

Error of the Newton-Cotes and Gauss-Legendre Quadrature Formulas

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Abstract. It was shown by P. J. Davis that the Newton-Cotes quadrature formula is convergent if the integrand is an analytic function that is regular in a sufficiently large region of the complex plane containing the interval of integration. In the present paper, a bound on the error of the Newton-Cotes quadrature formula for analytic functions is derived. Also the bounds on the Legendre polynomial and the Legendre function of the second kind are obtained. These bounds are employed to derive a bound on the error of the Gauss-Legendre quadrature formula for analytic functions.

1. Introduction. Let z_0, z_1, \dots, z_{n-1} be n distinct points lying in the complex plane and let C be a closed contour containing these points in its interior. Suppose that $f(z)$ is a regular function within C . Let

$$(1) \quad w_n(z) = \prod_{i=0}^{n-1} (z - z_i).$$

If now the points $z = a$ and $z = b$ also lie inside C , then, following the method given in [1, pp. 117-118], we have for any weight function $g(t)$,

$$(2) \quad \int_a^b g(t)f(t) dt = \sum_{k=0}^{n-1} \lambda_k f(z_k) + E_n(f),$$

where $\lambda_0, \lambda_1, \dots, \lambda_{n-1}$ are the weights for interpolating integration at z_0, z_1, \dots, z_{n-1} and

$$(3) \quad E_n(f) = \frac{1}{\pi i} \int_C \frac{f(z)v_n(z) dz}{w_n(z)},$$

$$(4) \quad v_n(z) = \frac{1}{2} \int_a^b \frac{w_n(t)g(t) dt}{z - t},$$

and

$$(5) \quad \lambda_k = \int_a^b \frac{g(t)w_n(t) dt}{(t - z_k)w'_n(z_k)} \quad (k = 0, 1, \dots, n - 1).$$

Here $E_n(f)$ designates the error of the n -point interpolating quadrature formula given by

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$$(6) \quad \int_a^b g(t)f(t) dt \approx \sum_{k=0}^{n-1} \lambda_k f(z_k).$$

The problem of estimating the error $E_n(f)$ for analytic functions is connected with the estimation of $v_n(z)$ and $w_n(z)$ on C . In this paper, we shall bound the error of two special quadrature formulas over the interval $[-1, 1]$ (i.e., $a = -1$, $b = +1$) with the weight function $g(t) = 1$. For the contour C we shall take the ellipse E_ρ in the complex plane defined by

$$(7) \quad z = \frac{1}{2}(\xi + \xi^{-1}), \quad \xi = \rho e^{i\theta}, \quad 0 \leq \theta \leq 2\pi \quad \text{and} \quad \rho > 1.$$

The ellipse E_ρ has foci at $z = \pm 1$ and sum of its semi-axes is ρ (> 1). Let

$$A(E_\rho) = \left\{ f: \begin{array}{l} f \text{ is analytic on } [-1, 1] \text{ and continuable analytically so as to be} \\ \text{single valued and regular in the closure of the ellipse } E_\rho. \end{array} \right.$$

Davis [2] discussed the convergence (as $n \rightarrow \infty$) of the Newton-Cotes quadrature formula for functions $f \in A(E_\rho)$. In fact, it was shown by him that the Newton-Cotes quadrature formula is convergent provided $f \in A(E_\rho)$, where $\rho > 2$. Moreover, as $n \rightarrow \infty$, the error $E_n(f)$ tends to zero with geometric rapidity. In Section 2 we derive an upper bound on the error $|E_{NC_n}(f)|$ of the Newton-Cotes quadrature formula given in Theorem 1. For $\rho > 1 + \sqrt{2}$, this bound on $|E_{NC_n}(f)|$ converges (as $n \rightarrow \infty$) to zero with geometric rapidity.

In Section 3 we derive an upper bound on $|Q_n(z)|$ and a lower bound on $|P_n(z)|$ for $z \in E_\rho$ and $\rho > \sqrt{2}$, where $P_n(z)$ and $Q_n(z)$ are the Legendre polynomial and Legendre function of the second kind, respectively. Using these bounds, we derive an upper bound on the error $|E_{G_n}(f)|$ of the Gauss-Legendre quadrature formula given in Theorem 2. This result differs from similar results due to Chawla and Jain, since this result is a bound, while theirs is an asymptotic bound, i.e., a bound on the first term of the asymptotic expansion.

2. Error of the Newton-Cotes Quadrature Formula. Newton-Cotes ($n + 1$)-point quadrature formula for the integral $\int_{-1}^{+1} f(t) dt$ is a special case of the nonsymmetric interpolating quadrature formula (2) when $a = -1$, $b = +1$, $g(t) = 1$, and the abscissas are given by

$$(8) \quad z_i = x_i = -1 + 2i/n \quad (i = 0, 1, \dots, n).$$

The weights λ_k (known as Cotes numbers) and the error $E_{NC_n}(f)$ of the Newton-Cotes quadrature formula are, respectively, given by

$$(9) \quad \lambda_k = \int_{-1}^{+1} \frac{w_{n+1}(x) dx}{(x - x_k)w'_{n+1}(x_k)} \quad (k = 0, 1, \dots, n)$$

and

$$(10) \quad E_{NC_n}(f) = \frac{1}{\pi i} \int_C \frac{f(z)Q_n^*(z) dz}{w_{n+1}(z)},$$

where

$$(11) \quad Q_n^*(z) \equiv v_{n+1}(z) = \frac{1}{2} \int_{-1}^{+1} \frac{w_{n+1}(x) dx}{z - x},$$

and $w_{n+1}(x)$ is defined by (1), with z_i given by (8).

2.1 An Upper Bound on $Q_n^*(z)$.

LEMMA 1. For $z \in E_\rho$,

$$(12) \quad Q_n^*(z) = \sum_{m=1}^{\infty} \frac{\sigma_{nm}^*}{\xi^m},$$

where

$$(13) \quad \sigma_{nm}^* = \int_0^\pi w_{n+1}(\cos \theta) \sin m\theta \, d\theta, \quad (n, m = 1, 2, 3, \dots)$$

and σ_{nm}^* is bounded as follows:

(a) Let $n \geq 1$ be an odd integer. Then

$$(14) \quad \begin{aligned} |\sigma_{nm}^*| &\leq 0, \quad m \text{ even,} \\ &\leq 4/3, \quad m = 1, \\ &\leq \sqrt{2(\pi/4)}, \quad m > 1, \end{aligned}$$

and

$$(15) \quad |Q_n^*(z)| \leq 4\rho/3(\rho^2 - 1).$$

(b) Let $n \geq 1$ be an even integer. Then

$$(16) \quad \begin{aligned} |\sigma_{nm}^*| &\leq 0, \quad m \text{ odd,} \\ &\leq 2 \left[\frac{m^2}{18} \left(\frac{3}{4m^2 - 1} + \frac{1}{4m^2 - 9} \right) \right]^{1/2} \leq 4 \left(\frac{2}{105} \right)^{1/2}, \quad m \geq 2 \end{aligned}$$

and

$$(17) \quad |Q_n^*(z)| \leq 4\sqrt{(2/105)(1/(\rho^2 - 1))}.$$

Proof. In (11), setting $x = \cos \theta$ and $z = \frac{1}{2}(\zeta + \zeta^{-1})$, we get

$$(18) \quad Q_n^*(z) = \frac{1}{\xi} \int_0^\pi \frac{w_{n+1}(\cos \theta) \sin \theta \, d\theta}{1 - 2\xi^{-1}\cos \theta + \xi^{-2}}.$$

Following [3, pp. 311-312], we get

$$(19) \quad \frac{\sin \theta}{\xi} [1 - 2\xi^{-1}\cos \theta + \xi^{-2}]^{-1} = \sum_{m=1}^{\infty} \frac{\sin m\theta}{\xi^m}.$$

The last series converges uniformly and absolutely for $0 \leq \theta \leq \pi$, and for all $|\xi| \geq \rho > 1$. Using (19) in (18), we obtain (12). We now proceed to find bounds for

$$(20) \quad \sigma_{nm}^* = \int_0^\pi \left[\prod_{i=0}^n (\cos \theta - x_i) \right] \sin m\theta \, d\theta.$$

Proof of (a). Let n be odd, say, $n = 2r - 1$ ($r = 1, 2, 3, \dots$). From (20)

$$\sigma_{nm}^* = \int_0^\pi \left[\prod_{i=0}^{r-1} (\cos^2 \theta - x_i^2) \right] \sin m\theta \, d\theta.$$

Breaking the range of integration into two intervals, $[0, \pi/2]$ and $[\pi/2, \pi]$, we easily get

$$(21) \quad \sigma_{nm}^* = [1 + (-1)^{m+1}] \int_0^{\pi/2} \left[\prod_{i=0}^{r-1} (\cos^2 \theta - x_i^2) \right] \sin m\theta \, d\theta.$$

Hence $\sigma_{nm}^* = 0$ if m is even. We now bound σ_{nm}^* for odd integer m . Consider the following two cases.

Case 1. Let $m = 1$. From (21)

$$|\sigma_{nm}^*| \leq 2 \int_0^{\pi/2} \sin^3 \theta \, d\theta = 4/3.$$

Case 2. Let $m > 1$. (21) yields

$$\begin{aligned} |\sigma_{nm}^*| &\leq 2 \int_0^{\pi/2} \sin^2 \theta |\sin m\theta| \, d\theta \\ &\leq 2 \left[\left(\int_0^{\pi/2} \sin^2 \theta \, d\theta \right) \left(\int_0^{\pi/2} \sin^2 \theta \sin^2 m\theta \, d\theta \right) \right]^{1/2} \\ &= \sqrt{2(\pi/4)}, \end{aligned}$$

where the second inequality is derived by employing Cauchy's inequality. This completes the proof of (14).

Proof of (b). Let n be an even integer, say, $n = 2r$ ($r = 1, 2, 3, \dots$). We have from (20),

$$\begin{aligned} \sigma_{nm}^* &= \int_0^\pi \left[\prod_{i=0, i \neq r}^{2r} (\cos \theta - x_i) \right] \cos \theta \sin m\theta \, d\theta \\ &= \int_0^\pi \left[\prod_{i=0}^{r-1} (\cos^2 \theta - x_i^2) \right] \cos \theta \sin m\theta \, d\theta \\ &= [1 + (-1)^{m+2}] \int_0^{\pi/2} \left[\prod_{i=0}^{r-1} (\cos^2 \theta - x_i^2) \right] \cos \theta \sin m\theta \, d\theta. \end{aligned}$$

Hence $\sigma_{nm}^* = 0$ for m odd. When m is even, we obtain

$$\begin{aligned} |\sigma_{nm}^*| &\leq 2 \int_0^{\pi/2} \sin^2 \theta \cos \theta |\sin m\theta| \, d\theta \\ &\leq 2 \left[\left(\int_0^{\pi/2} \sin^2 \theta \cos \theta \, d\theta \right) \left(\int_0^{\pi/2} \sin^2 \theta \sin^2 m\theta \cos \theta \, d\theta \right) \right]^{1/2} \\ &= 2 \left[\frac{m^2}{18} \left(\frac{3}{4m^2 - 1} + \frac{1}{4m^2 - 9} \right) \right]^{1/2} \leq 4\sqrt{(2/105)}. \end{aligned}$$

This proves (16). Bounds (15) and (17) follow from (12), (14), and (16). This completes the proof of Lemma 1.

2.2 A Lower Bound on $w_{n+1}(z)$.

LEMMA 2. For $z \in E_\rho$,

$$(22) \quad |w_{n+1}(z)| \geq ((\rho^2 - 1)/(2\rho))^{n+1}.$$

Proof. We consider the two cases when n is odd or even.

Case 1. When $n = 2r - 1$ ($r = 1, 2, 3, \dots$) is odd, we have for $z \in E_\rho$,

$$\begin{aligned} |w_{n+1}(z)| &= \frac{1}{(2\rho)^{n+1}} \prod_{i=0}^{r-1} |\xi^4 + 1 + 2\xi^2 - 4\xi^2 x_i^2| \\ &= \frac{1}{(2\rho)^{n+1}} \prod_{i=0}^{r-1} |(\xi^2 - q_i)(\xi^2 - \bar{q}_i)|, \end{aligned}$$

where $q_i = (2x_i^2 - 1) + \sqrt{-1(2x_i(1 - x_i^2)^{1/2})}$ and \bar{q}_i is the complex conjugate of q_i . Also $|q_i| = 1$. Hence,

$$|w_{n+1}(z)| \geq \frac{1}{(2\rho)^{n+1}} \prod_{i=0}^{r-1} (\rho^2 - 1)^2 = \left(\frac{\rho^2 - 1}{2\rho}\right)^{n+1}.$$

Case 2. When $n = 2r$ ($r = 1, 2, 3, \dots$) is even, we have for $z \in E_\rho$,

$$\begin{aligned} |w_{n+1}(z)| &= |z| \prod_{i=0}^{r-1} |z^2 - x_i^2| \\ &= \frac{1}{2|\xi|} |\xi^2 + 1| \left(\frac{1}{2|\xi|}\right)^{2r} \prod_{i=0}^{r-1} |(\xi^2 - q_i)(\xi^2 - \bar{q}_i)| \\ &\geq (\rho^2 - 1)/(2\rho)^{n+1}(\rho^2 - 1)^{2r} = ((\rho^2 - 1)/2\rho)^{n+1}. \end{aligned}$$

This completes the proof of Lemma 2.

2.3 *A Bound on $E_{NC_n}(f)$.* From (10), by selecting the contour C as an ellipse E_ρ ($\rho > 1$) it follows that

$$(23) \quad |E_{NC_n}(f)| \leq \frac{1}{\pi} \int_{E_\rho} \frac{|f(z)||Q_n^*(z)|}{|w_{n+1}(z)|} |dz|.$$

Employing (15), (17), and (22) we obtain the following theorem.

THEOREM 1. Let $f \in A(E_\rho)$, $\rho > 1$. Then for $n \geq 1$

$$(24) \quad |E_{NC_n}(f)| \leq K_\rho M(\rho)(2\rho/(\rho^2 - 1))^{n+1},$$

where

$$(25) \quad \begin{aligned} K_\rho &= \frac{4}{3} \frac{(\rho^2 + 1)}{(\rho^2 - 1)}, \quad n \text{ odd}, \\ &= 4 \left(\frac{2}{105}\right)^{1/2} \left(\frac{\rho^2 + 1}{\rho(\rho^2 - 1)}\right), \quad n \text{ even}, \end{aligned}$$

and

$$(26) \quad M(\rho) = \max|f(z)| \quad \text{on } E_\rho.$$

2.4 *Discussion of the Results.* Relation (24) gives a bound on $|E_{NC_n}(f)|$ for all $\rho > 1$ and all $n \geq 1$. From (24) it is easily seen that the bound on $|E_{NC_n}(f)|$ tends to zero as n tends to infinity only if $\rho > 1 + \sqrt{2}$. However, Davis [2] proved the stronger result that $|E_{NC_n}(f)|$ tends to zero as n tends to infinity provided that $\rho > 2$. Therefore, it is of interest to tighten the bound (24).

3. Error of the Gauss-Legendre Quadrature Formula. An important special case of the general interpolating quadrature formula (2) is the Gauss-Legendre quadrature

formula. The n -point Gauss-Legendre quadrature formula for $\int_{-1}^{+1} f(t) dt$ is obtained by letting $a = -1$, $b = +1$, $g(t) = 1$, and choosing $z_0, z_1, z_2, \dots, z_{n-1}$ as the n zeros of the Legendre polynomial $P_n(x)$. The weights λ_k and the error $E_{G_n}(f)$ of the Gauss-Legendre quadrature formula are, respectively, given by

$$(27) \quad \lambda_k = \int_{-1}^{+1} \frac{P_n(x) dx}{(x - z_k)P'_n(z_k)} \quad (k = 0, 1, \dots, n - 1)$$

and

$$(28) \quad E_{G_n}(f) = \frac{1}{\pi i} \int_C \frac{f(z)Q_n(z) dz}{P_n(z)},$$

where $Q_n(z)$, defined by

$$(29) \quad Q_n(z) = \frac{1}{2} \int_{-1}^{+1} \frac{P_n(t) dt}{z - t},$$

is the Legendre function of the second kind.

3.1 An Upper Bound on $Q_n(z)$.

LEMMA 3. For $z \in E_\rho$

$$(30) \quad Q_n(z) = \frac{1}{\xi^{n+1}} \sum_{r=0}^{\infty} \frac{\sigma_{n,n+2r+1}}{\xi^{2r}},$$

where

$$(31) \quad 0 < \sigma_{n,n+2r+1} \leq b_n \quad \text{for } r = 0, 1, 2, 3, \dots$$

Moreover,

$$(32) \quad |Q_n(z)| \leq \rho b_n / (\rho^2 - 1)\rho^n,$$

where

$$(33) \quad b_n = (2)^{2n+1}(n!)^2/(2n + 1)! \quad (\leq 2 \text{ for all } n = 0, 1, 2, \dots).$$

Proof. Setting $t = \cos \theta$ and $z = \frac{1}{2}(\xi + \xi^{-1})$ in (29) and proceeding as in the proof of Lemma 1, we get

$$(34) \quad Q_n(z) = \sum_{m=1}^{\infty} \frac{\sigma_{nm}}{\xi^m},$$

where

$$(35) \quad \sigma_{nm} = \int_0^\pi P_n(\cos \theta) \sin(m\theta) d\theta.$$

Heine [4, p. 311] gave the following evaluation of σ_{nm} :

$$(36) \quad \sigma_{nm} = \Gamma\left(\frac{m+n+1}{2}\right)\Gamma\left(\frac{m-n}{2}\right) / \Gamma\left(\frac{m-n+1}{2}\right)\Gamma\left(\frac{m+n+2}{2}\right),$$

when $m > n$ and $m - n$ is odd,

= 0, otherwise.

Writing $m - n = 2r + 1$ ($r = 0, 1, 2, \dots$), we obtain from (36)

$$\frac{\sigma_{n,n+2r+1}}{\sigma_{n,n+2r+3}} = \frac{(r + 1)(n + r + 3/2)}{(r + 1/2)(n + r + 1)} > 1.$$

Hence, for fixed n , the sequence $\{\sigma_{n,n+2r+1}\}$ for varying r is strictly monotonically decreasing, yielding

$$(37) \quad \sigma_{n,n+2r+1} < \sigma_{n,n+1} = b_n = \frac{(n!)^2(2)^{2n+1}}{(2n + 1)!}.$$

The results (30) and (31) follow from (34), (36), and (37). Bound (32) follows from (30) and (31). This completes the proof of the lemma.

A similar result based on $|\sigma_{n,k}| \leq 2$ was used to derive an asymptotic bound ($n \rightarrow \infty$) on $|E_{G_n}(f)|$ (see [5]). Using Stirling's formula

$$(38) \quad b_n \approx 2\sqrt{\pi n}/(2n + 1) \text{ as } n \rightarrow \infty.$$

This extra $n^{-1/2}$ factor in (32) is vital to obtain a better bound.

3.2 A Lower Bound on $P_n(z)$.

LEMMA 4. For $z \in E_\rho$,

$$(39) \quad \begin{aligned} |P_n(z)| &\geq a_n(\rho^2 + \rho^{-2n} - 2)\rho^n/(\rho^2 - 1) \\ &\geq a_n(\rho^2 - 2)\rho^n/(\rho^2 - 1), \end{aligned}$$

where

$$(40) \quad a_n = \frac{(2n)!}{(2)^{2n}(n!)^2} = \frac{2}{(2n + 1)b_n} \quad \left(\approx \frac{1}{\sqrt{\pi n}} \text{ as } n \rightarrow \infty \right).$$

The bound (39) is significant if $\rho > \sqrt{2}$.

Proof. It is shown in [3, Lemmas 12.4.1 and 12.4.3] that for $z \in E_\rho$

$$(41) \quad P_n(z) = \sum_{j=0}^n a_j a_{n-j} (\xi)^{n-2j}$$

and

$$(42) \quad a_j a_{n-j} \leq a_n, \quad j = 0, 1, 2, \dots, n,$$

where a_n is given by (40). From (41)

$$\begin{aligned} |P_n(z)| &= \left| 1 + \sum_{j=1}^n \frac{a_j a_{n-j}}{a_n} \xi^{-2j} \right| (a_n \rho^n) \\ &\geq a_n \rho^n \left[1 - \left| \sum_{j=1}^n \frac{a_j a_{n-j}}{a_n} \xi^{-2j} \right| \right] \\ &\geq a_n \rho^n \left[1 - \sum_{j=1}^n \rho^{-2j} \right] \quad (\text{using (42)}) \\ &= a_n \rho^n \left[\frac{\rho^2 + \rho^{-2n} - 2}{\rho^2 - 1} \right] \geq a_n \rho^n \frac{(\rho^2 - 2)}{(\rho^2 - 1)}. \end{aligned}$$

This establishes the lemma.

3.3 *A Bound on $E_{G_n}(f)$.* From (27) by selecting the contour C as an ellipse E_ρ it follows that

$$(43) \quad |E_{G_n}(f)| \leq \frac{1}{\pi} \int_{E_\rho} \frac{|f(z)| |Q_n(z)| |dz|}{|P_n(z)|}.$$

Let $\rho > \sqrt{2}$. Employing (32) and (39), we obtain

$$(44) \quad |E_{G_n}(f)| \leq d_n \frac{M(\rho)}{\rho^{2n}} \left(\frac{\rho^2 + 1}{\rho^2 - 2} \right),$$

where

$$(45) \quad d_n = \frac{(2)^{4n+1}(n!)^4}{(2n)!(2n+1)!}$$

and $M(\rho)$ is given by (26).

It is easily seen that the sequence $\{d_n\}$ is strictly monotonically increasing and $\lim_{n \rightarrow \infty} d_n = \pi$. Thus

$$(46) \quad 0 < d_n \leq \pi,$$

and we have the following theorem.

THEOREM 2. *Let $f \in A(E_\rho)$, $\rho > \sqrt{2}$. Then*

$$(47) \quad |E_{G_n}(f)| \leq d_n \frac{(\rho^2 + 1)}{(\rho^2 - 2)} \frac{M(\rho)}{\rho^{2n}},$$

where $M(\rho)$ and d_n are, respectively, given by (26) and (45).

In view of (46), an overall bound is given by

COROLLARY. *Let $n \rightarrow \infty$, then for $\rho > \sqrt{2}$*

$$(48) \quad |E_{G_n}(f)| \leq \pi \frac{(\rho^2 + 1)}{(\rho^2 - 2)} \frac{M(\rho)}{\rho^{2n}}.$$

We mention here that Chawla [6, Theorem 1] obtained the following asymptotic ($n \rightarrow \infty$) result by using Davis' method.

If $f \in A(E_\rho)$ and $\rho > 1$, then

$$(49) \quad |E_{G_n}(f)| \leq \pi \frac{M(\rho)}{\rho^{2n}} (1 + \rho^{-4})^{1/2} (1 + O(1)).$$

3.4 *Discussion of the Results.* The asymptotic ($n \rightarrow \infty$) bound (48) is not better than the asymptotic bound (49). But the bound (47) is valid for all n and $\rho > \sqrt{2}$ as compared to the asymptotic bound (49) which is valid for $n \rightarrow \infty$ and $\rho > 1$.

As a consequence of (47) we have the following asymptotic bound valid for $\rho \rightarrow \infty$

$$(50) \quad |E_{G_n}(f)| \leq d_n \frac{M(\rho)}{\rho^{2n}} \left[1 + \frac{3}{\rho^2 - 2} \right] = d_n \frac{M(\rho)}{\rho^{2n}} [1 + O(\rho^{-2})].$$

This bound is compatible with the asymptotic ($\rho \rightarrow \infty$) bound of Chawla (unpublished work), having the same leading term.

The bound (47) can be compared in some sense with the bound of Stenger [7] given by

$$(51) \quad |E_{G_n}(f)| \leq \frac{32}{\pi} \frac{M_1(\rho)}{\rho^{2n}},$$

where $M_1(\rho) = \max_{z \in E_n} |\text{Real part of } f(z)|$ and $\rho > 1$. Now, if we compare the coefficients $((\rho^2 + 1)/(\rho^2 - 2))d_n$ and $32/\pi$ of (47) and (51), respectively, it is clear that the former is less than the latter, for

$$(52) \quad \rho > \left(\frac{64 + \pi d_n}{32 - \pi d_n} \right)^{1/2}.$$

The relation (52) is definitely true if

$$(53) \quad \rho > \left(\frac{64 + \pi^2}{32 - \pi^2} \right)^{1/2} \quad (\approx 1.83).$$

Thus we see that Stenger's bound is better for small ρ , but ours is better for large ρ . For small $\rho < \sqrt{2}$ ours does not exist. For large ρ ours is smaller by a factor $\pi^2/32 = 0.31$. The cross-over point is near $\rho = 1.83$. These numbers depend on n but only slightly.

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