi/2, |v| < \pi/2, u + v > 0\}.$$
 (5.21)

This integral occurred in a discussion of the asymptotic behavior of the sum

$$S(3,n) = \sum_{k=0}^{2n} (-1)^{k+n} \left(\frac{2n}{k}\right)^3; \qquad (5.22)$$

see [5, p. 72, Sect. 4.7]. Making the change of variables

$$u = (\sqrt{3}/2)x - \frac{1}{2}y + \pi/6, \qquad v = y + \pi/6, \tag{5.23}$$

we may rewrite (5.20) as

$$T_n = \left(\frac{\sqrt{3}}{2}\right)^{2n+1} \iint_D e^{-2nf(x,y)} \, dx \, dy, \tag{5.24}$$

where D is given by

$$D = \left\{ (x, y): \frac{\sqrt{3}}{2}x - \frac{1}{2}y < \frac{\pi}{3}, y < \frac{\pi}{3}, \frac{\sqrt{3}}{2}x + \frac{1}{2}y > -\frac{\pi}{3} \right\} \quad (5.25)$$

and

$$f(x, y) = -\left[\log \cos\left(\frac{\sqrt{3}}{2}x - \frac{1}{2}y + \frac{\pi}{6}\right) - \log\frac{\sqrt{3}}{2}\right] - \left[\log \cos\left(y + \frac{\pi}{6}\right) - \log\frac{\sqrt{3}}{2}\right] - \left[\log \sin\left(\frac{\sqrt{3}}{2}x + \frac{1}{2}y + \frac{\pi}{3}\right) - \log\frac{\sqrt{3}}{2}\right].$$
 (5.26)

The constant c in this case is again $+\infty$, and hence, as in Example 1, the integral I_2 in (2.6) is absent. In view of the identity

$$\tan(w + \pi/6) = \tan(\pi/6) + \sec^2(\eta + (\pi/6))w, \qquad (5.27)$$

where η is some number between 0 and w, it is easy to see that

$$x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} \ge \frac{3}{2}(x^2 + y^2).$$
(5.28)

Thus the constants δ and ε are both equal to $\frac{3}{4}$. By using (5.27), an estimate corresponding to (3.28) can also be obtained. Indeed, we have

$$x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} \leq 2(x^2 + y^2)\left(\frac{4}{3}\right)^2 e^{2t}.$$
(5.29)

Unfortunately this estimate is not sufficient to yield an inequality of the form

$$|F_{\ell}(\xi_{t},\eta)| \leqslant Kte^{\alpha t}, \tag{5.30}$$

for some constants K and α , as in the case of (3.30). Consequently, our analysis in Example 1 cannot be repeated here. The general result (4.51)–(4.53) still applies, however. Let us take $t_0 = \pi^2/108$ so that $\varepsilon t_0 = \pi^2/144$. By essentially the same argument as given in Example 2, the following values are obtained:

$$M_{00}^{(1)} = 1/3\sqrt{3} + \pi/16 = 0.3888, \tag{5.31}$$

$$M_{10}^{(1)} = M_{01}^{(1)} = 1/\sqrt{3} + \pi/4 = 1.3627,$$
 (5.32)

$$M_{20}^{(1)} = M_{02}^{(1)} = 2/\sqrt{3} + 3\pi/4 = 3.5109,$$
 (5.33)

$$M_{11}^{(1)} = 2/\sqrt{3} + \pi/2\sqrt{3} = 2.0616, \qquad (5.34)$$

$$M_{10}^{(2)} = 1 + 5\pi/12\sqrt{3} = 1.7557, \tag{5.35}$$

$$M_{01}^{(2)} = 1 + 5\pi/18 = 1.8727.$$
 (5.36)

It may be noted that the only difference between this example and the previous one is that the cubic terms in the Taylor expansion of (5.26) do not all vanish, whereas these terms in (5.4) are all absent. The constant C in (4.45) is hence given by C = 11.46337. Laplace approximation (4.51) now yields

$$T_n = (\sqrt{3}/2)^{2n+1} [(\pi/2n) + E_1(n) + E_2(n)], \qquad (5.37)$$

where

$$|E_1(n)| \le 2.8659/n^2 \tag{5.38}$$

and

$$|E_2(n)| \le (7\pi/6n) \, e^{-n\pi^2/72}. \tag{5.39}$$

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