ma
the
ma
tisch

cen
trum

MC

AFDELING NUMERIEKE WISKUNDE NW 86/80 AUGUSTUS
(DEPARTMENT OF NUMERICAL MATHEMATICS)

H.J.J. TE RIELE

NUMERICAL SOLUTION OF TWO COUPLED NONLINEAR EQUATIONS RELATED TO THE LIMITS OF BUCHSTAB'S ITERATION SIEVE

amsterdam 1980

stichting
mathematisch
centrum

AFDELING NUMERIEKE WISKUNDE NW 86/80 AUGUSTUS
(DEPARTMENT OF NUMERICAL MATHEMATICS)

H.J.J. TE RIELE

NUMERICAL SOLUTION OF TWO COUPLED NONLINEAR EQUATIONS RELATED TO THE LIMITS OF BUCHSTAB'S ITERATION SIEVE

kruislaan 413 1098 SJ amsterdam

Printed at the Mathematical Centre, 413 Kruislaan, Amsterdam.

The Mathematical Centre, founded the 11-th of February 1946, is a non-profit institution aiming at the promotion of pure mathematics and its applications. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O.).

1980 Mathematics subject classification: 65H10, 65D30, 65Q05

Numerical solution of two coupled nonlinear equations related to the limits of Buchstab's iteration sieve

by

H.J.J. te Riele

ABSTRACT

Details are presented of numerical computations concerning the solution of two coupled nonlinear equations which arise in connection with the so-called Buchstab iteration sieve in number theory [2]. The computations involve (among others) a function which is given as an infinite range integral over an integrand which has a weak singularity in one of the endpoints, and a function which is the solution of a differential-difference equation.

KEY WORDS & PHRASES: *sieve methods, nonlinear equations, Newton's method, quadrature over an infinite range, differential-difference equation*

1. INTRODUCTION

In this report we present the details of numerical computations concerning the solution of two coupled nonlinear equations in two real unknowns α and β, where $\alpha \geq \beta$. These equations arise in connection with the so-called Buchstab iteration sieve [2] in number theory. They read as follows:

CASE 1. $\beta \leq \alpha \leq \beta+1$

(1) $$\begin{cases} \alpha \dfrac{p(\alpha)}{\sigma(\alpha)} + \kappa \displaystyle\int_{\beta-1}^{\alpha} \dfrac{p(x+1)}{\sigma(x)}\,dx = 2, \\ \alpha \dfrac{q(\alpha)}{\sigma(\alpha)} - \kappa \displaystyle\int_{\beta-1}^{\alpha} \dfrac{q(x+1)}{\sigma(x)}\,dx = 0; \end{cases}$$

CASE 2. $\alpha \geq \beta+1$

(2) $$\begin{cases} \alpha \dfrac{p(\alpha)}{\sigma(\alpha)} + \kappa \displaystyle\int_{\alpha-2}^{\alpha} \dfrac{p(x+1)}{\sigma(x)}\,dx + \kappa(\alpha-1)^{1-\kappa} p(\alpha-1) \displaystyle\int_{\beta}^{\alpha-1} \dfrac{t^{\kappa-1}}{\sigma(t-1)}\,dt = 2, \\ \alpha \dfrac{q(\alpha)}{\sigma(\alpha)} - \kappa \displaystyle\int_{\alpha-2}^{\alpha} \dfrac{q(x+1)}{\sigma(x)}\,dx - \kappa(\alpha-1)^{1-\kappa} q(\alpha-1) \displaystyle\int_{\beta}^{\alpha-1} \dfrac{t^{\kappa-1}}{\sigma(t-1)}\,dt = 0. \end{cases}$$

Here, κ is some given number in the interval $(1,2]$. The functions p and q are given by:

(3) $$p(s) = \int_0^{\infty} \exp(-sz - \kappa\psi(z))\,dz, \qquad s > 0,$$

where

$$\psi(z) = \int_0^{z} \frac{1-e^{-u}}{u}\,du;$$

(4) $$q(s) = \frac{1}{\Gamma(1-2\kappa)} \int_0^{\infty} z^{-2\kappa} \exp(-sz + \kappa\psi(z))\,dz, \qquad s > 0,$$

provided that $\kappa < \frac{1}{2}$; if $\kappa \geq \frac{1}{2}$ one should take the analytic continuation of $q(s)$ with respect to κ. The function σ is the continuous solution of the following differential-difference equation:

$$(5)\qquad \begin{cases} s^{-\kappa}\sigma(s) = A^{-1}, & \text{if } 0 < s \le 2, \\ \dfrac{d}{ds}\left(s^{-\kappa}\sigma(s)\right) = -\kappa s^{-\kappa-1}\sigma(s-2), & \text{if } s > 2, \end{cases}$$

where $A = 2^{\kappa}e^{\gamma\kappa}\Gamma(1+\kappa)$, γ the Euler constant. Note that p, q and σ depend on κ, and that (2) reduces to (1) for $\beta = \alpha-1$.

2. NUMERICAL SOLUTION OF (1) AND (2)

We have written two FORTRAN-programs for the numerical solution of (1), resp. (2), given any fixed $\kappa \in (1,2]$. We intended to compute α and β with an accuracy of at least 7D. As a partial check, we had at our disposal a small unpublished table, constructed by Diamond and Jurkat, of 4D - approximations of the solutions of (1) and (2), for $\kappa = 1.0(0.1)2.0$.

Equation (1) was solved by the Newton-method. Defining

$$g_1(\alpha,\beta) := \alpha\frac{p(\alpha)}{\sigma(\alpha)} + \kappa\int_{\beta-1}^{\alpha}\frac{p(x+1)}{\sigma(x)}\,dx - 2,$$

and

$$g_2(\alpha,\beta) := \alpha\frac{q(\alpha)}{\sigma(\alpha)} - \kappa\int_{\beta-1}^{\alpha}\frac{q(x+1)}{\sigma(x)}\,dx,$$

and assuming an initial vector $(\alpha_0,\beta_0)^T$ to be given, the Newton-iteration process reads

$$\begin{pmatrix}\alpha_{n+1}\\ \beta_{n+1}\end{pmatrix} = \begin{pmatrix}\alpha_{n}\\ \beta_{n}\end{pmatrix} - J^{-1}(\alpha_n,\beta_n)\begin{pmatrix}g_1(\alpha_n,\beta_n)\\ g_2(\alpha_n,\beta_n)\end{pmatrix}, \qquad n = 0,1,\ldots,$$

where

$$J(\alpha,\beta) = \begin{pmatrix}\dfrac{\partial g_1}{\partial\alpha} & \dfrac{\partial g_1}{\partial\beta}\\ \dfrac{\partial g_2}{\partial\alpha} & \dfrac{\partial g_2}{\partial\beta}\end{pmatrix}$$

is the Jacobian matrix of the system (1). The iteration was terminated as soon as the maximal absolute Newton-correction of $(\alpha_n,\beta_n)^T$ was $<10^{-8}$. In this process, we not only needed to compute p, q and σ, but also p', q' and σ'/σ, which occur in the Jacobian matrix. The corresponding computational details are given in Section 3.

Equation (2) is somewhat easier to solve than (1). By eliminating β, which in both equations of (2) only occurs as lower bound of the integral

$$\int_{\beta}^{\alpha-1} \frac{t^{\kappa-1}}{\sigma(t-1)}\, dt,$$

we obtain one equation with one unknown α:

$$\frac{\alpha}{\sigma(\alpha)}\{p(\alpha)q(\alpha-1)+q(\alpha)p(\alpha-1)\} + \\ + \kappa \int_{\alpha-2}^{\alpha} \{q(\alpha-1)p(x+1) - p(\alpha-1)q(x+1)\}\frac{dx}{\sigma(x)} = 2q(\alpha-1).$$

This equation was solved by the Newton-method, yielding α. Next, β was obtained from the first equation of (2), again by the Newton method.

The integrals involved in (1) and (2) were evaluated using the CLENSHAW-CURTISS method [1] as implemented in the NAG-FORTRAN library [3, SUBROUTINE DO1AAF]. The function $\sigma(s)$ occurring in these integrals has a discontinuity in one of its (higher) derivatives at the points $s = 2,4,6,\ldots,2\ell,\ldots$. Therefore, if any of these points occurred in the integration interval, the integral was split up in pieces such that these points became *endpoints* of the subintervals of integration (for example $\int_1^5 = \int_1^2 + \int_2^4 + \int_4^5$). In this way these discontinuities did not affect the desired accuracy. For the parameter "relative accuracy" in the subroutine DO1AAF we took the value 10^{-8}.

With the two programs for the solution of (1) and (2) we found (by numerical experiments) that there is one critical value κ_0 (≈ 1.8344311) in the interval (1,2] with the properties that $\alpha = \beta+1$ (≈ 4.8818986) for $\kappa = \kappa_0$, that $\alpha < \beta+1$ for $1 < \kappa < \kappa_0$ and that $\alpha > \beta+1$ for $\kappa_0 < \kappa \le 2$. Keeping this in mind we used (1) or (2) to compute α and β for $\kappa = 1.01\ (0.01) 2.00$ (Table 1), and for a few more rational values of κ which may be useful for future applications (Table 2). Several checks indicate that the absolute errors in the α's and β's never exceed the value 5.10^{-8}.

KAPPA	ALPHA	BETA	KAPPA	ALPHA	BETA
1.01	2.1652207	2.0223726	1.51	3.9413435	3.1384748
1.02	2.2400528	2.0446520	1.52	3.9711338	3.1611472
1.03	2.3006341	2.0668912	1.53	4.0008524	3.1838378
1.04	2.3540469	2.0891064	1.54	4.0305001	3.2065462
1.05	2.4029996	2.1113059	1.55	4.0600789	3.2292722
1.06	2.4488648	2.1334948	1.56	4.0895910	3.2520153
1.07	2.4924487	2.1556765	1.57	4.1190389	3.2747752
1.08	2.5342706	2.1778535	1.58	4.1484253	3.2975517
1.09	2.5746869	2.2000278	1.59	4.1777528	3.3203443
1.10	2.6139543	2.2222008	1.60	4.2070239	3.3431530
1.11	2.6522642	2.2443736	1.61	4.2362411	3.3659772
1.12	2.6897637	2.2665474	1.62	4.2654068	3.3888169
1.13	2.7265682	2.2887231	1.63	4.2945233	3.4116717
1.14	2.7627702	2.3109014	1.64	4.3235927	3.4345414
1.15	2.7984447	2.3330831	1.65	4.3526173	3.4574257
1.16	2.8336539	2.3552688	1.66	4.3815989	3.4803245
1.17	2.8684494	2.3774592	1.67	4.4105396	3.5032376
1.18	2.9028748	2.3996548	1.68	4.4394412	3.5261647
1.19	2.9369671	2.4218562	1.69	4.4683054	3.5491056
1.20	2.9707579	2.4440641	1.70	4.4971338	3.5720602
1.21	3.0042747	2.4662788	1.71	4.5259282	3.5950283
1.22	3.0375410	2.4885009	1.72	4.5546899	3.6180098
1.23	3.0705774	2.5107310	1.73	4.5834204	3.6410044
1.24	3.1034021	2.5329696	1.74	4.6121211	3.6640121
1.25	3.1360309	2.5552172	1.75	4.6407933	3.6870328
1.26	3.1684777	2.5774742	1.76	4.6694383	3.7100662
1.27	3.2007549	2.5997412	1.77	4.6980572	3.7331124
1.28	3.2328735	2.6220187	1.78	4.7266511	3.7561711
1.29	3.2648433	2.6443073	1.79	4.7552212	3.7792423
1.30	3.2966728	2.6666073	1.80	4.7837685	3.8023258
1.31	3.3283698	2.6889193	1.81	4.8122939	3.8254217
1.32	3.3599413	2.7112439	1.82	4.8407985	3.8485298
1.33	3.3913933	2.7335815	1.83	4.8692830	3.8716500
1.34	3.4227315	2.7559327	1.84	4.8977566	3.8947822
1.35	3.4539607	2.7782980	1.85	4.9262591	3.9179264
1.36	3.4850855	2.8006779	1.86	4.9547956	3.9410825
1.37	3.5161097	2.8230729	1.87	4.9833656	3.9642503
1.38	3.5470369	2.8454835	1.88	5.0119692	3.9874296
1.39	3.5778703	2.8679104	1.89	5.0406058	4.0106205
1.40	3.6086127	2.8903540	1.90	5.0692755	4.0338227
1.41	3.6392667	2.9128150	1.91	5.0979778	4.0570363
1.42	3.6698346	2.9352938	1.92	5.1267125	4.0802610
1.43	3.7003184	2.9577910	1.93	5.1554795	4.1034968
1.44	3.7307199	2.9803072	1.94	5.1842784	4.1267435
1.45	3.7610407	3.0028429	1.95	5.2131089	4.1500012
1.46	3.7912823	3.0253988	1.96	5.2419708	4.1732697
1.47	3.8214459	3.0479747	1.97	5.2708639	4.1965490
1.48	3.8515328	3.0705706	1.98	5.2997879	4.2198389
1.49	3.8815439	3.0931862	1.99	5.3287425	4.2431393
1.50	3.9114805	3.1158210	2.00	5.3577274	4.2664503

Table 1. Solutions of (1) - (2) for $\kappa = 1.01(0.01)2.00$

KAPPA	ALPHA	BETA
1.0001	2.0157572	2.0002252
1.0002	2.0223222	2.0004502
1.001	2.0503075	2.0022478
4/3	3.4018518	2.7410304
5/3	4.4008971	3.4955983
7/6	2.8568940	2.3700618
11/6	4.8787736	3.8793594
8/7	2.7730138	2.3172387
9/7	3.2511596	2.6347537
10/7	3.6959687	2.9545759
9/8	2.7082466	2.2776350
11/8	3.5315852	2.8342762

Table 2. Solutions of (1) for some rational values of κ.

3. COMPUTATIONAL DETAILS

3.1. Computation of p(s) and p'(s)

We first tried to compute p(s), as given in (3), by standard Laguerre-Gauss quadrature, i.e., with weight function exp(-z) and integrand $\exp((1-s)z-\kappa\psi(z))$. The accuracy obtained was estimated by repeating the quadrature with several different sets of quadrature abscissas and weights, and comparing the results. It turned out that even with 48 abscissas we could not obtain sufficient accuracy. Therefore, we replaced the integral $\int_0^\infty$ by $\int_0^B$, where B was chosen such that $|\int_B^\infty|$ was sufficiently small. This was achieved as follows. Since $\psi(z)=\gamma+\log z+E_1(z)$, where E_1 is the exponential integral $E_1(z) = \int_z^\infty \exp(-t)/t\,dt$, the neglected part $\int_B^\infty$ can be approximated (provided that B is not too small) by

$$\int_B^\infty \exp(-sz-\kappa\gamma-\kappa\log z)\,dz,$$

which is smaller than $\exp(-\kappa\gamma)B^{-\kappa}\exp(-Bs)/s$. In our computations we only needed values of p(s) for s > 1. With this information we chose B such that $\exp(-Bs) < 10^{-15}$, thus guaranteeing that the neglected part of the integral in p(s) was sufficiently small. The remaining finite integral $\int_0^B$ was computed by a method of PATTERSON ([4,5]) as available in the NAG-FORTRAN library ([3, SUBROUTINE D01ACF]); the relative accuracy actually used was 10^{-7}, but checks with smaller relative accuracies indicated that at least 9 correct digits were obtained. The function $\psi(z)$, occurring in p (and q) was evaluated for $z > 1$ by $\psi(z) = \gamma + \log z + E_1(z)$, with the exponential integral $E_1(z)$ taken from the NAG-FORTRAN library ([3, SUBROUTINE S13AAF]). For $0 < z \le 1$ we used the rapidly converging series expansion $\psi(z) = -\Sigma_{n=1}^{\infty} (-z)^n/(n!n)$.

The functions p, as given in (3), and p' given by

$$p'(s) = -\int_0^\infty z\exp(-sz-\kappa\psi(z))dz$$

were computed to at least 9D accuracy with the provisions described above. This could be checked in the case $\kappa = s = 1$, for which we have

$$p(1) = \int_0^\infty \exp(-z-\gamma-\log z - E_1(z))dz = e^{-\gamma}\int_0^\infty d\exp(-E_1(z)) = e^{-\gamma},$$

since $E_1(z) \to 0$ as $z \to \infty$ and $E_1(z) \sim -\log z$ as $z \to 0$. Table 3 shows a selection of values of p(s) and p'(s) for $\kappa = 1.0(0.1)2.0$.

3.2. Computation of q(s) and q'(s)

Since we wanted to solve (1) and (2) for $\kappa \in (1,2]$ we had to take the analytic continuation of q(s) (see (4)) with respect to κ. To this end, we write (4) as

$$\text{(6)}\qquad q(s) = \frac{1}{\Gamma(1-2\kappa)}\int_0^\infty z^{-2\kappa} f(s,z)dz, \qquad s > 0,\ \kappa < \frac{1}{2},$$

where

$$f(s,z) = \exp(-sz+\kappa\psi(z)).$$

This function f and its derivatives with respect to z are continuous on $[0,\infty)$ and tend to zero exponentially fast as $z \to \infty$. Therefore, integrating (6) n times by parts, we obtain

$$(7)\qquad q(s) = \frac{(-1)^n}{\Gamma(n+1-2\kappa)} \int_0^\infty z^{n-2\kappa} \frac{\partial^n}{\partial z^n} f(s,z)\,dz, \qquad s > 0,\ \kappa < \frac{1}{2}(n+1).$$

It follows that, if $n > 3$, this formula can be used for all $\kappa \in (1,2]$. To obtain some extra smoothness for the integrand in (7) near $z = 0$, we took $n = 5$. This increased the complexity of the integrand and, consequently, the cost of computing q, but experiments have shown that this also increased the accuracy which can be obtained for q. The fifth derivative of f with respect to z was computed as follows. Defining $\phi(z) := \kappa\psi(z) = \kappa(1-e^{-z})/z$, we obtain after some calculations

$$\frac{\partial^v f(s,z)}{\partial z^v} = f(s,z)\{\phi^{iv} + 5\phi'''(\phi-s) + 10\phi''(\phi-s)^2 + 10\phi'(\phi-s)^3 + $$
$$+ (\phi-s)^5 + 10\phi'\phi'' + 15(\phi')^2(\phi-s)\},$$

where $\phi^i = \phi^i(z)$. The derivatives of ϕ were computed for $z > 1$ by using the following recursion formula:

$$\phi^{i+1}(z) = \{(-1)^i e^{-z} - (i+1)\phi^i(z)\}/z, \qquad i = 0,1,2,\ldots;$$

for $0 < z \le 1$, ϕ and its derivatives were computed from their rapidly converging series expansions. Similarly as in Section 3.1 for p, we replaced the integral $\int_0^\infty$ in (7) by $\int_0^B$, where B was chosen such that the neglected part of the integral was sufficiently small. The remaining finite integral was computed with the SUBROUTINE D01ACF from the NAG-FORTRAN library. The results could be checked in the following cases:

$$q(s) = \begin{cases} s-1, & \text{if } \kappa = 1, \\ s^2 - 3s + 3/2 & \text{if } \kappa = 3/2, \\ s^3 - 6s^2 + 9s + 8/3, & \text{if } \kappa = 2. \end{cases}$$

The function $q'(s)$, given by

$$(8)\qquad q'(s) = \frac{2\kappa-1}{\Gamma(2-2\kappa)} \int_0^\infty z^{1-2\kappa} f(s,z)\,dz, \qquad s > 0,\ \kappa < 1,$$

was computed in a manner completely analogous to the computation of $q(s)$. In

Table 3 one finds a selection of values of q(s) and q'(s) for $\kappa = 1.0(0,1)2.0$.

3.3. Computation of $\sigma(s)$ and $\sigma'(s)/\sigma(s)$

In our computations we only needed values of $\sigma(s)$ for s in the interval (0, 5.5). From (5) it follows that

$$\sigma(s) = \begin{cases} A^{-1}s^{\kappa}, & \text{if } 0 < s \le 2, \\ A^{-1}s^{\kappa}(1-\kappa \int_2^s (1-\frac{2}{u})^{\kappa} \frac{du}{u}), & \text{if } 2 < s \le 4. \end{cases}$$

The integral $\int_2^s$ was computed to machine precision (about 14D) using a standard library quadrature routine, and no numerical problems occurred. In the range $4 < s \le 6$ we computed a table of $\sigma(s)$ for $s = 4+j/40$, $j = 1,2,\ldots,80$, from the differential equation in (5), using a standard fourth order Runge-Kutta method (SUBROUTINE DO2AAF from [3]). Values of $\sigma(s)$ in intermediate points were computed with five point Lagrangian interpolation. We estimate the obtained accuracy to be at least 10D.

The function $\sigma'(s)/\sigma(s)$, values of which were needed for s in the interval (2, 5.5), was computed with the following formula, which easily follows from (5):

$$\sigma'(s)/\sigma(s) = \frac{\kappa}{s}\left(1-\frac{\sigma(s-2)}{\sigma(s)}\right), \qquad \text{if } s > 2.$$

In Table 3 we give a selection of values of $\sigma(s)$ and $\sigma'(s)/\sigma(s)$ for $\kappa = 1.0(1.1)2.0$.

KAPPA = 1.0

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.1403648709		.5
1.0	.5614594836	-.3505359929	-.0000000000	1.0000000000	.2807297418		1.0
1.5	.4301784783	-.1976626886	.5000000000	1.0000000000	.4210946127		1.5
2.0	.3505359929	-.1286087744	1.0000000000	1.0000000000	.5614594836	.5000000000	2.0
2.5	.2964940329	-.0909194604	1.5000000000	1.0000000000	.6855816465	.3181046508	2.5
3.0	.2572175488	-.0679031461	2.0000000000	1.0000000000	.7814406218	.2135845284	3.0
3.5	.2272986511	-.0527465057	2.5000000000	1.0000000000	.8537959242	.1447991758	3.5
4.0	.2037094383	-.0422063366	3.0000000000	1.0000000000	.9060303346	.0950770736	4.0
4.5	.1846127699	-.0345664015	3.5000000000	1.0000000000	.9413229291	.0603739635	4.5
5.0	.1688253462	-.0288448195	4.0000000000	1.0000000000	.9643635066	.0379365008	5.0
5.5	.1555488067	-.0244450184	4.5000000000	1.0000000000	.9789728387	.0232482844	5.5
6.0	.1442240973	-.0209867296	5.0000000000	1.0000000000			6.0
6.5	.1344476010	-.0182178693	5.5000000000	1.0000000000			6.5

KAPPA = 1.1

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.1102175910		.5
1.0	.5356887523	-.3203537688	-.2463297961	.8830258587	.2362565782		1.0
1.5	.4145607516	-.1841318604	.2499138752	1.0832464873	.3690492225		1.5
2.0	.3399296764	-.1212357396	.8251443985	1.2100371320	.5064270618	.5500000000	2.0
2.5	.2887762415	-.0864160324	1.4544348577	1.3030715954	.6339250811	.3634992565	2.5
3.0	.2513313154	-.0649351900	2.1250543857	1.3769127976	.7372852371	.2491715540	3.0
3.5	.2226524593	-.0506804895	2.8293050024	1.4384036490	.8183448041	.1725521835	3.5
4.0	.1999442741	-.0407072711	3.5620299584	1.4912798477	.8791239780	.1165838431	4.0
4.5	.1814972357	-.0334426342	4.3195293376	1.5377978634	.9219423139	.0763650951	4.5
5.0	.1662031925	-.0279798592	5.0990149045	1.5794236055	.9509783831	.0494359209	5.0
5.5	.1533105252	-.0237645663	5.8983067741	1.6171630950	.9700726760	.0312817535	5.5
6.0	.1422905595	-.0204414980	6.7156513973	1.6517369020			6.0
6.5	.1327601521	-.0177740738	7.5496057681	1.6836791109			6.5

Table 3. Selected values of p, p', q, q', σ and σ'/σ.

KAPPA = 1.2

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0860213723		.5
1.0	.5119151123	-.2934831327	-.4517757023	.6004752208	.1976252178		1.0
1.5	.3999241381	-.1718103461	-.0303940054	1.0500721473	.3214784550		1.5
2.0	.3298884626	-.1144239702	.5756919677	1.3591824366	.4540235252	.6000000000	2.0
2.5	.2814169556	-.0822125886	1.3176558517	1.6003077496	.5825219008	.4091181007	2.5
3.0	.2456880274	-.0621434553	2.1693553997	1.8011513681	.6915215552	.2856867345	3.0
3.5	.2181790522	-.0487253067	3.1143651697	1.9751625141	.7801751140	.2015796494	3.5
4.0	.1963066428	-.0392816296	4.1413191870	2.1298911407	.8490479038	.1395767106	4.0
4.5	.1784786533	-.0323695436	5.2418298045	2.2700107208	.8994633068	.0939645982	4.5
5.0	.1636565392	-.0271510584	6.4094172711	2.3986245119	.9348880222	.0624758802	5.0
5.5	.1511322306	-.0231106366	7.6389019022	2.5179047509	.9589898723	.0406825246	5.5
6.0	.1404054997	-.0199161781	8.9260325876	2.6294356597			6.0
6.5	.1311124561	-.0173455279	10.2672464578	2.7344111160			6.5

KAPPA = 1.3

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0667532370		.5
1.0	.4899376581	-.2695022594	-.5827669604	.1599122332	.1643657496		1.0
1.5	.3861870981	-.1605703655	-.3153253727	.8680479613	.2784389333		1.5
2.0	.3203719668	-.1081222875	.2574940933	1.4041152938	.4047159486	.6500000000	2.0
2.5	.2743935982	-.0782849500	1.0743611952	1.8522508388	.5321295032	.4547683543	2.5
3.0	.2402739731	-.0595151782	2.1007556613	2.2459607347	.6449004645	.3228896880	3.0
3.5	.2138695803	-.0468736550	3.3140913372	2.6020690700	.7398703286	.2316470837	3.5
4.0	.1927905588	-.0379249701	4.6981965428	2.9302966200	.8161576871	.1638391295	4.0
4.5	.1755528205	-.0313442929	6.2407802645	3.2368147738	.8740173719	.1130041687	4.5
5.0	.1611823448	-.0263565325	7.9320980902	3.5258149497	.9160543070	.0769605017	5.0
5.5	.1490116646	-.0224819356	9.7641787712	3.8002914665	.9455839942	.0514213759	5.5
6.0	.1385672044	-.0194098569	11.7303425548	4.0624690180			6.0
6.5	.1295031885	-.0169315716	13.8248841802	4.3140529765			6.5

Table 3. Continued

KAPPA = 1.4

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0515206099		.5
1.0	.4695792585	-.2480488996	-.6070361687	-.3993142535	.1359637047		1.0
1.5	.3732761826	-.1502993200	-.5695819419	.5171595176	.2398560914		1.5
2.0	.3113432878	-.1022848155	-.1117855615	1.2984618629	.3588103679	.7000000000	2.0
2.5	.2676853236	-.0746111698	.7168371809	2.0065252269	.4833708683	.5003117907	2.5
3.0	.2350763901	-.0570386611	1.8868842503	2.6670906230	.5981161557	.3605840467	3.0
3.5	.2097157529	-.0451187902	3.3782701392	3.2935429883	.6980271392	.2625519967	3.5
4.0	.1893903852	-.0366331638	5.1760844063	3.8938507438	.7808681756	.1891743540	4.0
4.5	.1727157621	-.0303642313	7.2686374310	4.4732070906	.8458142436	.1333155147	4.5
5.0	.1587777209	-.0255945125	9.6464065804	5.0352223720	.8945123152	.0927778447	5.0
5.5	.1469466756	-.0218772441	12.3014120964	5.5825306117	.9297698396	.0634447887	5.5
6.0	.1367740364	-.0189216711	15.2268208768	6.1171266203			6.0
6.5	.1279310807	-.0165315791	18.4166810894	6.6405666126			6.5

KAPPA = 1.5

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0395595594		.5
1.0	.4506834075	-.2288112938	-.5000000000	-1.0000000000	.1118913309		1.0
1.5	.3611251238	-.1408978232	-.7500000000	-.0000000000	.2055575005		1.5
2.0	.3027686651	-.0968703751	-.5000000000	1.0000000000	.3164764753	.7500000000	2.0
2.5	.2612728645	-.0711713057	.2500000000	2.0000000000	.4367377179	.5456521966	2.5
3.0	.2300833885	-.0547031732	1.5000000000	3.0000000000	.5517900252	.3986105894	3.0
3.5	.2057097976	-.0434544782	3.2500000000	4.0000000000	.6552323658	.2941213064	3.5
4.0	.1861008092	-.0354023701	5.5000000000	5.0000000000	.7436324464	.2154068047	4.0
4.5	.1699637151	-.0294268803	8.2500000000	6.0000000000	.8151283970	.1547366364	4.5
5.0	.1564399232	-.0248633369	11.5000000000	7.0000000000	.8703656977	.1098075234	5.0
5.5	.1449352127	-.0212954125	15.2500000000	8.0000000000	.9115196799	.0766813287	5.5
6.0	.1350244307	-.0184508035	19.5000000000	9.0000000000			6.0
6.5	.1263949169	-.0161449562	24.2500000000	10.0000000000			6.5

Table 3. Continued

KAPPA = 1.6

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0302267524		.5
1.0	.4331115280	-.2115205584	-.2527189028	-1.5263025888	.0916303788		1.0
1.5	.3496740377	-.1322780055	-.8099226422	-.6471901437	.1753014451		1.5
2.0	.2946171720	-.0918419545	-.8591695294	.4813660627	.2777713662	.8000000000	2.0
2.5	.2551383943	-.0679472157	-.3030197688	1.7645760966	.3925986811	.5907254546	2.5
3.0	.2252838826	-.0524988615	.9238961515	3.1592926344	.5064610327	.4368411411	3.0
3.5	.2018444225	-.0418749519	2.8707825637	4.6413424756	.6120443908	.3262082310	3.5
4.0	.1829168212	-.0342290141	5.5772126320	6.1953879989	.7049223665	.2423818682	4.0
4.5	.1672931157	-.0285299205	9.0763932036	7.8108611189	.7822844360	.1771158018	4.5
5.0	.1541663431	-.0241614439	13.3970152608	9.4800427830	.8437795073	.1279266810	5.0
5.5	.1429753199	-.0207353561	18.5643994474	11.1970458846	.8908627840	.0910474730	5.5
6.0	.1333168908	-.0179964806	24.6012529776	12.9572289825			6.0
6.5	.1248935316	-.0157711386	31.5281954415	14.7568355451			6.5

KAPPA = 1.7

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0229878929		.5
1.0	.4167406598	-.1959442920	.1194641569	-1.8315414214	.0746878843		1.0
1.5	.3388687246	-.1243620511	-.7066537155	-1.3447628356	.1488008109		1.5
2.0	.2868604434	-.0871662427	-1.1265684301	-.2559250124	.2426616521	.8500000000	2.0
2.5	.2492654023	-.0649223784	-.8955803838	1.2377897284	.3512107075	.6354917694	2.5
3.0	.2206675269	-.0504166703	.1627928684	3.0421199791	.4625814376	.4751732970	3.0
3.5	.1981127809	-.0403748718	2.1890474056	5.1020877257	.5689790361	.3586890792	3.5
4.0	.1798336939	-.0331097659	5.3014146619	7.3815940712	.6652113836	.2699647665	4.0
4.5	.1647005871	-.0276711805	9.6029257965	9.8550133092	.7476423126	.2003137708	4.5
5.0	.1519544997	-.0234873649	15.1855211899	12.5031289002	.8149712193	.1470144257	5.0
5.5	.1410651314	-.0201960510	22.1326540263	15.3109359843	.8678825928	.1064526157	5.5
6.0	.1316499850	-.0175579700	30.5210468783	18.2663506055			6.0
6.5	.1234258072	-.0154095906	40.4219353768	21.3594016497			6.5

Table 3. Continued

KAPPA = 1.8

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0174045983		.5
1.0	.4014614735	-.1818811978	.5692400134	-1.7577806094	.0606063313		1.0
1.5	.3286600539	-.1170809360	-.4121458522	-1.9644495293	.1257425496		1.5
2.0	.2794724315	-.0828132207	-1.2295403445	-1.1653261062	.2110435035	.9000000000	2.0
2.5	.2436385818	-.0620817309	-1.4538653401	.3791029877	.3127323238	.6799295954	2.5
3.0	.2162246592	-.0484482693	-.7483444103	2.5376500863	.4205168392	.5135259390	3.0
3.5	.1945084404	-.0389492906	1.1726943008	5.2304556098	.5264995956	.3914601746	3.5
4.0	.1768469640	-.0320415218	4.5620143202	8.4031455504	.6249599109	.2980389303	4.0
4.5	.1621829274	-.0268486261	9.6491328812	12.0158891630	.7115831066	.2242047508	4.5
5.0	.1498020324	-.0228397183	16.6460948569	16.0379809864	.7842006426	.1669549374	5.0
5.5	.1392028663	-.0196765301	25.7512194133	20.4448482544	.8427119775	.1228031538	5.5
6.0	.1300223430	-.0171345774	37.1516828292	25.2162588835			6.0
6.5	.1219906714	-.0150598029	51.0253833112	30.3351796553			6.5

KAPPA = 1.9

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0131210344		.5
1.0	.3871765610	-.1691565518	1.0130470241	-1.1693449378	.0489694318		1.0
1.5	.3190034218	-.1103733356	.0736382652	-2.3330463893	.1058031157		1.5
2.0	.2724291877	-.0787558008	-1.0953090840	-2.1395863140	.1827603817	.9500000000	2.0
2.5	.2382437279	-.0594115261	-1.8767600119	-.8080640307	.2772376451	.7240309089	2.5
3.0	.2119462477	-.0465859882	-1.7333655008	1.5447993792	.3805495114	.5518354663	3.0
3.5	.1910253529	-.0375936203	-.1742505610	4.8446098176	.4850105910	.4244350338	3.5
4.0	.1739524145	-.0310213864	3.2602247835	9.0387135422	.5846034622	.3265041615	4.0
4.5	.1597370993	-.0260603504	9.0068209857	14.0872323568	.6744959096	.2486764780	4.5
5.0	.1477066941	-.0222172033	17.4845536129	19.9585149486	.7517593481	.1876394864	5.0
5.5	.1373868243	-.0191758799	29.0981087950	26.6265690506	.8155270436	.1400056709	5.5
6.0	.1284326532	-.0167256450	44.2402507690	34.0694930907			6.0
6.5	.1205870953	-.0147212913	63.2935957150	42.2684586517			6.5

<u>Table 3.</u> Continued

KAPPA = 2.0

S	P(S)	P'(S)	Q(S)	Q'(S)	SIG(S)	SIG'(S)/SIG(S)	S
0.0					0.0000000000		0.0
.5					.0098511485		.5
1.0	.3737989601	-.1576183758	1.3333333333	.0000000000	.0394045940		1.0
1.5	.3098582741	-.1041846786	.7083333333	-2.2500000000	.0886603364		1.5
2.0	.2657086680	-.0749695092	-.6666666667	-3.0000000000	.1576183758	1.0000000000	2.0
2.5	.2330676460	-.0568992041	-2.0416666667	-2.2500000000	.2447303327	.7677975398	2.5
3.0	.2078238432	-.0448227584	-2.6666666667	.0000000000	.3428841203	.5900526512	3.0
3.5	.1876578281	-.0363036035	-1.7916666667	3.7500000000	.4448547430	.4575418473	3.5
4.0	.1711460591	-.0300466576	1.3333333333	9.0000000000	.5445435200	.3552747668	4.0
4.5	.1573602202	-.0253045649	7.4583333333	15.7500000000	.6367661948	.2736297284	4.5
5.0	.1456663447	-.0216185948	17.3333333333	24.0000000000	.7179601481	.2089676029	5.0
5.5	.1356153811	-.0186932366	31.7083333333	33.7500000000	.7865399401	.1579692985	5.5
6.0	.1268796593	-.0163305489	51.3333333333	45.0000000000			6.0
6.5	.1192140912	-.0143935956	76.9583333333	57.7500000000			6.5

Table 3. Continued

ACKNOWLEDGEMENTS

I want to acknowledge the expert advice by Jan van de Lune and Nico Temme concerning some crucial points in this research.

REFERENCES

[1] CLENSHAW, C.W. & A.R. CURTIS, *A method for numerical integration on an automatic computer,* Numer. Math. 2 (1960), pp. 197-205.

[2] IWANIEC, H., J. VAN DE LUNE & H.J.J. TE RIELE, *The limits of Buchstab's iteration sieve,* Proc. Kon. Ned. Akad. Wetensch. A83 (1980), pp. - .

[3] NAG Library Manual, *Numerical Algorithms Group,* Oxford, 1974.

[4] PATTERSON, T.N.L., *The optimum addition of points to quadrature,* Math. Comp. 22 (1968), pp. 847-856.

[5] PATTERSON, T.N.L., *On some Gauss and Lobatto based integration formulae,* Math. Comp. 22 (1968), pp. 877-881.