

# Chebyshev Approximations for Dawson's Integral

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**Abstract.** Rational Chebyshev approximations to Dawson's integral are presented in well-conditioned forms for  $|x| \leq 2.5$ ,  $2.5 \leq |x| \leq 3.5$ ,  $3.5 \leq |x| \leq 5.0$  and  $5.0 \leq |x|$ . Maximal relative errors range down to between  $2 \times 10^{-20}$  and  $7 \times 10^{-22}$ .

**1. Introduction.** Dawson's integral,

$$(1.1) \quad F(x) \equiv e^{-x^2} \int_0^x e^{t^2} dt,$$

appears in a variety of applications including spectroscopy, heat conduction, and electrical oscillations in certain special vacuum tubes. It is closely related to the (modified) complex error function,

$$(1.2) \quad w(z) \equiv e^{-z^2} \operatorname{erfc}(-iz) = e^{-z^2} \left\{ 1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right\} = e^{-z^2} + \frac{2i}{\sqrt{\pi}} F(z).$$

Because of its many applications this latter function has been extensively studied and tabulated. Its more important mathematical properties are included in Gautschi's [1] summary, while Armstrong [2] reviews both its applications and some computational methods. Many schemes for computing  $w(z)$  are less effective near the real axis, and algorithms for computation there frequently begin with a value of  $F(x)$ .

Extensive tabulations of Dawson's integral exist. Perhaps the most accurate is that of Lohmander and Rittsten [3], which gives 10D values for much of the range, and selected values to 20D. More recently, Hummer [4] has published 18D values of the coefficients in the expansion

$$(1.3) \quad F(x) = \sum_{k=0}^{33} a_k T_{2k+1}(x/5), \quad |x| \leq 5,$$

where  $T_{2k+1}(s)$  is the Chebyshev polynomial of the first kind of degree  $2k + 1$ .

In this paper we present a set of nearly-best rational approximations to  $F(x)$  for all real  $x$  and with relative accuracies up to 22S. These approximations are not only more accurate than Hummer's, but may be made the basis of significantly faster subroutines.

**2. Functional Properties.** Dawson's integral is a special case of the confluent hypergeometric function:

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$$(2.1) \quad F(z) = {}_1F_1(1; 3/2; -z^2).$$

It follows that Dawson's integral is an antisymmetric function, and that values for all real  $x$  can be obtained from computations valid for  $[0, \infty)$ .

Differentiating (1.1) we find that for all complex  $z$

$$(2.2) \quad F'(z) = -2zF(z) + 1,$$

while for  $k \geq 1$  the derivatives can be shown to obey the recurrence

$$(2.3) \quad F^{(k+1)}(z) + 2zF^{(k)}(z) + 2kF^{(k-1)}(z) = 0.$$

These results allow the computation of the Taylor series expansion about any point at which  $F(z)$  is known with sufficient accuracy. In particular, since  $F(0) = 0$ , the Maclaurin series

$$(2.4) \quad F(z) = z \sum_{k=0}^{\infty} \frac{(-1)^k k!}{(2k+1)!} (2z)^{2k}; \quad |z| < \infty$$

is easily obtained.

Although (2.4) converges for all finite  $z$  (hence  $F(z)$  is an entire function), the ratio of successive terms is only  $-2z^2/(2k+3)$ . Practical convergence is thus delayed until  $k$  becomes greater than  $|z^2| - 3/2$ , and serious cancellation errors may occur in summing (2.4) for even moderately large  $z$ . A more efficient expansion of  $F(z)$  in the neighborhood of the origin is the continued fraction

$$(2.5) \quad F(z) = \frac{z}{1+} \frac{2z^2/3}{1-} \frac{4z^2/15}{1+} \frac{6z^2/35}{1-} \dots + \frac{(-1)^{k+1} (2kz^2)/(2k-1)(2k+1)}{1+\dots},$$

which can be obtained either by applying the QD algorithm to (2.4), or as a special case of the continued fraction for  $1/{}_1F_1(1; \gamma; x)$  given by Perron [5, p. 123, Eq. (8)]. Thacher [6] shows that (2.5) converges throughout the complex plane, is uniformly more efficient than (2.4) and is numerically stable in the first octant of the complex plane. For large  $|z|$ , however, convergence is slow, and some 70 convergents are needed to attain 25D accuracy at  $z = 6$ .

Thus, for large  $z$ , expansions about the point at  $\infty$  are desirable. By deforming the path in the integral representation of the (modified) complex error function [1, Eq. 7.1.4], it can be shown that  $F(x)$  can be represented as the Cauchy principal value

$$(2.6) \quad F(x) = \frac{1}{2\sqrt{\pi}} \mathop{\int}\limits_{-\infty}^{\infty} \frac{e^{-t^2}}{x-t} dt.$$

Replacing  $1/(x-t)$  by the identity

$$(2.7) \quad \frac{1}{x-t} = \frac{1}{x} \left\{ \sum_{k=0}^{n-1} \left( \frac{t}{x} \right)^k + \frac{(t/x)^n}{1-t/x} \right\}$$

and integrating, we have

$$(2.8) \quad F(x) = \frac{1}{2x} \left\{ \sum_{k=0}^{[(n-1)/2]} \frac{\Gamma(k + \frac{1}{2})}{\Gamma(\frac{1}{2})} x^{-2k} + \frac{x^{-n}}{\Gamma(\frac{1}{2})} \mathop{\int}\limits_{-\infty}^{\infty} \frac{t^n e^{-t^2}}{1-t/x} dt \right\},$$

where  $[x]$  is the greatest integer contained in  $x$ . Equation (2.8) is the familiar

asymptotic series with two different expressions for the remainder, depending on whether  $n$  is even or odd. (We are indebted to the referee for pointing out that Stieltjes [7] gives a similar remainder term for  $n$  even.) The development of recurrences and converging factors does not seem worthwhile in view of the good accuracy of (2.8) (almost 29D for  $x = 8$ ).

TABLE I.  $\epsilon_{\ell m} = -100 \log_{10} \max \left| \frac{F(x) - F_{\ell m}(x)}{F(x)} \right|$

$0 \leq  x  \leq 2.5$									
$\ell$	1	2	3	4	5	6	7	8	9
0	33	73	124	182	246	316	391	471	
1	126*	185	251	323	399	480	565		
2	209	284	363	447	534	624			
3	259	378	469*	563	660				
4		493	573	677	782	889			
5		593	653	790	903*				
6						1144*			
7							1398		
8								1663*	
9									1939*
*****									
$2.5 \leq  x  \leq 3.5$									
$\ell$	1	2	3	4	5	6	7	8	9
0	279	417†	453	596†	626	718	828	868	963
1	384*	450		624	624	792	862		
2		524		727	727	930	1019		
3			727		883				
4				964*	928				
5					1020				
6					1104*	1245			
7						1338	1551	1574	
8							1574*		
9								1839*	
*****									
$3.5 \leq  x  \leq 5.0$									
$\ell$	1	2	3	4	5	6	7	8	9
0	353	481	596	767†	768	865	945	1024	1102
1	507*	652	709	768		925	997		
2		707		847	976	1040	1135		
3			860*	995	1033	1098	1195	1296	
4				1032					
5					1242*				
6						1359			
7							1576*		
8								1751*	
9									1973*
*****									
$5.0 \leq  x $									
$\ell$	1	2	3	4	5	6	7	8	9
0	521	659	783	893	991	1076	1154	1232	1327
1	707*	838	952	1050	1138	1229	1330	1337	
2	858	978	1080	1175	1296	1312	1337		
3	973		119*	1302	1312				
4	1068			1311					
5					1449*				
6						1571			
7							1685*		
8								1802*	
9									191*
*****									

† Nonstandard error curve

\* Coefficients for these approximations only are given in Tables II-V.

The continued fraction

$$(2.9) \quad F(x) \sim \frac{x}{2} \left\{ \frac{1}{x^2-1} \frac{1/2}{1-x^2} \frac{2/2}{x^2-1} \dots - \frac{2k/2}{x^2-1} \frac{(2k+1)/2}{1-x^2} \dots \right\}$$

corresponding to (2.8) diverges for all real  $x$ , but appropriate convergents can be profitably used for computation. Gautschi [9] has recently observed that it is in fact asymptotic in the sense of Poincaré.

TABLE II.  $F(x) \approx x \frac{\sum_{j=0}^n p_j x^{2j}}{\sum_{j=0}^n q_j x^{2j}} \quad |x| \leq 2.5$

n	j	$p_j$			$q_j$		
1	0	1.145		( 00)	1.085		( 00)
	1	-0.426		(-02)	1.000		( 00)
3	0	4.76800 8		( 01)	4.76791 2		( 01)
	1	-4.30297 8		( 00)	2.75055 1		( 01)
	2	1.36584 5		( 00)	6.90076 0		( 00)
	3	-3.56642 4		(-02)	1.00000 0		( 00)
5	0	1.08326 55887 3		( 04)	1.08326 55877 2		( 04)
	1	-1.28405 83227 9		( 03)	5.93771 27693 5		( 03)
	2	4.19672 97228 0		( 02)	1.48943 55724 2		( 03)
	3	-1.51982 15242 2		( 01)	2.19728 33183 3		( 02)
	4	1.67795 11618 9		( 00)	1.99422 33636 4		( 01)
	5	-2.38594 56569 6		(-02)	1.00000 00000 0		( 00)
6	0	2.31569 75201 341		( 05)	2.31569 75201 425		( 05)
	1	-2.91794 64300 780		( 04)	1.25200 37031 851		( 05)
	2	9.66963 98191 665		( 03)	3.13846 20138 163		( 04)
	3	-4.35011 60207 595		( 02)	4.74470 98440 662		( 03)
	4	5.46161 22556 699		( 01)	4.66849 06545 115		( 02)
	5	-8.54176 81195 954		(-01)	2.93919 95612 556		( 01)
	6	2.08468 35103 886		(-02)	1.00000 00000 000		( 00)
8	0	1.73971 38358 72305 762		( 08)	1.73971 38358 72305 803		( 08)
	1	-2.35903 54309 49078 422		( 07)	9.23905 68081 99581 718		( 07)
	2	7.94595 11256 26974 712		( 06)	2.31472 94223 70433 794		( 07)
	3	-4.49438 95997 95344 826		( 05)	3.59959 82595 90670 414		( 06)
	4	6.26435 22480 53304 262		( 04)	3.83498 04512 71685 588		( 05)
	5	-1.64294 23044 87861 388		( 03)	2.90022 12938 95164 274		( 04)
	6	1.10415 15859 64097 196		( 02)	1.54480 44953 25198 331		( 03)
	7	-1.23896 01126 69044 439		( 00)	5.42357 27435 06117 292		( 01)
	8	1.70141 56251 64813 150		(-02)	1.00000 00000 00000 000		( 00)
9	0	5.83917 15512 36746 64696 3		( 09)	5.83917 15512 36746 64671 7		( 09)
	1	-8.10874 57862 86504 21438 5		( 08)	3.08190 64555 29180 70960 1		( 09)
	2	2.74522 24075 69207 53304 4		( 08)	7.72014 13077 99080 38383 4		( 08)
	3	-1.66059 10282 27997 89467 4		( 07)	1.21117 71647 64931 95888 2		( 08)
	4	2.37774 44786 51142 48955 9		( 06)	1.32000 94110 32992 82644 7		( 07)
	5	-7.23343 62824 52533 46646 8		( 04)	1.04469 18186 92075 89871 5		( 06)
	6	5.42029 78360 01654 65492 4		( 03)	6.06500 93218 89635 57172 5		( 04)
	7	-7.87402 38311 16328 77922 8		( 01)	2.52420 27853 26999 70863 5		( 03)
	8	2.44411 40962 76240 45913 0		( 00)	6.96419 57634 28417 04830 2		( 01)
	9	-1.57085 62593 09369 50290 0		(-02)	1.00000 00000 00000 00000 0		( 00)

3. Generation of the Approximations. The approximation forms and corresponding intervals used are

$$\begin{aligned}
 F_{lm}(x) &= xR_{lm}(x^2), & |x| \leq 2.5 \\
 (3.1) \quad &= \frac{1}{x} R_{lm}(1/x^2), & 2.5 \leq |x| \leq 3.5; 3.5 \leq |x| \leq 5.0 \\
 &= \frac{1}{2x} \left[ 1 + \frac{1}{x^2} R(1/x^2) \right], & 5.0 \leq |x|
 \end{aligned}$$

where the  $R_{lm}(z)$  are rational functions of degree  $l$  in the numerator and  $m$  in the

TABLE III.  $F(x) \approx \frac{1}{x} \left\{ \alpha_0 + \frac{\beta_0}{\alpha_1 + x^2} + \dots + \frac{\beta_{n-1}}{\alpha_n + x^2} \right\}$ ,  $2.5 \leq |x| \leq 3.5$

n	j	$\alpha_j$	$\beta_j$
1	0	4.99160 (-01)	2.51472 (-01)
	1	-1.96079 (00)	
4	0	5.00652 75443 7 (-01)	2.14221 96577 8 (-01)
	1	-4.91605 36574 1 (00)	3.73902 76351 2 (01)
	2	4.07068 10166 7 (00)	1.38216 34118 2 (01)
	3	-1.26817 90159 8 (01)	8.87619 38676 4 (01)
5	0	5.01401 06611 704 (-01)	1.88975 53014 354 (-01)
	1	-7.44990 50579 364 (00)	7.02049 80729 194 (01)
	2	7.50778 16490 106 (00)	4.18218 06337 830 (01)
	3	-2.66290 01073 842 (01)	3.73430 84728 334 (01)
	4	3.09840 87863 402 (01)	1.25993 23546 764 (03)
7	0	5.00236 89608 86678 82 (-01)	2.26064 66607 43091 60 (-01)
	1	-5.97678 08682 34888 63 (00)	1.15840 29255 18881 28 (02)
	2	1.52644 09962 36985 89 (01)	7.29177 55641 55315 00 (01)
	3	-8.89106 47974 78123 30 (00)	1.12461 66202 45754 35 (02)
	4	-7.57931 91808 93692 74 (-02)	7.21193 21760 02290 59 (00)
	5	-4.00000 89364 35497 21 (01)	1.24486 78826 22516 16 (03)
	6	2.93365 74739 54485 30 (01)	-6.73106 06974 48133 14 (-01)
8	0	4.99753 72322 38672 65701 (-01)	2.82505 12959 56025 34507 (-01)
	1	5.14905 19894 61839 18332 (00)	-1.71845 97911 60867 73018 (02)
	2	6.76056 09265 22734 73204 (00)	2.85094 29523 41035 37104 (02)
	3	5.31365 22629 36985 87395 (00)	5.71551 83515 55917 20071 (01)
	4	-1.46536 07407 01534 12337 (01)	2.09472 56189 26938 46157 (02)
	5	4.70341 81870 14092 00108 (00)	-2.57668 08798 49772 32129 (00)
	6	9.69230 82777 47642 74334 (01)	1.05565 30121 09847 04166 (04)
	7	-1.07998 24592 49835 68179 (02)	4.65888 43814 36620 82502 (-01)
9	0	5.00260 18362 20279 67838 339(-01)	2.06522 69153 96421 05009 383(-01)
	1	-1.73717 17784 36727 91148 539(01)	9.51190 92396 03814 58746 503(02)
	2	4.65842 08794 00152 95572 731(01)	1.70641 26974 52362 27356 448(02)
	3	-7.33080 08989 64028 70749 508(00)	3.02890 11061 01226 63923 423(02)
	4	4.56604 25072 51633 10121 912(00)	4.06209 74221 89356 89922 236(01)
	5	-2.27571 82952 50758 91337 450(01)	4.53642 11110 25777 27152 835(02)
	6	1.25808 70373 89512 51884 757(01)	-7.08465 68667 65730 00364 345(00)
	7	2.61935 63126 88259 92834 528(01)	1.10067 08103 45155 32890 922(03)
	8	-3.79258 97727 10428 80785 664(01)	1.82180 09331 35144 78378 375(00)
9	-1.70953 80470 08554 94930 087(00)		

denominator. Experiences with other choices of intervals and forms closely paralleled previous experiences in approximating

$$(3.2) \quad \text{Ei}(v) = - \int_{-\infty}^v \frac{e^t}{t} dt$$

[8], including the existence of "barriers" and entire counter-diagonals of cases in the Walsh array with nonstandard error curves. Aside from the form in the first interval, the final choice of forms and intervals was achieved by analogy with the  $Ei(x)$  case.

TABLE IV.  $F(x) \approx \frac{1}{x} \left( \alpha_0 + \frac{\beta_0}{\alpha_1 + x^2} + \dots + \frac{\beta_{n-1}}{\alpha_n + x^2} \right)$ ,  $3.5 \leq |x| \leq 5.0$

n	j	$\alpha_j$			$\beta_j$								
1	0	5.00221	90	(-01)	2.40464	13	(-01)						
	1	-1.99531	75	(00)									
3	0	5.00009	65199	(-01)	2.49246	32421	(-01)						
	1	-1.58539	35006	(00)	-5.37142	72981	(-01)						
	2	-1.63850	24821	(01)	1.77617	78077	(01)						
	3	-4.10832	33779	(00)									
5	0	5.00001	53840	8193	(-01)	2.49811	16284	5499	(-01)				
	1	-1.53672	6927	1915	(00)	-6.53419	35986	0764	(-01)				
	2	-1.77068	69371	7670	(01)	2.34866	41097	6332	(02)				
	3	7.49584	01627	8357	(00)	-2.29875	84192	8600	(00)				
	4	4.02187	49020	5698	(01)	2.53388	00696	3558	(03)				
	5	-5.93915	91850	0315	(01)								
7	0	4.99999	90270	50535	94	(-01)	2.50011	45961	18389	42	(-01)		
	1	-1.49838	04203	66907	23	(00)	-1.48715	81178	71947	48	(00)		
	2	-4.98544	89298	66076	69	(00)	3.30707	72467	61143	70	(01)		
	3	5.06460	15374	22307	72	(00)	1.46515	16778	31092	86	(02)		
	4	-1.50507	70349	66919	57	(01)	7.51701	27774	40669	33	(01)		
	5	-9.16804	87981	35517	10	(00)	2.56105	72234	22263	53	(01)		
	6	-2.66167	67489	63992	81	(01)	2.87776	12297	31873	57	(02)		
	7	4.76405	64527	32287	81	(00)							
8	0	5.00000	24559	63383	2639	(-01)	2.49955	21697	80615	1194	(-01)		
	1	-1.51367	66880	71179	3746	(00)	-9.52887	96162	11405	9108	(-01)		
	2	-1.64140	11434	80851	0959	(01)	2.82166	88221	34411	2618	(02)		
	3	1.25225	24765	67802	1319	(01)	2.12179	97847	65171	2123	(01)		
	4	-3.07219	08168	86247	9422	(01)	6.12148	21935	89774	4415	(02)		
	5	1.28215	21658	43074	6296	(01)	-1.19322	18919	12575	0535	(01)		
	6	4.84015	36834	58465	7257	(00)	3.42841	52809	32221	0445	(02)		
	7	-2.73122	93682	83313	8394	(01)	3.88492	00485	30068	5817	(00)		
	8	-5.44601	26093	27636	7554	(00)							
9	0	4.99999	81092	48588	24981	0	(-01)	2.50041	49236	99223	81760	6	(-01)
	1	-1.48432	34182	33439	65307	5	(00)	-2.31251	57538	51451	43070	0	(00)
	2	7.50964	45983	89196	12289	4	(00)	-6.88024	95250	45122	54535	0	(01)
	3	-3.35044	14982	05924	49071	5	(01)	1.24018	50000	99171	63022	7	(03)
	4	2.69790	58673	54676	49968	7	(01)	-9.18871	38529	32158	73406	3	(00)
	5	4.84507	26508	14914	52130	0	(01)	3.48817	75882	22863	53588	2	(03)
	6	-6.68407	24033	76967	56837	9	(01)	1.40238	37312	61493	85227	7	(01)
	7	-7.36315	66912	68305	26753	7	(00)	9.98607	19803	94520	81913	3	(01)
	8	-1.86647	12333	84938	52581	7	(01)	4.47820	90802	59717	49851	5	(01)
	9	-4.55169	50325	50948	15111	5	(00)						

With a simple change of variable in (1.1) we have

$$(3.3) \quad e^{z^2} F(z) = \int_0^{\sqrt{z}} \frac{e^y}{2\sqrt{y}} dy.$$

Comparison of (3.2) and (3.3), ignoring the difference in the lower limit of integration, indicates a similarity of the integrals involved provided  $v = \sqrt{z}$ , i.e.,  $v^2 = z$ . The approximating forms and intervals for  $Ei(x)$  were



with the aid of (2.2) and (2.3). All expansion coefficients used were derived in 40S arithmetic. The final master function routines in 25S arithmetic were extensively checked by comparing calculations based on two different methods wherever possible, and by direct comparison against calculations in 40S arithmetic. These checks indicated an accuracy of from 23S to 25S in our master routine.

#### 4. Results.

Table I lists the values of

$$\varepsilon_{im} = -100 \log_{10} \max \left| \frac{F(x) - F_{im}(x)}{F(x)} \right|,$$

where the maximum is taken over the appropriate interval, for the initial segments of the various  $L_\infty$  Walsh arrays. Tables II-V present coefficients for selected approximations along the main diagonals of these arrays. Each approximation listed, with the coefficients just as they appear here, was tested against the master function routines with 5000 pseudo-random arguments. In all cases the maximal error agreed in magnitude and location with the values given by the Remes algorithm.

In all intervals except the first the approximations were found to be slightly ill-conditioned when expressed as ratios of polynomials. For these intervals the approximations are presented here as well-conditioned  $J$ -fractions:

$$R_{nn}(1/x^2) = \alpha_0 + \frac{\beta_0}{\alpha_1 + x^2} + \cdots + \frac{\beta_{n-1}}{\alpha_n + x^2}.$$

The coefficients are all presented to an accuracy slightly greater than that warranted by the maximal errors in the approximations. Reasonable additional rounding will not seriously affect the overall accuracy of the approximations. Subroutines based on these coefficients and achieving essentially machine accuracy have been written for the CDC 3600 and the IBM System/360 at Argonne National Laboratory.

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