## Analysis of a constrained initial value for an ODE arising in the study of a power-flow model

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#### Abstract.

We consider in this work the ODE  $f''(t) = k/f(t), t \ge 0$ , with initial values f(0) = 1, f'(0) = w, where w = w(k) should be such that f(1) = 1 + k. Here k is an arbitrary positive real number. This initial value problem arises in the analysis of a particular model (Distflow model) for charging electric vehicles when one passes from the intrinsic discrete setting of separate charging stations to an analytically more tractable continuous setting. The mathematical challenge is to show existence and uniqueness of w = w(k) for any k > 0, and to analyze, bound, approximate and compute w(k) as a function of k. In the context of the study of the Distflow model, several results have been presented in a somewhat scattered way, with particular attention for small k > 0. In the present work, the results for w(k) are developed more systematically, where k is also allowed to be large positive.

#### 1 Introduction

The Distflow model is a particular model for charging electric vehicles at N+1 charging stations located along a power line, with the requirement that the ratio between the voltages at the root station (with index N) and the last station (with index 0) at the power line should stay below a level  $1/(1 - \Delta)$  with tolerance  $\Delta$  small (typically of the order 0.1). A full description of the Distflow model, including a comparison with a linearized version of it, appears in [1], Subsections 2.3.1–2. Under the Distflow model, the normalized voltages  $V_n$ , n = 0, 1, ..., N - 1, N, with  $V_N$  the voltage at the root station and  $V_0$  the voltage at the last station, satisfy a recursion

$$V_0 = 1$$
,  $V_1 = 1 + k_0$ ;  $V_{n+1} - 2V_n + V_{n-1} = \frac{k_n}{V_n}$ ,  $n = 1, ..., N - 1$ , (1)

see [1], (2.16–18). The  $k_n$ , comprising given charging rates  $p_n$  and resistance/reactance values r and x as well as the arrival rate  $\lambda$  of the vehicles at the stations, are normally small (of the order  $a/N^2$  with 0 < a < 0.1).

For analytically comparing the Distflow model to its linearized version, it is assumed that all  $k_n$  are equal to a particular  $k = a/N^2$ . A key step in [1] is then to establish a relationship between the sequence  $V_n$ , n = 0, 1, ..., N, and the solution  $f_0(t)$ ,  $t \ge 0$ , of the second-order boundary value problem

$$f_0''(t) = \frac{1}{f_0(t)}, \quad t \ge 0; \qquad f_0(0) = 1, \quad f_0'(0) = 0.$$
 (2)

In particular, it is shown in [1], Section 5.4 that  $V_n - f_0(\frac{n}{N}\sqrt{a}) \to 0$ , n = 0, 1, ..., N as  $N \to \infty$  with  $k_n = k = a/N^2$  and a > 0 fixed. In [2], this convergence result is refined by considering appropriately sampledand-shifted versions  $f_0(\frac{N+\beta}{N}\sqrt{a})$  of  $f_0$ , so that the initial conditions  $V_0 = 1$ ,  $V_0 = 1 + k$  can be accommodated more accurately. In [3], the solution f of the initial value problem

$$f''(t) = \frac{k}{f(t)}, \quad t \ge 0; \qquad f(0) = 1, \quad f'(0) = w,$$
 (3)

with w such that f(1) = 1 + k, is compared to the  $V_n$ , n = 0, 1, ..., in (1) with  $k_0 = k_n = k$ , n = 1, 2, ..., with respect to the asymptotic behaviour as  $t \to \infty$ ,  $n \to \infty$ . (In [3], Section 1, the ODE f''(t) = k/f(t),  $t \ge 0$ , is placed in the more general context of Emden-Fowler equations.) It is shown in [3] that

$$\frac{f(t)}{t(2k\ln t)^{1/2}} \to 1, \quad t \to \infty; \qquad \frac{V_n}{n(2k\ln n)^{1/2}} \to 1, \quad n \to \infty.$$
(4)

Furthermore in [3], there are presented various results on comparing the f of (3) and  $g(t) = t(2k \ln t)^{1/2}$ ,  $t \ge 1$ .

In the present work, we collect and extend the results that appear in [1] and [3] on the solution f of the initial value problem in (3), with focus on the constraint that f'(0) = w should be such that f(1) = 1 + k. Here we shall also consider large k > 0, that are excluded in the Distflow model for natural and practical reasons. Many of the results that we establish also hold when the condition f(1) = 1 + k is replaced by  $f(1) = 1 + k\alpha$  with  $\alpha \ge 1/2$ , and we shall sometimes present details for this.

#### 2 Overview of results

We consider the solution of the initial value problem in (3). In Section 3, we present the three following representations of the function f(t). We have for  $t \ge 0$ 

$$\int_{1}^{f(t)} \frac{ds}{(w^2 + 2k\ln s)^{1/2}} = t , \qquad (5)$$

$$(W^2 {+} {\ln f(t)})^{1/2}$$

$$\int_{W} e^{v^2} dv = t e^{W^2} \sqrt{\frac{1}{2}k} , \qquad W = \frac{w}{\sqrt{2k}} , \qquad (6)$$

$$f(t) = c f_0(a + bt) ,$$
 (7)

where  $f_0$  in (7) is the solution of the second-order boundary value problem in (2), and

$$a = \sqrt{2} \int_{0}^{W} e^{v^{2}} dv , \qquad b = \sqrt{k} e^{W^{2}} , \qquad c = e^{-W^{2}} , \qquad (8)$$

with  $W = w/\sqrt{2k}$  as in (6).

The function  $f_0$  can be expressed in terms of the inverse of the imaginary error function. That is, we have for  $t \ge 0$ 

$$f_0(t) = \exp(U^2(t)) , \qquad \int_0^{U(t)} e^{v^2} dv = t/\sqrt{2} . \qquad (9)$$

Hence, with  $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} \exp(-s^2) ds$  the standard error function,

$$U(t) = \frac{1}{i} \operatorname{erf}^{-1} \left( it \sqrt{\frac{2}{\pi}} \right) \,. \tag{10}$$

In Section 4, we present the condition f(1) = 1 + k in the form

$$\int_{1}^{1+k} \frac{ds}{(w^2 + 2k\ln s)^{1/2}} = 1 , \qquad (11)$$

and we show existence and uniqueness of w > 0 such that (11) holds. In fact, we show this for the more general problem where we require  $f(1) = 1 + k\alpha$  with  $\alpha \ge 1/2$ . We also show that w satisfies (11) if and only if

$$\int_{W}^{V} e^{v^2} dv = e^{W^2} \sqrt{\frac{1}{2}k} , \quad W = \frac{w}{\sqrt{2k}} , \quad V = (W^2 + \ln(1+k))^{1/2} .$$
(12)

We furthermore show that the solution w = w(k) of (11) can be expressed in terms of f(t) in (3) according to

$$\frac{w}{k} = 1 - \int_{0}^{1} \left( \int_{0}^{t} \frac{ds}{f(s)} \right) dt , \qquad (13)$$

where we should realize that the f(s) at the right-hand side of (13) comprises both k and w implicitly.

In Section 5, we prove monotonicity properties of both w = w(k) and of f(t) = f(t; k),  $f'(t) = \frac{d}{dt} f(t; k)$  for fixed  $t \ge 0$  as a function of k > 0. In particular, it is shown that w(k)/k strictly increases in  $k \ge 0$ . We do this for the more general problem where we require  $f(1) = 1 + k\alpha$  with  $\alpha \ge 1/2$ .

In Section 6, we present a method to compute the coefficients  $c_k$  of the power series  $\sum_{j=0}^{\infty} c_j k^j$  of w(k). We thus find

$$w(k) = \frac{1}{2}k + \frac{1}{8}k^2 - \frac{7}{180}k^3 + \frac{1667}{120960}k^4 - \frac{10621}{1814400}k^5 + \dots$$
(14)

In Section 7, we present several inequalities for w = w(k). From  $f(s) \ge 1$ ,  $s \in [0,1]$ , it is readily obtained from (13) that  $\frac{1}{2}k < w(k) < k$ . Next, by convexity of f(s),  $0 \le s \le 1$  and f'(0) = w, f(1) = 1 + k, we have 1 + ws < f(s) < 1 + ks, 0 < s < 1. Inserting this into (13), and evaluating the integrals that show up in closed form, we get for w = w(k)

$$k(1+w^{-1})(1-w^{-1}\ln(1+w)) < w < k(1+k^{-1})(1-k^{-1}\ln(1+k)) =: w_U(k) .$$
(15)

We shall show that the mapping

$$w \in \left[\frac{1}{2}k, k\right] \mapsto k(1+w^{-1})(1-w^{-1}\ln(1+w)) =: \varphi_k(w)$$
(16)

is a strictly increasing contraction of  $[\frac{1}{2}k, k]$ . Starting from a lower bound  $w^{(0)}$  of w(k), for instance  $w^{(0)} = \frac{1}{2}k$ , the iterands  $w^{(n+1)} = \varphi_k(w^{(n)})$ , n = 0, 1, ..., form a sequence of lower bounds of w(k) that converges to the unique fixed point  $w_L = w_L(k)$  of  $\varphi_k$ . Thus, with  $w_U$  given in (15), we have  $w_L < w < w_U$ . It appears that  $w_L$  and  $w_U$  are tight bounds of w = w(k). It has been found numerically that  $0 < w_U - w_L < 0.20$  for all k > 0. Furthermore, we show rigourously that

$$w_U - w_L = \frac{1}{12}k^2 + O(k^3) , \qquad k \downarrow 0 , \qquad (17)$$

$$k - \ln(1+k) < w_L < w < w_U < k + 1 - \ln(1+k) , \qquad (18)$$

$$w_U - w_L = O\left(\frac{\ln^2 k}{k}\right), \qquad k \to \infty.$$
 (19)

It also appears, numerically, that  $\frac{1}{2}(w_U + w_L)$  is a very good approximation of w (absolute error of the order 0.002, all k > 0).

In Section 8, we present a Newton method to compute w for small to moderately large k. This is based on (12) that we write as the equation

$$e^{-W^2} \int_{W}^{V} e^{v^2} dv - \sqrt{\frac{1}{2}k} = 0$$
,  $V = (W^2 + \ln(1+k))^{1/2}$ , (20)

from which  $W = w/\sqrt{2k}$  is to be solved.

In Section 9, we present a numerial method to compute w that is based on the equation (11) that we write in the form

$$y \int_{1}^{1+k} \frac{1/k}{(1+y^2 \ln s)^{1/2}} \, ds = u \; ; \qquad y = \frac{\sqrt{2k}}{w} = \frac{1}{W} \, , \quad u = \sqrt{\frac{2}{k}} \; . \tag{21}$$

For small values of y, we can expand  $(1 + y^2 \ln s)^{-1/2}$  in powers of  $y^2 \ln s$ ,  $s \in [1, 1 + k]$ . Upon interchanging series and integral in (21), we arrive at the equation

$$y \sum_{n=0}^{\infty} A_n y^{2n} = u ; \qquad y = \frac{\sqrt{2k}}{w}, \quad u = \sqrt{\frac{2}{k}} .$$
 (22)

Here  $A_0 = 1$  and the  $A_n$ , n = 1, 2, ..., can be computed recursively. This approach turns out to be feasible from values of k = 7 onwards.

From (22) there emerge two methods to compute w via  $y = \frac{\sqrt{2k}}{w}$ . A direct method is based on successive substitution in (22), starting with  $y^{(0)} = u$ ,

where the series in (22) is truncated at sufficiently large N. The second method is based on Bürmann-Lagrange inversion for which we write the equation in (22) as

$$y F(y) = u$$
,  $w = k F(y)$ , (23)

with  $F(y) = \sum_{n=0}^{\infty} A_n y^{2n}$ . This yields an expansion

$$\frac{w}{k} = 1 + \sum_{r=1}^{\infty} B_r \, u^{2r} \,, \tag{24}$$

where the  $B_r$  can be expressed explicitly in terms of  $A_1, A_2, ..., A_r$ .

In Section 10, we present results of numerical computations. Thus we show tables comprising w and the lower and upper bound  $w_L$  and  $w_U$  for wfor various values of k. The computation of  $w_L$  is done by iteration of the function  $\varphi_k$  in (16) while  $w_U$  can be computed directly, see (15). For the computation of w = w(k), we vary between the Newton method described in Section 10 (small to moderately large k) and the iteration method via yfor solving (22) (larger values of k). A special role is played here by the Bürmann-Lagrange (BL) approach embodied by (23). It appears that the BL-method produces surprisingly good results for all k, no matter how small or large. At the moment, we are just at the beginning of understanding why this is so.

#### **3** Representations of f

Let k > 0 be fixed, and consider for  $w \ge 0$  the solution f of

$$f(t) f''(t) = k, \quad t \ge 0; \qquad f(0) = 1, \quad f'(0) = w.$$
 (25)

From basic theory of ordinary differential equations, it follows that f(t) exists for all  $t \ge 0$  as a positive, increasing and convex function. From (25) we get for any t > 0

$$f'(u) f''(u) = k f'(u) / f(u) , \qquad 0 \le u \le t .$$
 (26)

Integrating (26) over u from 0 to t, using f(0) = 1 and f'(0) = w, we get for  $t \ge 0$ 

$$\frac{1}{2} (f'(t))^2 - \frac{1}{2} w^2 = k \ln f(t) , \qquad f'(t) = (w^2 + 2k \ln f(t))^{1/2} , \qquad (27)$$

and so

$$\frac{f'(u)}{(w^2 + 2k\ln f(u))^{1/2}} = 1 , \qquad 0 \le u \le t .$$
(28)

Integrating (28) over u from 0 to t and substituting  $s = f(u) \in [1, f(t)]$ , we get

$$\int_{1}^{f(t)} \frac{ds}{(w^2 + 2k\ln s)^{1/2}} = t , \qquad t \ge 0 , \qquad (29)$$

and this is (5).

We next substitute for t > 0 in the integral in (29)

$$v = (W^2 + \ln s)^{1/2} \in [W, (W^2 + \ln f(t))^{1/2}], \qquad 1 \le s \le f(t), \qquad (30)$$

where  $W = w/\sqrt{2k}$ , so that

$$s = e^{-W^2} e^{v^2}$$
,  $ds = e^{-W^2} 2v e^{v^2} dv$ . (31)

We then get

$$t = \int_{1}^{f(t)} \frac{ds}{(w^2 + 2k \ln s)^{1/2}} = \int_{W}^{(W^2 + \ln f(t))^{1/2}} \frac{e^{-W^2} 2v e^{v^2}}{v \sqrt{2k}} dv$$
$$= \sqrt{\frac{2}{k}} e^{-W^2} \int_{W}^{(W^2 + \ln f(t))^{1/2}} e^{v^2} dv , \qquad (32)$$

and this gives (6).

Next, we write (32) as

$$\int_{0}^{(W^{2}+\ln f(t))^{1/2}} e^{v^{2}} dv = \int_{0}^{W} e^{v^{2}} dv + t \sqrt{\frac{k}{2}} e^{W^{2}}$$
$$= \frac{1}{\sqrt{2}} \left( \sqrt{2} \int_{0}^{W} e^{v^{2}} dv + \sqrt{k} e^{W^{2}} t \right) .$$
(33)

With

$$a = \sqrt{2} \int_{0}^{W} e^{v^2} dv , \qquad b = e^{W^2} \sqrt{k} , \qquad c = e^{-W^2}$$
(34)

as in (8), we then get

$$\int_{0}^{(\ln(f(t)/c))^{1/2}} e^{v^2} dv = \frac{1}{\sqrt{2}} \left(a + bt\right) \,. \tag{35}$$

Define U(x) for  $x \ge 0$  implicitly by

$$\int_{0}^{U(x)} e^{v^2} dv = x/\sqrt{2} .$$
(36)

Then it follows from (35) that

$$(\ln(f(t)/c))^{1/2} = U(a+bt) , \qquad f(t) = c \exp(U^2(a+bt)) .$$
 (37)

Finally, let

$$g(x) := \exp(U^2(x)) , \qquad x \ge 0 .$$
 (38)

We shall show that

$$g''(x) = \frac{1}{g(x)}, \quad x \ge 0; \qquad g(0) = 1, \quad g'(0) = 0,$$
 (39)

i.e., that  $g = f_0$  with  $f_0$  defined in (2). That g(0) = 1 follows from U(0) = 0, see (36). From (36), we also get

$$U'(x) \exp(U^2(x)) = 1/\sqrt{2} , \qquad x \ge 0 .$$
 (40)

From (40) we get, using the definition of g in (38)

$$g'(x) = 2U(x) U'(x) \exp(U^2(x)) = \sqrt{2} U(x) , \qquad x \ge 0 .$$
 (41)

Therefore g'(0) = 0 as U(0) = 0, while we get from (41) and (40)

$$g''(x) = \sqrt{2} U'(x) = \exp(-U^2(x)) = \frac{1}{g(x)}, \qquad x \ge 0.$$
 (42)

This establishes (39), and we get (7) from (34) and (37).

The standard error function erf is defined by

$$\operatorname{erf}(z) = \frac{2}{\sqrt{\pi}} \int_{0}^{z} e^{-w^{2}} dw , \qquad z \in \mathbb{C} .$$
 (43)

We have for U > 0

$$\int_{0}^{U} e^{v^{2}} dv = \frac{\sqrt{\pi}}{2i} \operatorname{erf}(i U) .$$
 (44)

Therefore, by (36)

$$\operatorname{erf}(iU(x)) = ix\sqrt{\frac{2}{\pi}}, \qquad x \ge 0,$$
(45)

so that

$$U(x) = \frac{1}{i} \operatorname{inverf}\left(ix \sqrt{\frac{2}{\pi}}\right), \qquad x \ge 0, \qquad (46)$$

where inverf =  $erf^{-1}$  is the inverse of the error function.

The function inverf is analytic in the whole complex plane, with the exception of the two branch cuts  $(-\infty, -1]$  and  $[1, \infty)$ . Hence U(x) and  $f_0(x) = \exp(U^2(x))$  are analytic in the whole complex plane with the exception of the two branch cuts  $(-i\infty, -i\sqrt{\frac{\pi}{2}}]$  and  $[i\sqrt{\frac{\pi}{2}}, i\infty)$ . As a consequence,  $f_0(x)$  has a power series

$$f_0(x) = \sum_{l=0}^{\infty} c_l x^l , \qquad (47)$$

with radius of convergence  $\sqrt{\frac{\pi}{2}}$ , and below we shall identify the  $c_l$  in terms of the sequence A002067 from the On-line Encyclopedia of Integer Sequences [4].

From  $f_0(0) = 1$ , f'(0) = 0, f''(x)f(x) = 1, it can be shown that

$$c_0 = 1, \ c_1 = 0, \ c_2 = \frac{1}{2}; \ c_{l+2} = -\sum_{j=0}^{l-1} \frac{(j+2)(j+1)}{(l+2)(l+1)} c_{j+2} c_{l-j}, \ l = 1, 2, \dots$$
  
(48)

Next, it can be shown by induction that

$$c_{2m+1} = 0, \quad m = 0, 1, \dots; \qquad c_{4i+4} < 0 < c_{4i+2}, \quad i = 0, 1, \dots.$$
 (49)

Letting  $d_m = c_{2m}$ , the recursion in (48) can be written as

$$d_0 = 1, \ d_1 = \frac{1}{2}; \ d_{m+1} = -\sum_{r=0}^{m-1} \frac{(2k+2)(2k+1)}{(2m+2)(2m+1)} d_{r+1} d_{m-r}, \ r = 1, 2, \dots$$
(50)

When we finally write

$$d_m = \frac{b_m}{(2m)!}$$
,  $m = 1, 2, ...,$  (51)

it can be shown that

$$b_1 = 1, \quad b_2 = -1; \qquad b_{m+1} = -\sum_{r=0}^{m-1} {\binom{2m}{2r}} b_{r+1} b_{m-r}, \quad m = 1, 2, \dots.$$
 (52)

As a consequence, we have

$$f_0(x) = 1 + \sum_{m=1}^{\infty} d_m x^{2m} = 1 + \sum_{m=1}^{\infty} \frac{b_m}{(2m)!} x^{2m}$$
$$= 1 + \frac{1}{2!} x^2 - \frac{1}{4!} x^4 + \frac{7}{6!} x^6 - \frac{127}{8!} x^8 + \frac{4369}{10!} x^{10} - \frac{243649}{12!} x^{12} + \dots$$
(53)

Entering the integer sequence 1, 1, 7, 127, 4369, OEIS comes up with the sequence A002067. For the matter of the power series coefficients of  $f_0(x)$  and inverf(z), also see [2], Section 2, [5] and [6].

## 4 Representations of w constrained such that f(1) = 1 + k

When we take t = 1 in (29), the condition f(1) = 1 + k yields the equation

$$\int_{1}^{1+k} \frac{ds}{(w^2 + 2k \ln s)^{1/2}} = 1 .$$
 (54)

We shall show that for any k > 0, there is a unique w > 0 such that (54) holds. More generally, we shall show that for any k > 0 and any  $\alpha \ge 1/2$ , there is a unique w > 0 such that  $f(1) = 1 + k\alpha$ . In this more general case, we have the equation

$$\int_{1}^{1+k\alpha} \frac{ds}{(w^2 + 2k \ln s)^{1/2}} = 1$$
(55)

for w.

The left-hand side of (55) is a continuous, strictly decreasing function of  $w \ge 0$ , with limit equal to 0 as  $w \to \infty$ . It is therefore sufficient to show that for  $\alpha \ge 1/2$ 

$$F(k) := \int_{1}^{1+k\alpha} \frac{ds}{(\ln s)^{1/2}} > \sqrt{2k} , \qquad k > 0 .$$
 (56)

We have F(0) = 0, and

$$F'(k) = \frac{\alpha}{(\ln(1+k\alpha))^{1/2}} , \qquad k > 0 .$$
(57)

Since  $0 < \ln(1 + k\alpha) < k\alpha$  for k > 0, we have  $F'(k) > (\alpha/k)^{1/2}$ , k > 0. Hence, for any k > 0

$$F(k) = F(0) + \int_{0}^{k} F'(k_1) \, dk_1 > \int_{0}^{k} (\alpha/k_1)^{1/2} \, dk_1 = \alpha^{1/2} \, 2\sqrt{k} \ge \sqrt{2k} \quad (58)$$

when  $\alpha \geq 1/2$  and this gives (56).

Next, from the representation (6) of f with t = 1, we have f(1) = 1 + k if and only if w satisfies

$$\int_{W}^{V} e^{v^2} dv = e^{W^2} \sqrt{\frac{1}{2}k} , \qquad W = \frac{w}{\sqrt{2k}} , \quad V = (W^2 + \ln(1+k))^{1/2} .$$
(59)

This is (12).

Finally, from f(0) = 1, f'(0) = w, f''(s) = k/f(s),  $s \ge 0$ , we get

$$f(u) = 1 + wu + \int_{0}^{u} \left( \int_{0}^{t} \frac{k \, ds}{f(s)} \right) \, dt \, , \qquad u \ge 0 \; . \tag{60}$$

Taking u = 1 and using f(1) = 1 + k, we get

$$\frac{w}{k} = 1 - \int_{0}^{1} \left( \int_{0}^{t} \frac{ds}{f(s)} \right) dt , \qquad (61)$$

and this is (13).

# 5 Monotonicity properties of w and f as functions of k

We let  $\alpha \ge 1/2$  be fixed, and we let w > 0 be such that f(0) = 1, f'(0) = w, f''(t) = k/f(t),  $t \ge 0$ , while w is such that  $f(1) = 1 + k\alpha$ . We shall show that both w and f(t), f'(t) (with t fixed) are increasing functions of k.

We first show that w increases as a function of k, and for this we use that w = w(k) is such that (55) holds. By differentiating this identity (55), it follows that

$$0 = \frac{d}{dk} \left[ \int_{1}^{1+k\alpha} \frac{ds}{(w^{2}(k) + 2k \ln s)^{1/2}} \right]$$
$$= \frac{\alpha}{(w^{2}(k) + 2k \ln(1+k\alpha))^{1/2}} + \int_{1}^{1+k\alpha} \frac{d}{dk} \left[ \frac{1}{(w^{2}(k) + 2k \ln s)^{1/2}} \right] ds$$

$$= \frac{\alpha}{(w^2(k) + 2k \ln(1+k\alpha))^{1/2}} - \int_{1}^{1+k\alpha} \frac{w(k) w'(k) + \ln s}{(w^2(k) + 2k \ln s)^{3/2}} \, ds \,. \tag{62}$$

Hence

$$w(k) w'(k) \int_{1}^{1+k\alpha} \frac{ds}{(w^{2}(k) + 2k \ln s)^{3/2}}$$
  
=  $\frac{\alpha}{(w^{2}(k) + 2k \ln(1+k\alpha))^{1/2}} - \int_{1}^{1+k\alpha} \frac{\ln s}{(w^{2}(k) + 2k \ln s)^{3/2}} ds$ . (63)

We have for  $1 \leq s \leq 1 + k \alpha$ 

$$\frac{\ln s}{(w^2(k) + 2k \ln s)^{3/2}} \le \frac{\ln(1+k\alpha)}{w^2(k) + 2k \ln(1+k\alpha)} \frac{1}{w^2(k) + 2k \ln s)^{1/2}} .$$
 (64)

Therefore

$$\int_{1}^{1+k\alpha} \frac{\ln s}{(w^{2}(k)+2k \ln s)^{3/2}} ds$$

$$\leq \frac{\ln(1+k\alpha)}{w^{2}(k)+2k \ln(1+k\alpha)} \int_{1}^{1+k\alpha} \frac{ds}{(w^{2}(k)+2k \ln s)^{1/2}}$$

$$= \frac{\ln(1+k\alpha)}{w^{2}(k)+2k \ln(1+k\alpha)},$$
(65)

where we have used (55). It follows from (63) that

$$w(k) w'(k) \int_{1}^{1+k\alpha} \frac{ds}{(w^2(k) + 2k \ln s)^{3/2}}$$
  

$$\geq \frac{\alpha}{(w^2(k) + 2k \ln(1+k\alpha))^{1/2}} - \frac{\ln(1+k\alpha)}{w^2(k) + 2k \ln(1+k\alpha)}. \quad (66)$$

We shall show that the right-hand side of (66) is positive. To that end, we note that

$$\alpha (w^2(k) + 2k \ln(1+k\alpha))^{1/2} > (2\alpha \cdot k\alpha \cdot \ln(1+k\alpha))^{1/2} > \ln(1+k\alpha) , \quad (67)$$

where the latter inequality follows from  $2\alpha \ge 1$  and  $u > \ln(1+u)$  for u > 0. It then follows from (66) that w'(k) > 0.

Next, we recall the identity (29): for fixed t > 0 we have

$$\int_{1}^{f(t)} \frac{ds}{(w^2 + 2k \ln s)^{1/2}} = t .$$
 (68)

For any s > 1, the integrand  $(w^2(k) + 2k \ln s)^{-1/2}$  decreases strictly in k > 0. Since t is fixed, it follows that f(t) = f(t; k) increases strictly in k > 0. Furthermore recalling the identity in (27): for fixed t > 0 we have

$$f'(t) = (w^2(k) + 2k \ln f(t; k))^{1/2}, \qquad (69)$$

we conclude that f'(t) = f'(t; k) increases strictly in k > 0.

Finally, from the generalization of (61),

$$\frac{w}{k} = \alpha - \int_{0}^{1} \left( \int_{0}^{t} \frac{ds}{f(s;k)} \right) dt$$
(70)

and strict increasingness of f(s; k) for any  $s \in (0, 1)$  as a function of k > 0, we conclude that w/k increases strictly in k > 0.

### 6 Power series of w(k)

We aim at a power series of w(k). By the representation  $f(t) = c f_0(a+bt)$ , see (7) and (8), and the fact that  $f_0(z)$  is analytic, at least in the disk  $|z| < \sqrt{\pi/2}$ , it follows that f(t) is analytic in a disk of radius larger than 1 when k is sufficiently small. Thus, for such k there is a power series

$$f(t) = \sum_{j=0}^{\infty} a_j t^j \tag{71}$$

having a radius of convergence that exceeds 1.

The condition f(1) = 1 + k can for sufficiently small k be expressed as

 $1 + k = a_0 + a_1 + a_2 + a_3 + a_4 + \dots$ (72)

in which  $a_0 = 1$ ,  $a_1 = w$ ,  $a_2 = \frac{1}{2}k$ . Therefore,

$$w = \frac{1}{2}k - a_3 - a_4 - \dots = \frac{1}{2}k - \sum_{s=3}^{\infty} \frac{f^{(s)}(0)}{s!} .$$
 (73)

In the sequel we denote for notational convenience  $f^{(s)}(t)$  by  $f_s(t)$ , s = 1, 2, ... We have by straightforward computation, using  $f_2(t) = k/f(t)$  all the time,

$$f_{2} = \frac{k}{f} , \qquad f_{3} = \frac{-kf_{1}}{f^{2}} , \qquad f_{4} = \frac{-k^{2} + 2kf_{1}^{2}}{f^{3}} ,$$
$$f_{5} = \frac{7k^{2}f_{1} - 6kf_{1}^{3}}{f^{4}} , \qquad f_{6} = \frac{7k^{3} - 46k^{2}f_{1}^{2} + 24kf_{1}^{4}}{f^{5}} , \dots, \qquad (74)$$

where we have deleted the argument t from f(t) and all  $f_s(t)$ . We thus postulate for r = 1, 2, ... the forms

$$f_{2r} = \frac{a_{0,2r} k^r + a_{1,2r} k^{r-1} f_1^2 + \dots + a_{r-1,2r} k f_1^{2r-2}}{f^{2r-1}} , \qquad (75)$$

$$f_{2r+1} = \frac{a_{0,2r+1} k^r f_1 + a_{1,2r+1} k^{r-1} f_1^3 + \dots + a_{r-1,2r+1} k f_1^{2r-1}}{f^{2r}} .$$
(76)

From (75), (76), we obtain  $f_{2r}(0)$ ,  $f_{2r+1}(0)$  by replacing f by 1 and  $f_1$  by w. The *a*-coefficients in (75, 76) are integers that can be obtained recursively straightforwardly as follows. We have

$$a_{0,3} = -1, a_{1,3} = a_{2,3} = \dots = 0 , \qquad (77)$$

and, for  $r = 1, 2, \ldots$ ,

$$\begin{cases}
 a_{0,2r+2} = a_{0,2r+1}, \\
 a_{j,2r+2} = (2j+1) a_{j,2r+1} - 2r a_{j-1,2r+1}, \quad j = 1, 2, ..., r-1, \\
 a_{r,2r+2} = -2r a_{r-1,2r+1},
\end{cases}$$
(78)

together with

$$\begin{cases}
 a_{j,2r+3} = 2(j+1) a_{j+1,2r+2} - (2r+1) a_{j,2r+2}, \quad j = 0, 1, ..., r-1, \\
 a_{r,2r+3} = -(2r+1) a_{r,2r+2}.
\end{cases}$$
(79)

In the table below, we list  $a_{i,j}$  for j = 3, 4, ..., 10 and  $i = 0, 1, ..., \lfloor \frac{1}{2}j \rfloor - 1$  $(\lfloor x \rfloor = \text{largest integer} \leq x).$ 

	0	1	2	3	4
3	-1				
4	-1	2			
5	7	-6			
6	7	-46	24		
7	-127	326	-120		
8	-127	1740	-2756	720	
9	4369	-23208	23612	-5040	
10	4369	-104576	303724	-224176	40320

We observe that  $a_{0,2r}$  coincide with the  $b_r$  of (52–53) for r = 2, 3, .... Thus, we have for r = 1, 2, ...

$$f_{2r}(0) = \sum_{l=0}^{r-1} a_{l,2r} k^{r-l} w^{2l} = k^r \sum_{l=0}^{r-1} a_{l,2r} Z^{2l} , \qquad (80)$$

$$f_{2r+1}(0) = \sum_{l=0}^{r-1} a_{l,2r+1} k^{r-l} w^{2l+1} = k^{r+1/2} \sum_{l=0}^{r-1} a_{l,2r+1} Z^{2l+1} , \qquad (81)$$

where we have set  $Z = w/\sqrt{k}$ ,  $w = Z\sqrt{k}$ . Observe that

$$w = \sum_{j=1}^{\infty} \alpha_j \, k^j \Leftrightarrow Z = \sum_{j=1}^{\infty} \alpha_j \, k^{j-1/2} \,. \tag{82}$$

Therefore, from (73) and (80-81), we get

$$Z = \frac{1}{2}\sqrt{k} - \sum_{r=1}^{\infty} \frac{k^r}{(2r+1)!} \sum_{l=0}^{r-1} a_{l,2r+1} Z^{2l+1}$$
$$- \sum_{r=1}^{\infty} \frac{k^{r+1/2}}{(2r+2)!} \sum_{l=0}^{r} a_{l,2r+2} Z^{2l} .$$
(83)

By successive substitution, we can now compute the coefficients

$$C_{k^{j-1/2}}(Z)$$
 of  $k^{j-1/2}$  in Z. (84)

Thus, we start with  $C_{k^{1/2}}(Z) = 1/2$ , and to find  $C_{k^{3/2}}(Z)$ , we insert  $Z = \frac{1}{2}\sqrt{k} + O(k^{3/2})$  into the right-hand side of (83), only retaining terms that do contribute to  $C_{k^{3/2}}(Z)$ . This gives

$$Z = \frac{1}{2}\sqrt{k} - \left(\frac{k}{6}a_{0,3}Z + \ldots\right) - \left(\frac{k^{3/2}}{24}\left(a_{0,4}Z^0 + a_{1,4}Z^2\right) + \ldots\right), \quad (85)$$

so that

$$C_{k^{3/2}}(Z) = -\frac{1}{6}a_{0,3} \cdot \frac{1}{2} - \frac{1}{24}a_{0,4} = \frac{1}{12} + \frac{1}{24} = \frac{1}{8}.$$
 (86)

Similarly, to find  $C_{k^{5/2}}(Z)$ , we write

$$Z = \frac{1}{2}\sqrt{k} - \left(\frac{k}{6}a_{0,3}Z + \frac{k^2}{120}(a_{0,5}Z + a_{1,5}Z^3) + ...\right) - \left(\frac{k^{3/2}}{24}(a_{0,4}Z^0 + a_{1,4}Z^2) + \frac{k^{5/2}}{720}(a_{0,6}Z^0 + a_{1,6}Z^2 + a_{2,6}Z^4) + ...\right), \quad (87)$$

and we insert  $Z = \frac{1}{2} k^{1/2} + \frac{1}{8} k^{3/2} + O(k^{5/2})$  into the right-hand side of (87). This then gives

$$C_{k^{5/2}}(Z) = -\frac{1}{6}a_{0,3}\frac{1}{8} - \frac{1}{120}a_{0,5}\frac{1}{2} - \frac{1}{24}a_{1,4}(\frac{1}{2})^2 - \frac{1}{720}a_{0,6}$$
$$= \frac{1}{48} - \frac{7}{240} - \frac{1}{48} - \frac{7}{720} = \frac{-7}{180}.$$
 (88)

With sufficient labour, one can then establish furthermore

$$C_{k^{7/2}}(Z) = \frac{1667}{120960} , \qquad C_{k^{9/2}} = \frac{-10621}{1814400}$$
 (89)

so that (due to (82)) we get (14):

$$w = \frac{1}{2}k + \frac{1}{8}k^2 - \frac{7}{180}k^3 + \frac{1667}{120960}k^4 - \frac{10621}{1814400}k^5 + \dots$$
 (90)

## 7 Bounds for w

We have the representation, see (13),

$$\frac{w}{k} = 1 - \int_{0}^{1} \left( \int_{0}^{t} \frac{ds}{f(s)} \right) dt , \qquad (91)$$

where f satisfies f''(s) = k/f(s),  $s \ge 0$ , and f(0) = 1, f'(0) = w > 0 and f(1) = 1 + k. Since f(s) > 1, 0 < s < 1, we get from (91)

$$\frac{1}{2} = 1 - \int_{0}^{1} \left( \int_{0}^{t} ds \right) dt < \frac{w}{k} < 1, \text{ i.e.}, \quad \frac{1}{2}k < w < k .$$
(92)

Next, by convexity of f and f(0) = 1, f(1) = 1 + k, f'(0) = w, we have

$$1 + ws < f(s) < 1 + ks$$
,  $0 < s < 1$ . (93)

Then, using

$$\int_{0}^{t} \frac{ds}{1+as} = \frac{1}{a} \ln(1+at) , \qquad \int_{0}^{1} \ln(1+at) dt = (1+a^{-1}) \ln(1+a) - 1 , \quad (94)$$

we get from (91) the bound

$$k(1+w^{-1})(1-w^{-1}\ln(1+w)) < w < k(1+k^{-1})(1-k^{-1}\ln(1+k)) .$$
(95)

Define

$$\varphi_k : w \in [\frac{1}{2}k, k] \mapsto k(1 + w^{-1})(1 - w^{-1}\ln(1 + w)) .$$
 (96)

From the above reasoning, it follows that  $\varphi_k(b)$  is a lower bound for w when  $b \in [\frac{1}{2}k, k]$  is a lower bound for w.

**Proposition 1**  $\varphi_k$  is a strictly increasing contraction of  $[\frac{1}{2}k, k]$ .

**Proof** It is sufficient to show that

(i) 
$$\varphi_k(\frac{1}{2}k) \ge \frac{1}{2}k$$
, (ii)  $\varphi_k(k) \le k$ , (iii)  $\varphi'_k(w) \in (0,1)$ ,  $\frac{1}{2}k \le w \le k$ . (97)

To prove item (i) in (97), we must show that

$$\left(\frac{1}{2}k+1\right)\left(\frac{1}{2}k-\ln(1+\frac{1}{2}k)\right) \ge \frac{1}{2}\left(\frac{1}{2}k\right)^2, \qquad k>0.$$
 (98)

With  $y = \frac{1}{2}k > 0$ , this follows from the elementary inequality

$$(y+1) \ln(y+1) < y + \frac{1}{2}y^2$$
,  $y > 0$ . (99)

To prove item (ii) in (97), we must show that

$$(1+k) \ln(1+k) \ge k$$
,  $k > 0$ , (100)

and this latter inequality follows by elementary means.

Finally, to prove item (iii) in (97), we compute for w > 0,

$$\frac{1}{k}\varphi_k'(w) = \frac{d}{dw} \left[ 1 + \frac{1}{w} - \left(\frac{1}{w} + \frac{1}{w^2}\right) \ln(1+w) \right] = \frac{-2}{w^2} + \left(\frac{1}{w^2} + \frac{2}{w^3}\right) \ln(1+w) .$$
(101)

Hence, we must show that

$$0 < (2+w) \ln(1+w) - 2w < \frac{1}{k} w^3 , \qquad \frac{1}{2} k \le w \le k .$$
 (102)

To prove the first inequality in (102), we note that there is equality for w = 0, and that

$$\frac{d}{dw}\left[(2+w)\,\ln(1+w) - 2w\right] = \frac{1}{1+w} + \ln(1+w) - 1 \tag{103}$$

vanishes at w = 0, while

$$\left(\frac{d}{dw}\right)^2 \left[(2+w)\,\ln(1+w) - 2w\right] = \frac{-1}{(1+w)^2} + \frac{1}{1+w} > 0 \;, \qquad w > 0 \;. \tag{104}$$

Therefore, the first inequality in (102) holds for w > 0.

Next, the second inequality in (102) holds if and only if

$$\ln(1+w) < \frac{\frac{1}{k}w^3 + 2w}{2+w} , \qquad \frac{1}{2}k \le w \le k .$$
 (105)

We first show that the inequality in (105) holds for  $w = \frac{1}{2}k$ , i.e., that

$$\ln(1+\frac{1}{2}k) < \frac{\frac{1}{8}k^2+k}{2+\frac{1}{2}k} = \frac{\frac{1}{2}(\frac{1}{2}k)^2+2(\frac{1}{2}k)}{2+\frac{1}{2}k} , \qquad k > 0 .$$
(106)

Setting  $y = \frac{1}{2}k$ , we have to show that

$$\ln(1+y) < \frac{\frac{1}{2}y^2 + 2y}{y+2} , \qquad y > 0 .$$
(107)

Now

$$\left(\ln(1+y) - \frac{\frac{1}{2}y^2 + 2y}{y+2}\right)(y=0) = 0 = \left(\ln(1+y) - \frac{\frac{1}{2}y^2 + 2y}{y+2}\right)'(y=0), (108)$$

and

$$\left(\ln(1+y) - \frac{\frac{1}{2}y^2 + 2y}{y+2}\right)'' = \frac{-1}{(1+y)^2} + \frac{4}{(y+2)^3} < 0 , \qquad y > 0 .$$
 (109)

From this (107) and (106) follow. We finally show that

$$\frac{1}{1+w} < \frac{d}{dw} \left[ \frac{\frac{1}{k} w^3 + 2w}{2+w} \right] = \frac{\frac{2}{k} w^3 + \frac{6}{k} w^2 + 4}{(2+w)^2} , \qquad w \ge \frac{1}{2} k .$$
(110)

The inequality in (110) can be worked out to the inequality

$$1 < \frac{8}{k}w + \frac{6}{k} + \frac{2}{k}w^2 , \qquad w \ge \frac{1}{2}k , \qquad (111)$$

and this latter inequality holds indeed. From (106) and (110), we get (105), and the proof of the proposition is complete.

**Remark 1** From a computation, it follows that

$$\frac{1}{k}\varphi_k''(w) = \frac{1}{w^4} \left[ 5w + 1 - (2w + 6) \ln(1 + w) + 1 + w - \frac{1}{1 + w} \right].$$
(112)

The expression between [] in (112) and its derivative vanish at w = 0, while its second derivative is negative for w > 0. Hence, the function  $\varphi_k$  is concave in w > 0, and the contraction constant of  $\varphi_k$  as a contraction of  $[\frac{1}{2}k, k]$ equals  $\varphi'_k(\frac{1}{2}k)$ .

Let

$$w_U = w_U(k) = \varphi_k(k) = k + 1 - (1 + k^{-1}) \ln(1 + k) , \qquad (113)$$

and let  $w_L = w_L(k)$  be the unique fixed point of  $\varphi_k$  as a contraction of  $[\frac{1}{2}k, k]$ .

**Proposition 2** We have

$$w_L(k) < w(k) < w_U(k)$$
 . (114)

**Proof** The second inequality in (114) follows from the second inequality in (95). Next, from Proposition 1 we have for  $b \in [\frac{1}{2}k, k]$ 

$$b > w_L(k) \Leftrightarrow b > \varphi_k(b)$$
 . (115)

The first inequality in (114) thus follows from the first inequality in (95).

The computation of  $w_L$  is done by iteration. Thus, one starts with an arbitrary  $w^{(0)} \in [\frac{1}{2}k, k]$ , and one defines  $w^{(n+1)} := \varphi_k(w^{(n)})$  for n = 0, 1, .... Then one has  $w^{(n)} \uparrow w_L$  or  $w^{(n)} \downarrow w_L$  according as  $w^{(0)} < w_L$  or  $w^{(0)} > w_L$ . The asymptotic convergence rate is given by

$$\lim_{n \to \infty} \frac{w_L - w^{(n+1)}}{w_L - w^{(n)}} = \varphi'_k(w_L) .$$
(116)

From

$$w_L = \varphi_k(w_L) = k(1 + w_L^{-1})(1 - w_L^{-1} \ln(1 + w_L))$$
(117)

and, see (101),

$$\varphi_k'(w_L) = k \left(\frac{-2}{w_L^2} + \left(\frac{1}{w_L^2} + \frac{2}{w_L^3}\right) \ln(1 + w_L)\right), \qquad (118)$$

one computes

$$\varphi_k'(w_L) = \frac{k}{w_L} - 1 - \frac{1}{1 + w_L} .$$
(119)

An explicit lower bound for w is given according to

$$w > w_L > \varphi_k(\frac{1}{2}k) = k + 2 - 2(1 + \frac{2}{k}) \ln(1 + \frac{1}{2}k) = w_U - \ln(k) + O(1) .$$
(120)

The following result improves upon this.

Proposition 3 We have

$$k - \ln(1+k) < w_L < w < w_U < k+1 - \ln(1+k)$$
,  $k > 0$ . (121)

**Proof** The inequality for  $w_U$  is obvious from (113), and so there remains only the first inequality for  $w_L$  to be proved.

We shall show below that  $w_L(k) = \frac{1}{2}k + \frac{1}{12}k^2 + \dots$ . Since  $k - \ln(1+k) = \frac{1}{2}k^2 - \frac{1}{3}k^3 + \dots$ , we see that the first inequality in (121) holds for small positive k, with equality for  $k \downarrow 0$ . We have

$$\frac{d}{dk}\left(k - \ln(1+k)\right) = 1 - \frac{1}{1+k} = \frac{k}{k+1} \ . \tag{122}$$

Furthermore, from (117) we compute

$$w'_{L}(k) = \frac{d}{dk} \left[ k(1 + w_{L}^{-1}(k))(1 - w_{L}^{-1} \ln(1 + w_{L})) \right]$$
  

$$= (1 + w_{L}^{-1}(k)(1 - w_{L}^{-1}(k) \ln(1 + w_{L}(k)))$$
  

$$+ \frac{d}{dw} \left[ k(1 + w^{-1})(1 - w^{-1} \ln(1 + w)) \right] (w = w_{L}(k)) w'_{L}(k)$$
  

$$= \frac{1}{k} w_{L}(k) + \frac{d\varphi_{k}}{dw} (w_{L}(k)) w'_{L}(k)$$
  

$$= \frac{1}{k} w_{L}(k) + \left( \frac{k}{w_{L}(k)} - 1 - \frac{1}{1 + w_{L}(k)} \right) w'_{L}(k) , \qquad (123)$$

where (119) has been used in the last step. It follows that

$$w'_{L}(k) = \frac{\frac{1}{k} w_{L}(k)}{2 + \frac{1}{1 + w_{L}(k)} - \frac{k}{w_{L}(k)}} .$$
(124)

We shall show that the right-hand side of (124) exceeds k/(k+1), see (122). From  $\frac{1}{k}w_L(k) < 1$ , we have  $(1+w_L)^{-1} < (\frac{w_L}{k} + w_L)^{-1}$ , and so

$$w_L'(k) > \frac{\frac{1}{k} w_L}{2 + \left(\frac{w_L}{k} + w_L\right)^{-1} - \frac{k}{w_L}} = \frac{\frac{1}{k} w_L}{2 - \frac{k}{w_L} \frac{k}{k+1}} .$$
(125)

Now set  $t = w_L/k$  and s = k/(k+1). Then we have

$$w_L'(k) - \frac{k}{k+1} > \frac{t}{2 - \frac{1}{t}s} - s = \frac{t - 2s + \frac{1}{t}s^2}{2 - \frac{1}{t}s} = \frac{(t-s)^2}{2t-s} \ge 0 , \qquad (126)$$

where it also has been used that  $2t = 2w_L/k > 1 > k/(k+1) = s$ . This completes the proof.

**Remark 2** From the proof of Proposition 3 it also follows that  $w_L(k) - (k - \ln(1+k))$  is strictly increasing in k > 0.

**Proposition 4** We have for small k > 0 the expansions

$$w_U(k) = \frac{1}{2}k + \frac{1}{6}k^2 - \frac{1}{12}k^3 + \frac{1}{20}k^4 - \frac{1}{30}k^5 + \dots , \qquad (127)$$

$$w_L(k) = \frac{1}{2}k + \frac{1}{12}k^2 - \frac{1}{144}k^3 - \frac{1}{540}k^4 + \frac{19}{25920}k^5 + \dots$$
(128)

**Proof** We have from (113) that

$$w_U(k) = (k+1)(1 - \frac{1}{k}\ln(1+k)) = (k+1)\sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j+1}k^j$$
$$= \frac{1}{2}k + \sum_{j=2}^{\infty} (-1)^j \frac{k^j}{j(j+1)} = \frac{1}{2}k + \frac{1}{6}k^2 - \frac{1}{12}k^3 + \dots, \quad (129)$$

and this establishes (127).

As to (128), we note that the fixed-point equation (117) can be written as

$$w^{3} = k (1+w)(w - \ln(1+w)) = k(1+w) \sum_{j=2}^{\infty} \frac{(-1)^{j}}{j} w^{j}$$
$$= \frac{1}{2} k w^{2} - k \sum_{j=3}^{\infty} (-1)^{j} \frac{w^{j}}{j(j-1)}.$$
(130)

From this we get the equation

$$w = \frac{1}{2} k \left( 1 + \sum_{j=1}^{\infty} a_j w^j \right); \qquad a_j = \frac{2(-1)^j}{(j+1)(j+2)}, \quad j = 1, 2, \dots.$$
(131)

We can now use a simplified version of the successive substitution procedure, as used in Section 6, to obtain a power series for  $w_L(k)$  in powers of  $\frac{1}{2}k$ . Alternatively, we have from the Bürmann-Lagrange formula (compare Section 9)

$$w = \sum_{l=1}^{\infty} \frac{1}{l!} \left(\frac{d}{dw}\right)^{l-1} \left[ \left(1 + \sum_{j=1}^{\infty} a_j w^j\right)^l \right]_{w=0} \left(\frac{1}{2} k\right)^l \,. \tag{132}$$

In either case, the first 5 terms of the power series of  $w_L(k)$  follow upon sufficient labour, and the proof is complete.

Remark 3 We observe that

$$\frac{1}{2}\left(w_U(k) + w_L(k)\right) = \frac{1}{2}k + \frac{1}{8}k^2 - \frac{13}{288}k^3 + O(k^4) , \qquad (133)$$

while, see Section 6,

$$w(k) = \frac{1}{2}k + \frac{1}{8}k^2 - \frac{7}{180}k^3 + O(k^4) .$$
(134)

The Remark 3 shows that w(k) is well approximated by  $\frac{1}{2}(w_U(k)+w_L(k))$ for small k > 0. We shall now establish a similar result for large k. To that end, we introduce sharp and explicit lower bounds for  $w_L$  that are easier to manipulate than  $w_L$  itself. For this, we write  $\varphi_k(w)$  of (96) as

$$\varphi_k(w) = k + \frac{k}{w} - \frac{k}{w} \left(1 + w^{-1}\right) \ln(1 + w) .$$
(135)

We consider the function

$$E: Y \in \left[\frac{1}{2}k, k\right] \mapsto (1+Y^{-1}) \ln(1+Y) , \qquad (136)$$

and note that this function is increasing and concave and satisfies E(Y) > 1for Y > 0. For  $Y \in [w_L(k), k]$ , we define

$$\varphi_k(w; Y) := k + \frac{k}{w} - \frac{k}{w} E(Y) , \qquad w \in [\frac{1}{2}k, k] .$$
 (137)

**Lemma 1** Assume that  $Y \in [w_L(k), k]$  is such that  $E(Y) - 1 \leq \frac{1}{4}k$ . Then  $\varphi_k(\cdot; Y)$  is a strictly increasing contraction of  $[\frac{1}{2}k, k]$ . Furthermore, the unique fixed point w(k; Y) of  $\varphi_k(\cdot; Y)$  satisfies  $w(k; Y) \leq w_L(k)$ .

**Proof** The proof of the contraction matter is similar to, but much easier than, the proof of Proposition 1, due to the much simpler w-dependence of  $\varphi_k(w; Y)$ . For instance,  $\varphi_k(\frac{1}{2}k; Y) \geq \frac{1}{2}k$  amounts to  $k + 2 - 2E(Y) \geq \frac{1}{2}k$ , i.e., to  $E(Y) - 1 \leq \frac{1}{4}k$ , and

$$\frac{d}{dw}\left[\varphi_k(w;Y)\right] = -\frac{k}{w^2} + \frac{k}{w^2}E(Y) \in (0,1) , \qquad w \in \left[\frac{1}{2}k,k\right] , \qquad (138)$$

when  $0 < E(Y) - 1 < \frac{1}{4}k$ .

We next observe that

$$\varphi_k(w_L; Y) \le \varphi_k(w_L) = w_L \tag{139}$$

since  $E(Y) \ge E(w_L)$  by the assumption  $Y \in [w_L(k), k]$ , For  $b \in [\frac{1}{2}k, k]$  we have

$$b \ge w(k; Y) \Leftrightarrow \varphi_k(b; Y) \le b$$
. (140)

Taking  $b = w_L(k)$ , we see from (139) that  $w_L(k) \ge w(k; Y)$ , and the proof is complete.

The crucial observation now is the fact that the unique fixed point of  $\varphi_k(\cdot; Y)$  can be computed explicitly by solving the equation

$$w^{2} = kw + k(1 - E(Y))$$
(141)

in  $w \in [\frac{1}{2}k, k]$ . We find for the fixed point w(k; Y) of  $\varphi_k(\cdot; Y)$ 

$$w(k;Y) = \frac{1}{2}k + (\frac{1}{4}k^2 + k(1 - E(Y))^{1/2}, \qquad (142)$$

where the square root is well-defined and non-negative when  $E(Y) - 1 \leq \frac{1}{4}k$ .

Two obvious choices for Y are Y = k and  $Y = w_U$ . It is readily shown that  $E(k) - 1 \leq \frac{1}{4}k$  when  $k \geq 5$ , and that  $E(w_U) - 1 \leq \frac{1}{4}k$  when  $k \geq 2$  (this has to be established numerically). We let

$$\overline{w}_L := w(k; Y = k) = \frac{1}{2}k + (\frac{1}{4}k^2 - [(1+k)\ln(1+k) - k])^{1/2},$$
 (143)

$$\overline{w}_L := w(k; Y = w_U) = \frac{1}{2}k + (\frac{1}{4}k^2 - k\left[(1 + w_U^{-1})\ln(1 + w_U) - 1\right])^{1/2}.$$
 (144)  
Note that for general  $Y \in [w_L, k]$  we have, setting  $b = E(Y) - 1$ ,

$$w(k;Y) = \frac{1}{2}k + (\frac{1}{4}k^2 - kb)^{1/2} = \frac{1}{2}k + ((\frac{1}{2}k - b)^2 - b^2)^{1/2}$$
  
$$= \frac{1}{2}k + (\frac{1}{2}k - b)\left(1 - \left(\frac{b}{\frac{1}{2}k - b}\right)^2\right)^{1/2}$$
  
$$= k - b - \frac{\frac{1}{2}b^2}{\frac{1}{2}k - b} - \frac{\frac{1}{8}b^4}{(\frac{1}{2}k - b)^3} - \dots .$$
(145)

**Proposition 5** We have for large k

$$w_U - w_L = O\left(\frac{\ln^2(1+k)}{k}\right)$$
 (146)

**Proof** Choose Y = k in (145). Then

$$b = (1 + k^{-1}) \ln(1 + k) - 1 = k - w_U , \qquad \frac{1}{2}k - b = w_U - \frac{1}{2}k , \qquad (147)$$

and so

$$w_L > w(k; Y = k) = w_U - \frac{\frac{1}{2}(k - w_U)^2}{w_U - \frac{1}{2}k} - \frac{\frac{1}{8}(k - w_U)^4}{(w_U - \frac{1}{2}k)^3} - \dots$$
(148)

By Proposition 3, we have

$$k - w_U < \ln(1+k)$$
,  $w_U - \frac{1}{2}k > \frac{1}{2}k - \ln(1+k)$ . (149)

Therefore

$$0 < w_U - w_L < \frac{\frac{1}{2} \ln^2(1+k)}{\frac{1}{2} k - \ln(1+k)} + \frac{\frac{1}{8} \ln^4(1+k)}{(\frac{1}{2} k - \ln(1+k))^3} + \dots$$
$$= \frac{\ln^2(1+k)}{k} + O\left(\frac{\ln^3(1+k)}{k^2}\right), \qquad (150)$$

and the proof is complete.

**Remark 4** As the proof shows, the constant implied by the O in (146) is of the order unity.

The fact that  $w_U - w_L$  gets small as k gets large implies that  $\overline{\overline{w}}_L$  is a significantly better approximation of  $w_L$  than  $\overline{w}_L$  is.

**Proposition 6** We have for large k

$$0 < w_L - \bar{\bar{w}}_L = O\left(\left(\frac{\ln k}{k}\right)^2\right), \qquad 0 < w_L - \bar{w}_L = O\left(\frac{\ln k}{k}\right). \tag{151}$$

**Proof** To show the first item in (151), we start by noting that  $w_L$  is the fixed point of  $\varphi(\cdot; Y = w_L)$  while  $\overline{w}_L$  is the fixed point of  $\varphi(\cdot; Y = w_U)$ . Hence, by (142)

$$w_L - \overline{\overline{w}}_L = (\frac{1}{4}k^2 - k(E(w_L) - 1))^{1/2} - (\frac{1}{4}k^2 - k(E(w_U) - 1))^{1/2} .$$
(152)

From this we get

$$w_L - \bar{\bar{w}}_L < \frac{k(E(w_U) - E(w_L))}{(k^2 - 4k(E(w_U) - 1))^{1/2}} .$$
(153)

We shall estimate  $E(w_U) - E(w_L)$ , and to that end we note that

$$\frac{d}{dw}\left[(1+w^{-1}\ln(1+w))\right] = \frac{1}{w} - \frac{\ln(1+w)}{w^2} > 0 , \qquad w > 0 , \qquad (154)$$

$$\frac{d^2}{dw^2} \left[ (1+w^{-1}) \ln(1+w) \right] = \frac{2\ln(1+w) - w - w(1+w)^{-1}}{w^3} < 0 , \qquad w > 0 .$$
(155)

Hence

$$E(w_U) - E(w_L) < (w_U - w_L) \left(\frac{1}{w_L} - \frac{\ln(1 + w_L)}{w_L^2}\right).$$
(156)

We shall show that

$$\frac{1}{w_L} - \frac{\ln(1+w_L)}{w_L^2} < \frac{1}{k} .$$
(157)

Indeed, since  $w_L$  is the fixed point of  $\varphi_k$  in (101), we have for  $w = w_L$ 

$$w^{-1}\ln(1+w) = 1 - \frac{w}{k(1+w^{-1})} , \qquad (158)$$

so that

$$\frac{1}{w} - \frac{\ln(1+w)}{w^2} = \frac{1}{k(1+w^{-1})} < \frac{1}{k} , \qquad w = w_L .$$
 (159)

It then follows from (153), (156) and (157) that

$$w_L - \bar{\bar{w}}_L \le \frac{w_U - w_L}{(k^2 - 4k(E(w_U) - 1))^{1/2}} = O\left(\left(\frac{\ln k}{k}\right)^2\right), \quad (160)$$

where Proposition 5 has been used.

When we repeat the reasoning just given in which the  $w_U$  in (152) is replaced by k (so that at the left-hand side of (152) we get  $w_L - \bar{w}_L$ ), we arrive at (153) with  $E(k) - E(w_L)$  instead of  $E(w_U) - E(w_L)$ . Now, compare (156),

$$(k - w_L) \left(\frac{1}{k} - \frac{\ln(1+k)}{k^2}\right) < E(k) - E(w_L) < (k - w_L) \left(\frac{1}{w_L} - \frac{\ln(1+w_L)}{w_L^2}\right),$$
(161)

and so we get from (157) that  $E(k) - E(w_L) = O(k^{-1}(k - w_L))$ , and not more than that. Since by Proposition 3

$$-1 + \ln(1+k) < k - w_L < \ln(1+k) , \qquad (162)$$

we see that  $E(k) - E(w_L) = O(k^{-1} \ln k)$ , and not more than that. This completes the proof.

From the tight upper bound  $w_U$  and the lower bounds  $w_L$ ,  $\bar{w}_L$ ,  $\bar{\bar{w}}_L$  of w, we can form approximations  $\frac{1}{2}(w_U + w_L)$ ,  $\frac{1}{2}(w_U + \bar{\bar{w}}_L)$  and  $\frac{1}{2}(w_U + \bar{w}_L)$  of w. From (133) and (134), we have

$$w(k) - \frac{1}{2} \left( w_U(k) + w_L(k) \right) = \frac{1}{160} k^3 + O(k^4) , \qquad k \downarrow 0$$
 (163)

so that  $\frac{1}{2}(w_U + w_L) < w$  for small k. Numerically it appears that  $\frac{1}{2}(w_U + w_L) > \frac{1}{2}(w_U + \overline{w}_L) > w > \frac{1}{2}(w_U + \overline{w}_L)$  for large k.

#### 8 Newton method to compute w

We present a Newton method to compute w, or rather  $W = w/\sqrt{k}$ . This is based on (12) that we write as an equation in W,

$$H(W) := \int_{W}^{V} e^{v^2} dv - e^{W^2} \sqrt{\frac{1}{2}k} , \qquad V = (W^2 + \ln(1+k))^{1/2} .$$
(164)

As starting value  $W^{(0)}$  we choose

$$W^{(0)} = \frac{1}{2} \left( \frac{w_U}{\sqrt{2k}} + \frac{w_L}{\sqrt{2k}} \right) \,. \tag{165}$$

The Newton step is

$$W^{(j+1)} = W^{(j)} - \frac{H(W^{(j)})}{H'(W^{(j)})} , \qquad j = 0, 1, \dots,$$
(166)

for which we compute

$$\frac{H(W)}{H'(W)} = \frac{\int\limits_{W}^{V} e^{v^2} dv - e^{W^2} \sqrt{\frac{1}{2}k}}{\frac{W}{V} e^{V^2} - e^{W^2} - W e^{W^2} \sqrt{2k}} = \frac{e^{-W^2} \int\limits_{W}^{V} e^{v^2} dv - \sqrt{\frac{1}{2}k}}{\frac{W}{V} (1+k) - 1 - W \sqrt{2k}}, \quad (167)$$

where  $\exp(V^2) = (1+k) \exp(W^2)$  has been used.

The Newton step requires evaluation of the quantity

$$e^{-W^2} \int_{W}^{V} e^{v^2} dv = (1+k) F(V) - F(W) , \qquad (168)$$

where F(Y) is Dawson's integral

$$F(Y) = e^{-Y^2} \int_{0}^{Y} e^{v^2} dv , \qquad Y \ge 0 .$$
 (169)

When one has access to a package that can evaluate Dawson's integral to sufficient accuracy for any  $Y \ge 0$ , there is virtual no limitation on V, W

(and thus k) for using this Newton method. Otherwise, one can use for small-to-moderately large values of k the series representation

$$\int_{W}^{V} e^{v^2} dv = \sum_{l=0}^{\infty} \frac{V^{2l+1} - W^{2l+1}}{l!(2l+1)} .$$
(170)

For large values of k, there is the asymptotic result

$$F(Y) \sim \frac{1}{2Y} \sum_{k=0}^{\infty} \frac{\Gamma(k+\frac{1}{2})}{\Gamma(\frac{1}{2})} Y^{-2k} ,$$
 (171)

in which the series should be truncated at the integer k nearest to  $Y^2 - 1/3$ , yielding an approximation error for F(Y) of the order  $\exp(-Y^2)/(Y\sqrt{2})$ . For this matter, see [7], [8], [9]. The series representation in (170) is feasible for use with a CASIOfx-82MS for values of k up to 10–20.

We illustrate this for the case that k = 1. Then

$$w_U = 0.613705638$$
,  $w_L = 0.579151685$ ,  $\frac{1}{2}(w_U + w_L) = 0.596428661$ , (172)

and

$$W^{(0)} = \frac{w_U + w_L}{2\sqrt{2}} = 0.421738751, \quad V^{(0)} = ((W^{(0)})^2 + \ln 2)^{1/2} = 0.933279567.$$
(173)

We compute, using CASIOfx-82MS

L	$\sum_{l=1}^{L} \frac{(V^{(0)})^{2l+1} - (W^{(0)})^{2l+1}}{(W^{(0)})^{2l+1}}$
	$\sum_{l=0} \qquad l!(2l+1)$
0	0.511540818
1	0.757502345
2	0.826972318
3	0.841159943
4	0.844084344
5	0.844438737
6	0.844482275
7	0.844486970
8	0.844487421
9	0.844487460
10	0.844487463
11	0.844487463
12	0.844487463

Then, via (166-167), we get

$$W^{(1)} = 0.421416848, \quad V^{(1)} = ((W^{(1)})^2 + \ln 2)^{1/2} = 0.933134149.$$
 (174)

Next, we compute

$$\sum_{l=0}^{12} \frac{(V^{(1)})^{2l+1} - (W^{(1)})^{2l+1}}{l!(2l+1)} = 0.844524567 , \qquad (175)$$

and then we get  $W^{(2)} = 0.421416826$ . For confirmation, we also compute  $W^{(3)} = 0.421416826$ . Finally, we get  $w = W\sqrt{2} = 0.595973391$ . Observe that the  $\frac{1}{2}(w_U + w_L)$  of (172) deviates only  $4.55 \times 10^{-4}$  from w.

#### 9 Methods to compute w for large k

We present two methods to compute w for, hopefully all but at least large, k > 0. These methods are based on the condition, see (11) and Section 4,

$$\int_{1}^{1+k} \frac{1}{(w^2 + 2k \ln s)^{1/2}} \, ds = 1 \,. \tag{176}$$

Setting

$$y = \frac{\sqrt{2k}}{w} = \frac{1}{W} , \qquad u = \sqrt{\frac{2}{k}} , \qquad (177)$$

we have from (176) that

$$y \int_{1}^{1+k} \frac{1/k}{(1+y^2 \ln s)^{1/2}} \, ds = u \,, \tag{178}$$

with both u and y small in (178) when k is large. The integral at the lefthand side of (178) is analytic in  $y \in \mathbb{C}$  with  $|y| < (1/\ln(1+k))^{1/2}$ , and equals 1 at y = 0. For  $|y| < (1/\ln(1+k))^{1/2}$ , we can develop

$$(1+y^2 \ln s)^{-1/2} = \sum_{n=0}^{\infty} {\binom{-1/2}{n} y^{2n} \ln^n s}, \qquad 1 \le s \le 1+k.$$
(179)

Interchanging sum and integral, we get for (178)

$$y \int_{1}^{1+k} \frac{1/k}{(1+y^2 \ln s)^{1/2}} \, ds = y \sum_{n=0}^{\infty} A_n \, y^{2n} \,, \tag{180}$$

where

$$A_n = X_n Y_n; \qquad X_n = \binom{-1/2}{n}, \quad Y_n = \frac{1}{k} \int_{-1}^{1+k} \ln^n s \, ds, \quad n = 0, 1, \dots.$$
(181)

Since  $A_0 = 1$ , we thus have to solve the equation

$$y\left(1+\sum_{n=1}^{\infty}A_n y^{2n}\right) = u$$
, (182)

with  $u = \sqrt{2/k}$ .

The  $X_n$ ,  $Y_n$  in (181) can be computed recursively according to  $X_0 = 1 = Y_0$ , and

$$X_{n+1} = -\frac{n+1/2}{n+1} X_n, \quad Y_{n+1} = (1+\frac{1}{k})(\ln(1+k))^{n+1} - (n+1) Y_n, \quad n = 0, 1, \dots.$$
(183)

The recursion formula for Y in (183) follows from

$$\int_{1}^{1+k} \ln^{n+1} s \, ds = \int_{0}^{\ln(1+k)} x^{n+1} e^x \, dx = \int_{0}^{\ln(1+k)} x^{n+1} \, d(e^x)$$
$$= (1+k)(\ln(1+k))^{n+1} - (n+1) \int_{0}^{\ln(1+k)} x^n e^x \, dx \, . \ (184)$$

It is thus seen that the  $A_n$  in (181) are alternating, and that

$$\left|\frac{A_{n+1}}{A_n}\right| = \frac{n+1/2}{n+1} \frac{\int\limits_{1}^{1+k} \ln^{n+1} s \, ds}{\int\limits_{1}^{1+k} \ln^n s \, ds} \le \frac{n+1/2}{n+1} \ln(1+k) \,. \tag{185}$$

Hence, when  $y^2 \ln(1+k) < 1$ , we have that the series  $\sum_{n=1}^{\infty} A_n y^{2n}$  in (182) has alternating terms that decay monotonically to 0 in modulus. The condition  $y^2 \ln(1+k) < 1$  with  $y = \sqrt{2k}/w$  is satisfied when  $k \ge 7$ . This can be read off from the following table, comprising  $w_U$  and  $w_L$  from Section 7 with  $w \in [w_L, w_U]$ ,

k	$(2k \ln(1+k))^{1/2}$	$w_L(k)$	$w_U(k)$
6	4.8322	4.5639	4.7292
7	5.3955	5.4509	5.6234

Finally, we have the bounds

$$|X_n| = \left| \binom{-1/2}{n} \right| \le \frac{1}{\sqrt{\pi n}}, \quad Y_n \le \frac{1+k}{k} \frac{(\ln(1+k))^{n+1}}{n+\ln(1+k)}, \qquad n = 1, 2, \dots.$$
(186)

The bound on  $Y_n$  in (186) follows from, see (181, 184),

$$\int_{0}^{a} x^{n} e^{x} dx = a^{n} e^{a} \int_{0}^{a} \exp(x - a + n \ln(x/a)) dx$$
$$= a^{n} e^{a} \int_{0}^{a} \exp\left(-u + n \ln\left(1 - \frac{u}{a}\right)\right) du$$
$$< a^{n} e^{a} \int_{0}^{a} \exp\left(-u\left(1 + \frac{n}{a}\right)\right) du < \frac{a^{n} e^{a}}{1 + n/a}$$
(187)

with  $a = \ln(1+k)$ .

From (182), there emerge two methods to compute y. In the first method, we use successive substitution

$$y^{(0)} = u; \quad y^{(j+1)} = \frac{u}{1 + \sum_{n=1}^{N} A_n(y^{(j)})^{2n}}, \qquad j = 0, 1, \dots.$$
 (188)

This produces, for sufficiently large k, a sequence

$$y(k; N) = \lim_{j \to \infty} y^{(j)}, \qquad N = 1, 2, \dots$$
 (189)

of approximations of the solution y(k) of (178). The approximation error y(k; N) - y(k) can be assessed by consideration of the first deleted term  $A_{N+1}(y^{(j)})^{2N+2}$  in the denominator series in the iteration step in (188). Using the bounds in (186) and  $y = \sqrt{2k}/w < \sqrt{2k}/w_L$ , we have then, for sufficiently large k, that  $y(k; N) - y_k$  is of the order

$$\frac{(-1)^n}{\sqrt{\pi n}} \left(\frac{2k \ln(1+k)}{w_L^2}\right)^n \frac{\ln(1+k)}{n+\ln(1+k)} , \qquad n=N+1 .$$
(190)

The second method that emerges from (182) is based on the Bürmann-Lagrange formula. With y and u as in (177), we can write (182) as

$$w = k F(y) , \qquad F(y) = \sum_{n=0}^{\infty} A_n y^{2n} , \qquad (191)$$

where y satisfies

$$y F(y) = u. (192)$$

Letting G(y) = k F(y), we have that w has a power series

$$w(u) = G(0) + \sum_{j=1}^{\infty} \left[ \left( \frac{d}{dy} \right)^{j-1} \frac{G'(y)}{(F(y))^j} \right]_{y=0} u^j / j!$$
  
$$= k + k \sum_{r=1}^{\infty} \frac{1}{(2r)!} \left[ \left( \frac{d}{dy} \right)^{2r-1} \frac{F'(y)}{F^{2r}(y)} \right]_{y=0} u^{2r}$$
  
$$= k - k \sum_{r=1}^{\infty} \frac{1}{2r-1} \frac{1}{(2r)!} \left[ \left( \frac{d}{dy} \right)^{2r} \frac{1}{F^{2r-1}(y)} \right]_{y=0} u^{2r} .$$
(193)

Here it has been used that  $F'(y)/F^j(y)$  is an odd function, and that

$$\frac{F'(y)}{F^{2r}(y)} = \frac{-1}{2r-1} \frac{d}{dy} \left(\frac{1}{F^{2r-1}(y)}\right) .$$
(194)

Write

$$F(y) = \sum_{n=0}^{\infty} A_n y^{2n} = 1 + A(y) = 1 + \sum_{n=1}^{\infty} A_n y^{2n} , \qquad (195)$$

$$A_r(y) = \sum_{n=1}^r A_n y^{2n} , \qquad r = 1, 2, \dots , \qquad (196)$$

and abbreviate by  $C_{y^{2r}}$  the "coefficient of  $y^{2r}$  in". Then we have

$$\frac{1}{(2r)!} \left[ \left( \frac{d}{dy} \right)^{2r} \frac{1}{F^{2r-1}(y)} \right]_{y=0} = C_{y^{2r}} \left( \frac{1}{F^{2r-1}(y)} \right) = C_{y^{2r}} \left( (1+A(y))^{-2r+1} \right)$$
$$= C_{y^{2r}} \left( \sum_{i=0}^{\infty} \left( \frac{-2r+1}{i} \right) A^{i}(y) \right) = C_{y^{2r}} \left( \sum_{i=0}^{r} \left( \frac{-2r+1}{i} \right) A^{i}_{r}(y) \right). \quad (197)$$

Thus, we get

$$\frac{w}{k} = 1 + \sum_{r=1}^{\infty} B_r \, u^{2r} \,, \tag{198}$$

where for  $r = 1, 2, \dots$ 

$$B_r = \frac{-1}{2r-1} C_{y^{2r}} \left( \sum_{i=0}^r \left( \frac{-2r+1}{i} \right) A_r^i(y) \right) .$$
 (199)

Explicitly, we have

$$\underline{r=1} \ B_1 = -C_{y^2} \left( 1 + \sum_{i=1}^{1} {\binom{-1}{i}} (A_1 y^2)^i \right) = A_1 , \qquad (200)$$

$$\underline{r=2} \quad B_2 = -\frac{1}{3} C_{y^4} \left( 1 + \sum_{i=1}^2 {\binom{-3}{i}} (A_1 y^2 + A_2 y^4)^2 \right)$$
$$= -\frac{1}{3} C_{y^4} (-3(A_1 y^2 + A_2 y^4) + 6(A_1 y^2 + A_2 y^4)^2)$$
$$= -\frac{1}{3} (-3A_2 + 6A_1^2) = A_2 - 2A_1^2 , \qquad (201)$$

$$\underline{r=3} \quad B_3 = -\frac{1}{5} C_{y^6} \left( 1 + \sum_{i=1}^3 {\binom{-5}{i}} (A_1 y^2 + A_2 y^4 + A_3 y^6)^i \right)$$
$$= -\frac{1}{5} C_{y^6} (-5(A_1 y^2 + A_2 y^4 + A_3 y^6) + 15(A_1 y^2 + A_2 y^4 + A_3 y^6)^2$$
$$- 35(A_1 y^2 + A_2 y^4 + A_3 y^6)^3)$$
$$= -\frac{1}{5} (-5A_3 + 30A_1A_2 - 35A_1^3) = A_3 - 6A_1A_2 + 7A_1^3. \quad (202)$$

In a similar fashion it follows that

$$B_{4} = A_{4} - 8A_{1}A_{3} - 4A_{2}^{2} + 36A_{1}^{2}A_{2} - 30A_{1}^{4} , \qquad (203)$$
  

$$B_{5} = A_{5} - 10A_{1}A_{4} - 10A_{2}A_{3} + 55A_{1}^{2}A_{3} + 55A_{1}A_{2}^{2} - 220A_{1}^{3}A_{2} + 143A_{1}^{5} . \qquad (204)$$

We can get a Bürmann-Lagrange result for y itself from (192). Thus

$$y = \sum_{j=1}^{\infty} \frac{1}{j!} \left[ \left( \frac{d}{dy} \right)^{j-1} \left( \frac{1}{F(y)} \right)^{j} \right]_{y=0} u^{j}$$
$$= \sum_{r=0}^{\infty} \frac{1}{2r+1} \frac{1}{(2r)!} \left[ \left( \frac{d}{dy} \right)^{2r} \frac{1}{F^{2r+1}(y)} \right]_{y=0} u^{2r+1}$$
$$= \sum_{r=0}^{\infty} D_{r} u^{2r+1} , \qquad (205)$$

where

$$D_r = \frac{1}{2r+1} C_{y^{2r}} \left( \frac{1}{F^{2r+1}(y)} \right) = \frac{1}{2r+1} C_{y^{2r}} \left( \sum_{i=0}^r \left( -\frac{2r-1}{i} \right) A_r^i(y) \right).$$
(206)

This yields  $D_0 = 1$ , and

$$D_{1} = -A_{1}, D_{2} = -(A_{2} - 3A_{1}^{2}), \quad D_{3} = -(A_{3} - 8A_{1}A_{2} + 12A_{1}^{3}),$$
  

$$D_{4} = -(A_{4} - 10A_{1}A_{3} - 5A_{2}^{2} + 55A_{1}^{2}A_{2} - 55A_{1}^{4}),$$
  

$$D_{5} = -(A_{5} - 12A_{1}A_{4} - 12A_{2}A_{3} + 78A_{1}^{2}A_{3} + 78A_{1}A_{2}^{2} - 364A_{1}^{3}A_{2} + 273A_{1}^{5}).$$
  
(207)

## 10 Numerical illustration of the results

## **A** Power series of w(k)

We have computed w(1) at the end of Section 10 and in a similar fashion we can compute w(0.1), w(0.4) and w(2). In Section 6, we have given the first terms of the power series of w(k) as

$$w(k) = \frac{1}{2}k + \frac{1}{8}k^2 - \frac{7}{180}k^3 + \frac{1667}{120960}k^4 - \frac{10621}{1814400}k^5 + \dots$$
(208)

Below we display for k = 0.1, 0.4, 1, 2 the 5 successive partial sums that can be formed from the right-hand side of (208).

k = 0.1		0.050000000	k = 0.4		0.200000000
		0.051250000			0.220000000
		0.051211111			0.217511111
		0.051212489			0.217863915
		0.051212430			0.217803973
w(0.1)	=	0.051212433	w(0.4)	=	0.217814154
k = 1		0.500000000	k = 2		1.000000000
$\kappa = 1$			$\kappa = 2$		
		0.625000000			1.500000000
		0.586111111			1.188888889
		0.599892526			1.409391534
		0.594038800			1.222072310
w(1)	=	0.595973391	w(2)	=	1.313398698

## **B** Table containing w, $w_U$ , $w_L$ , $w_U - w_L$ and $\frac{1}{2}(w_U + w_L)$

In Section 7, we have studied

$$w_U = w_U(k) = k + 1 - (1 + k^{-1}) \ln(k + 1) , \qquad (209)$$

and

$$w_L = w_L(k)$$
, fixed point  $\in [\frac{1}{2}k, k]$  of  $w \mapsto k(1+w^{-1})(1-w^{-1}\ln(1+w))$ 
(210)

as an upper bound and a lower bound, respectively, of w for k > 0. Below, we present two tables containing w,  $w_U$ ,  $w_L$ ,  $w_U - w_L$  and  $\frac{1}{2}(w_U + w_L)$  for small-to-large values of k and for very large values of k, respectively (for brevity, we have deleted the argument k from the various w-functions). For  $k \leq 20$ , the Newton method proposed in Section has been used to compute w (via  $W = w/\sqrt{2k}$ ), with  $\frac{1}{2}(w_U + w_L)$  as initialization. For  $k \geq 50$ , the iteration method of Section 9 has been used (involving up to 7 coefficients  $A_n$  to approximate  $y(k) = \sqrt{2k}/w(k)$  satisfying (178), (180)) as well as the Bürmann-Lagrange method (involving up to 5 coefficients  $B_r$ , see (198), to approximate w(k)/k). This is good enough for the required accuracy in the two tables.

k	w	$w_U$	$w_L$	$w_U - v$	$w_L  \frac{1}{2} \left( w_U + w_L \right)$
0.1	0.05121	0.05158	0.05082	0.0007	6 0.05120
0.2	0.10470	0.10607	0.10327	0.0027	0.10467
0.5	0.27710	0.28360	0.26987	7 0.0137	0.27673
1.0	0.59597	0.61370	0.57521	l 0.0384	9 0.59446
2.0	1.31339	1.35208	1.26684	1 0.0852	1.30946
5.0	3.77707	3.84988	3.69399	0.1558	9 3.77193
10.0	8.27355	8.36231	8.18096	6 0.1813	4 8.27164
20.0	17.71361	17.80325	17.6281	0.1712	17.71569
50.0	46.91571	46.98953	46.8510	0.1385	46.92028
100.0	96.28162	96.33872	96.2334	15  0.1052	96.28609
k	k - w	$k - w_U$	$k - w_L$	$w_U - w_L$	$k - \frac{1}{2} \left( w_U + w_L \right)$
100	3.71838	3.66128	3.76655	0.10527	3.71391
200	4.37106	4.32982	4.40517	0.07535	4.36749
500	5.25385	5.22903	5.27420	0.04516	5.25162
1000	5.93182	5.91663	5.94508	0.02942	5.93037
2000	6.61541	6.60520	6.62383	0.01863	6.61451
5000	7.52446	7.51909	7.52892	0.00983	7.52401
10000	8.21458	8.21136	8.21729	0.00593	8.21432

#### Observations

- 1.  $w_U$  and  $w_L$  appear indeed to be an upper bound and a lower bound, respectively, for w.
- 2.  $w_U w_L$  is small for small values of k and for very large values of k, and has a maximum value, of the order 0.20, for k somewhere between 10 and 20. The limiting behaviour  $w_U - w_L = \frac{1}{12}k^2 + O(k^3)$ ,  $k \downarrow 0$ , and  $w_U - w_L = O(k^{-1} \ln^2 k)$ ,  $k \to \infty$ , is confirmed by the tables.
- 3.  $\frac{1}{2}(w_U + w_L)$  is consistently very close to w, with a largest deviation of about -0.005 around k = 5 and a largest deviation of about +0.005 around k = 50, and vanishing deviation as  $k \downarrow 0$  or  $k \to \infty$ . Furthermore,  $\frac{1}{2}(w_U + w_L) w$  is negative for small k and positive for large k, the take-over point being apparently somewhere between 10 and 20.
- 4. The leading-order term in k w(k) is given by  $(1 + k^{-1}) \ln(1 + k) 1 = k w_U$ , and this is confirmed by the second table.

## C Auxiliary lower bounds $\bar{w}_L, \ \bar{\bar{w}}_L$

We have  $\bar{w}_L < \bar{\bar{w}}_L < w_L$ , where  $\bar{w}_L$  and  $\bar{\bar{w}}_L$  are defined for sufficiently large k by

$$\frac{1}{2}k + (\frac{1}{4}k^2 - k(E(Y) - 1))^{1/2}, \qquad E(Y) = (1 + Y^{-1})\ln(1 + Y) \quad (211)$$

with Y = k and  $Y = w_U$ , respectively. We have the following table.

k	$w_L - \overline{\overline{w}}_L$	$w_L - \bar{w}_L$
10	$2.528\times 10^{-2}$	$2.244\times10^{-1}$
100	$1.126\times 10^{-3}$	$3.959\times 10^{-2}$
1000	$2.974\times10^{-4}$	$5.992\times10^{-3}$
10000	$5.939\times10^{-7}$	$8.226\times 10^{-4}$

The order estimates  $(k^{-1} \ln k)^2$  and  $k^{-1} \ln k$  of  $w_L - \overline{w}_L$  and  $w_L - \overline{w}_L$ , respectively, see Proposition 6, are confirmed. Note also that for the case k = 10000 we have

$$\frac{1}{2}\left(w_U + \bar{w}_L\right) = 9991.78526 < 9991.78541 = w < 9991.78567 = \frac{1}{2}\left(w_U + \bar{\bar{w}}_L\right).$$
(212)

#### **D** Computation of w by iteration method

From Section 9, we can compute, for sufficiently large k, approximations  $w(k; N) = \sqrt{2k}/y(k; N)$ , where y(k; N) is an approximation of the solution y of the equation

$$y \int_{1}^{1+k} \frac{1/k}{(1+y^2 \ln s)^{1/2}} \, ds = u \,, \qquad u = \sqrt{\frac{2}{k}} \,. \tag{213}$$

The y(k; N) arise in the following manner. For sufficiently small y, the equation (213) can be written as

$$y\left(1 + \sum_{n=1}^{\infty} A_n y^{2n}\right) = u$$
, (214)

and the y(k; N), N = 1, 2, ..., appear when we solve the equation

$$y\left(1 + \sum_{n=1}^{N} A_n y^{2n}\right) = u \tag{215}$$

instead of (214). The  $A_n$  can be computed recursively according to (181) and (183), initialized by  $A_0 = 1 = X_0 = Y_0$ .

We illustrate the method by considering the cases k = 5, 10, 50, 100, 500.

 $\underline{k=5}$  We compute  $A_n, n = 1, ..., 6$  as

$$A_1 = -0.575055681, \quad A_2 = 0.582097375, \quad A_3 = -0.701857126,$$
  
$$A_4 = 0.925379751, \quad A_5 = -1.289354589, \quad A_6 = 1.865734249.$$
(216)

Next, we try to compute the y(k; N), solving (215), by successive substitution starting with  $y^{(0)} = u = \sqrt{2/k}$  for N = 1, ..., 6. This gives

$$\begin{array}{cccccccc} N & y(5\,;\,N) & w(5\,;\,N) = \sqrt{10}/y(5\,;\,N) \\ 1 & - & - & - \\ 2 & 0.73600 & 4.29651 \\ 3 & - & - & - \\ 4 & 0.76188 & 4.15059 \\ 5 & - & - & - \\ 6 & 0.77227 & 4.09473 \end{array}$$

For odd N, the successive procedure to compute y(5; N) diverges, while for even N this procedure has converged (to 9 decimal places) after some 10–20 iterations. The true values are y(5) = 0.83722 and w(5) = 3.77707.

 $\underline{k=10}$  We have now

$$\begin{split} A_1 &= -0.818842400 \,, \quad A_2 = 1.143570867 \,, \quad A_3 = -1.880581713 \,, \\ A_4 &= 3.362204205 \,, \quad A_5 = -6.330802987 \,, \quad A_6 = 12.35276688 \,, \, (217) \end{split}$$

and successive substitution gives

N	y(10;N)	$w(10; N) = \sqrt{20}/y(10; N)$
1		_
2	0.51850	8.62513
3	0.56134	7.96688
4	0.53348	8.38288
5	0.54570	8.19520
6	0.53804	8.31175

There is divergence of the successive procedure for N = 1, slow convergence for N = 3, and reasonably fast convergence for the other cases. The y(10; N) and w(10; N) oscillate around the true values y(10) = 0.54053 and w(10) = 8.27355, and these latter values are approximated slowly with increasing N.

 $\underline{k} = 50$  We have now

$$A_1 = -1.505231073$$
,  $A_2 = 3.655317589$ ,  $A_3 = -10.23631483$ ,  
 $A_4 = 30.82828367$ ,  $A_5 = -97.14234171$ ,  $A_6 = 315.8321473$ , (218)

and successive substitution gives

$$\begin{array}{lll} N & y(50\,;\,N) & w(50\,;\,N) = \sqrt{100}/y(50\,;\,N) \\ 1 & 0.21494 & 46.52268 \\ 2 & 0.21293 & 46.96335 \\ 3 & 0.21317 & 46.90916 \\ 4 & 0.21314 & 46.91662 \\ 5 & 0.21314 & 46.91556 \\ 6 & 0.21314 & 46.91571 \end{array}$$

There is a rather rapid convergence (some 5 iterations for 5 decimal places accuracy) of the successive substitution procedure in all cases. Furthermore, the y(50; N) have converged to the value y(50) = 0.21314 from N = 4 onwards while the w(50; N) have converged to w(50) = 46.91571 (this is confirmed by increasing N somewhat further).

 $\underline{k = 100}$  We have now

$$A_1 = -1.830635861$$
,  $A_2 = 5.321170243$ ,  $A_3 = -17.72269910$ ,  
 $A_4 = 63.25917564$ ,  $A_5 = -235.7335925$ ,  $A_6 = 905.0310697$ , (219)

and successive substitution gives

N	y(100;N)	$w(100; N) = \sqrt{200}/y(100; N)$
1	0.14726	96.02972
2	0.14685	96.29943
3	0.14688	96.28025
4	0.14688	96.28173
5	0.14688	96.28161
6	0.14688	96.28162

There is rapid convergence (some 3 iterations for 5 decimal places accuracy). Furthermore, the y(100; N) have converged to the value y(100) = 0.14688 from N = 3 onwards, while the w(100; N) have converged to w(100) = 96.28162 from N = 6 onwards.

 $\underline{k} = 500$  We have now

$$A_1 = -2.614519657, \quad A_2 = 10.59952694, \quad A_3 = -48.72888441,$$
  
$$A_4 = 238.6522706, \quad A_5 = -1215.535310, \quad A_6 = 6361.230874, \quad (220)$$

and successive substitution gives

$$\begin{array}{lll} N & y(500\,;\,N) & w(500\,;\,N) = \sqrt{1000}/y(500\,;\,N) \\ 1 & 0.063928 & 494.65740 \\ 2 & 0.063916 & 494.74780 \\ 3 & 0.063917 & 494.74610 \\ 4 & 0.063917 & 494.74614 \\ 5 & 0.063917 & 494.74614 \\ 6 & 0.063917 & 494.74614 \end{array}$$

There is very rapid convergence of the successive substitution process and of the y(500; N) and w(500; N) towards their respective limit values y(500) = 0.063917 and w(500) = 494.74614.

#### Observations

- 1. No or slow convergence of the successive substitution process when  $k \leq 10$ , with limit values y(k; N) and w(k; N) far away from the true values y(k) and w(k) for N = 1, ..., 6. Reasonable to good convergence for  $50 \leq k \leq 100$ , and excellent convergence for k > 100 (both for the successive substitution process and for the values of y(k; N) and w(k; N)to their limit values y(k) and w(k)).
- 2. Convergence behaviour well understood due to error estimate (190). Transparent algorithm, easy to implement.

#### **E** Computation of w by Bürmann-Lagrange inversion

With 
$$y = \sqrt{2k}/w$$
 and  $u = \sqrt{2/k}$ , we can write (182), (214) as  
 $\frac{1}{k}w = F(y) = 1 + \sum_{n=1}^{\infty} A_n y^{2n}$ , (221)

where y satisfies y F(y) = u, and where the  $A_n$  are as in (180–181). From the Bürmann-Lagrange formula, see (193–204), we then get for sufficiently small u

$$\frac{1}{k}w = 1 + \sum_{r=1}^{\infty} B_r u^{2r} .$$
(222)

The first 5 coefficients  $B_r$  are given by

$$B_{1} = A_{1}, \quad B_{2} = A_{2} - 2A_{1}^{2}, \quad B_{3} = A_{3} - 6A_{1}A_{2} + 7A_{1}^{3},$$
  

$$B_{4} = A_{4} - 8A_{1}A_{3} - 4A_{2}^{2} + 36A_{1}^{2}A_{2} - 30A_{1}^{4},$$
  

$$B_{5} = A_{5} - 10A_{1}A_{4} - 10A_{2}A_{3} + 55A_{1}^{2}A_{3} + 55A_{1}A_{2}^{2} - 220A_{1}^{3}A_{2} + 143A_{1}^{5}.$$
  
(223)

We illustrate the method for the cases k = 1, 5, 10, 50, 100, 500.

k = 1 We require first 
$$A_1, ..., A_5$$
. We find as in 10.D  
 $A_1 = -0.193147190$ ,  $A_2 = 0.070618989$ ,  $A_3 = -0.031592933$ ,  
 $A_4 = 0.015662677$ ,  $A_5 = -0.008269279$ . (224)

These  $A_1, ..., A_5$  are converted to  $B_1, ..., B_5$  according to (223), and we find

$$B_1 = -0.193147180, \quad B_2 = -3.992677118 \times 10^{-3},$$
  

$$B_3 = -1.923968074 \times 10^{-4}, \quad B_4 = -1.192450263 \times 10^{-5},$$
  

$$B_5 = -8.363327884 \times 10^{-7}.$$
(225)

With

$$\frac{w}{k} = w = 0.595973391, \quad u = \sqrt{\frac{2}{k}} = \sqrt{2},$$
 (226)

we display in the table below the numerical values of

$$1 + \sum_{r=1}^{R} B_r u^{2r}, \quad 1 + \sum_{r=1}^{R} B_r u^{2r} - \frac{w}{k}, \qquad R = 1, ..., 5.$$
 (227)

Thus we get

 $\underline{k=5}$  We convert  $A_1, ..., A_5$  from (216) into  $B_1, ..., B_5$  according to (223), and we find

$$B_1 = -0.575055681$$
,  $B_2 = -0.079280698$ ,  $B_3 = -0.024578974$ ,

$$B_4 = -9.726328081 \times 10^{-3}, \quad B_5 = -4.342859392 \times 10^{-3}.$$
 (228)

With

$$\frac{w}{k} = \frac{1}{5}w = 0.755415578$$
,  $u = \sqrt{\frac{2}{k}} = \sqrt{0.4}$ , (229)

we then get

 $\underline{k=10}$  We convert  $A_1, ..., A_5$  from (217) into  $B_1, ..., B_5$  according to (223), and we find

$$B_1 = -0.818842400, \quad B_2 = -0.197434884, \quad B_3 = -0.10540912,$$
  
$$B_4 = -0.071604664, \quad B_5 = -0.054818398.$$
(230)

With

$$\frac{w}{k} = \frac{1}{10} w = 0.827355248 , \qquad u = \sqrt{\frac{2}{k}} = \sqrt{0.2} , \qquad (231)$$

we then get

 $\underline{k=50}$  We convert  $A_1, ..., A_5$  from (218) into  $B_1, ..., B_5$  according to (223), and we find

$$B_1 = -1.505231073, \quad B_2 = -0.876123575, \quad B_3 = -1.096760292,$$
  
$$B_4 = -1.736530296, \quad B_5 = -3.091653647.$$
(232)

With

$$\frac{w}{k} = \frac{1}{50} w = 0.938314 , \qquad u = \sqrt{\frac{2}{k}} = \sqrt{0.04} , \qquad (233)$$

we then get

 $\underline{k = 100}$  We convert  $A_1, ..., A_5$  from (219) into  $B_1, ..., B_5$  according to (223), and we find

$$B_1 = -1.830635861, \quad B_2 = -1.381285068, \quad B_3 = -2.220091357,$$
  
$$B_4 = -4.504203953, \quad B_5 = -10.26756326.$$
(234)

With

$$\frac{w}{k} = \frac{1}{100} w = 0.962816252 , \qquad u = \sqrt{\frac{2}{k}} = \sqrt{0.02} , \qquad (235)$$

we then get

R	$1 + \sum_{r=1}^R B_r u^{2r}$	$1 + \sum_{r=1}^{R} B_r  u^{2r} - w/k$
1	0.963387282	$5.710\times10^{-4}$
1	0.962834768	$1.851\times10^{-5}$
3	0.962817008	$7.559\times10^{-7}$
4	0.962816287	$3.490 \times 10^{-8}$
5	0.962816254	$1.900\times10^{-9}$

 $\underline{k=500}$  We convert  $A_1,...,A_5$  from (220) into  $B_1,...,B_5$  according to (223), and we find

$$B_1 = -2.614519657, \quad B_2 = -3.071899130, \quad B_3 = -7.557597885,$$
  
$$B_4 = -23.386121408, \quad B_5 = -81.19365308.$$
(236)

With

$$\frac{w}{k} = \frac{1}{500} w = 0.989492281 , \qquad u = \sqrt{\frac{2}{k}} = \sqrt{0.004} , \qquad (237)$$

we then get

#### Observations

- 1. The coefficients of the products of the numbers  $A_n$  from which the coefficients  $B_r$  are built, see (223), are all integer. This is a non-trivial matter because of the occurrence of the factor -1/(2r-1) in front of the  $C_{y^{2r}}$ , see (199).
- 2. It seems almost impossible to get a closed form for the  $B_r$  in (223).
- 3. In all considered cases, it appears that the  $B_r$  are negative and much smaller in modulus than the  $A_n$ . I have no mathematical result for this phenomenon. Because of the rapidly growing coefficients required to convert the  $A_n$  into  $B_r$ , loss-of-digits is a hazard here.
- 4. While  $\sum_{n=1}^{\infty} A_n y^{2n}$  diverges for small k when y is in the relevant range (near  $\sqrt{2k/w}$ ), it appears that the odds for the series  $\sum_{r=1}^{\infty} B_r u^{2r}$  to converge are much better. I have investigated this issue numerically, also for very small k (like 0.1), and then very small coefficients  $B_r$  appear (while u becomes large, but apparently not large enough to destroy convergence). I have no mathematical results for all this.
- 5. I have also investigated, numerically, the Bürmann-Lagrange series of the y satisfying y F(y) = u, see (205–207). The coefficients  $D_r$  are all positive in the cases I have considered, and clearly larger in modulus than the coefficients  $B_r$ . We should try to understand the mapping

$$y \in \mathbb{C} \mapsto y \int_{1}^{1+k} \frac{1/k}{(1+y^2 \ln s)^{1/2}} \, ds = y F(y) ,$$
 (238)

and especially the analyticity range of its inverse. We have that y F(y) increases in  $y \in \mathbb{R}$ , and that

$$\lim_{y \to \pm \infty, \, y \in \mathbb{R}} \, y \, F(y) = \pm \, \int_{1}^{1+k} \frac{1/k \, ds}{(\ln \, s)^{1/2}} = \pm \, \frac{2}{k} \, \int_{0}^{(\ln(1+k))^{1/2}} e^{v^2} \, dv =: \pm L \, .$$
(239)

Thus a natural candidate for the radius of convergence of the inverse mapping  $y = u \sum_{r=0}^{\infty} D_r u^{2r}$  would be L in (239). It appears from numerial experiments based on the first 5 coefficients  $D_r$  that  $D_r/D_{r+1}$  approaches  $L^2$  from above as r grows, and it does so quite convincingly when k is small. However, no mathematical proof for this. I have not found such a crisp numerical result for the coefficients  $B_r$ .

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