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Efficient solution of differential equations by analytic continuation

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Abstract. A new method is described for the automatic solution of linear ordinary differential equations by the use of Taylor series. This new method is shown to be superior in speed and accuracy to conventional methods. The method is illustrated for Coulomb wavefunctions, confluent hypergeometric functions, zeros of Bessel functions and s-wave phaseshift for e-H scattering in the static approximation.

1. Introduction

The basic idea of the method developed in this paper is very old since it is founded on Cauchy's method of limits, (Cauchy 1835) and, according to Ince (1927), the essence of the method goes back to Euler (1768). The standard method can be described as follows. Given a differential equation (DE) with initial values specified at z_0 we approximate the solution in the neighbourhood of z_0 by a truncated Taylor series, where the values of the derivatives evaluated at z_0 are determined from successive differentiations of the DE. A new Taylor series about $z_1 = z_0 + h$ is then constructed from the derivatives of the first, and so on. In this way we obtain an analytic continuation of the solution of the DE along a polygonal path $\{z_0, z_1, z_2, \dots\}$.

One difficulty with this method is the evaluation of the Taylor coefficients by successive differentiation of the DE. In practical terms it means that one has to construct a subroutine for the Taylor coefficients for each DE. This is rather inconvenient, since the coefficients rapidly increase in complexity. Attempts have been made to automatise this process (see, for example, Wilson 1949, Gibons 1960, Leavitt 1966, Barton *et al* 1971, Corliss and Chang 1982, Gofen 1982).

Another difficulty arises if the DE has singularities anywhere in the complex z plane. Then the radius of convergence of its Taylor series about z_0 is equal to the distance to the closest singularity. Therefore if a singularity is close to z_0 we need a truncated Taylor series with a great number of terms to achieve a given accuracy with a preset step size. In some cases even a 100-term series is not long enough (Chang 1974). In Corliss and Lowery (1977) some estimates are given for the radius of convergence of a long Taylor series in the presence of a singularity. This latter difficulty is very serious because the majority of ODES of mathematical physics are linear DES of the second order with a regular singularity at the origin.

In this paper we propose a modification of the method which avoids both the above mentioned difficulties. The idea is to continue analytically a Frobenius series rather than a Taylor series. For simplicity we choose the most frequent case, i.e. a second-order

linear DE with a regular singularity and with analytic coefficients which are finite polynomials. Of course the method works for arbitrary order and, as we shall see, for more general analytic coefficients than finite polynomials.

The main advantages of this method are great accuracy, stability and speed. The relative speed, i.e. the speed with respect to the speed of classical integration methods for DE (Adams, Runge-Kutta, Milne, Hamming, etc) which are based on polynomial interpolation, is greater, the greater the required accuracy. Moreover, the truncated series forms a polynomial approximation to the solution which can be evaluated at any point in the neighbourhood $|z - z_0| < h$ with preset precision. Also, because polynomials are very easy to handle, we can evaluate derivatives and integrals of the solution or find zeros of the solution in a straightforward manner.

2. Analytic continuation

Consider the second-order linear DE

$$z^2 u'' + zP(z)u' + Q(z)u = 0. \tag{2.1}$$

Assuming $P(z)$ and $Q(z)$ to be finite polynomials, i.e. $\deg P = p < \infty$ and $\deg Q = q < \infty$, we have

$$P(z) = \sum_{i=0}^p P_i z^i = \sum_{i=0}^p \tilde{P}_i (z - z_0)^i$$

$$Q(z) = \sum_{i=0}^q Q_i z^i = \sum_{i=0}^q \tilde{Q}_i (z - z_0)^i. \tag{2.2}$$

We can find the coefficients \tilde{Q}_i and \tilde{P}_i exactly in a finite number of steps by the following algorithm (generalised Horner's rule; see, for example, Knuth 1981)

$$\begin{aligned} \tilde{P}_i &\leftarrow P_i && \text{for } i = 0(1)p \\ \tilde{P}_j &\leftarrow \tilde{P}_j + z_0 \tilde{P}_{j+1} && \text{for } i = 0(1)p - 1, j = p - 1(-1)i. \end{aligned} \tag{2.3}$$

Now writing $z = (z - z_0) + z_0$ and $z^2 = (z - z_0)^2 + 2z_0(z - z_0) + z_0^2$ we rewrite (2.1) as

$$[(z - z_0)^2 + 2z_0(z - z_0) + z_0^2]u'' + [(z - z_0) + z_0] \sum \tilde{P}_i (z - z_0)^i u' + \sum \tilde{Q}_i (z - z_0)^i u = 0. \tag{2.4}$$

First assume the characteristic exponent r of the Frobenius expansion to be equal to zero. Then the solution is of the form

$$u = \sum c_i (z - z_0)^i. \tag{2.5}$$

Substituting (2.5) into (2.4) we get

$$\begin{aligned} c_0 &= u(z_0) && c_1 = u'(z_0), \\ c_{i+2} &= -F_i / z_0^2 (i + 2)(i + 1) \end{aligned} \tag{2.6}$$

where

$$\begin{aligned} F_i &= 2z_0(i + 1)ic_{i+1} + i(i - 1)c_i + \sum_{j=\max(1, i-p)}^i jc_j \tilde{P}_{i-j} \\ &+ z_0 \sum_{j=\max(1, i-p+1)}^{i+1} jc_j \tilde{P}_{i-j+1} + \sum_{j=\max(0, i-q)}^i c_j \tilde{Q}_{i-j} \quad i = 0, 1, 2, \dots \end{aligned}$$

Thus starting the solution by a Frobenius expansion (see the appendix) about the origin we can continue this solution using (2.6), to arbitrary points z_0 in the complex plane.

If the characteristic exponent is different from zero we can reduce this case to the previous one. Let $r \in \{r_1, r_2\}$ be a characteristic exponent and assume first that $r_1 - r_2$ is not an integer. Then two independent solutions are of the form

$$u = z^r f(z) \quad r \in \{r_1, r_2\} \tag{2.7}$$

where $f(z)$ is an analytic function. Substituting (2.7) into (2.1) we obtain

$$z^2 f'' + z(2r + P(z))f' + [r(r - 1) + rP(z) + Q(z)]f = 0. \tag{2.8}$$

Now the coefficients \tilde{P}_i and \tilde{Q}_i in

$$2r + P(z) = \sum_{i=0}^p \tilde{P}_i (z - z_0)^i$$

and

$$r(r - 1) + rP(z) + Q(z) = \sum_{i=0}^{\max(p,q)} \tilde{Q}_i (z - z_0)^i$$

are calculated as above and using (2.6) we get a Taylor polynomial for $f(z)$.

Lastly, if $r_1 - r_2 = n$ is an integer then

$$u_1 = z^r f_1(z) \tag{2.9}$$

where f_1 is calculated as above and

$$u_2 = C u_1 \ln(z) + z^{r_2} f_2(z) \tag{2.10}$$

(see the appendix, formula (A8), for the determination of the constant C). Substituting (2.10) into (2.1) we get

$$\begin{aligned} z^2 f_2'' + z(2r_2 + P(z))f_2' + [r_2(r_2 - 1) + r_2P(z) + Q(z)]f_2 \\ = -Cz^n [(2r_1 - 1 + P(z))f_1 + 2zf_1']. \end{aligned} \tag{2.11}$$

Let this be equal to $-G(z)$, say. If $n = 0$, i.e. $r_1 = r_2 = r$, then $f_2(z) = z \sum c_i z^i$ and therefore it is advantageous to write zf_2 instead of f_2 in (2.11) and we get

$$\begin{aligned} z^2 f_2'' + z[2(r + 1) + P(z)]f_2' + [(r + 1)r + (r + 1)P(z) + Q(z)]f_2 \\ = -C[z^{-1}(P(z) - P_0)f_1 + 2f_1'] = -G(z). \end{aligned} \tag{2.12}$$

Now

$$G(z) = \sum G_i (z - z_0)^i \tag{2.13}$$

where the G_i are evaluated from (2.11) or (2.12). Again the coefficients \tilde{P}_i and \tilde{Q}_i in the expansion of the coefficients of f_2 and f_2' in (2.11) or (2.12) can be calculated as above and the coefficients c_i in

$$f_2(z) = \sum c_i (z - z_0)^i \tag{2.14}$$

are given by

$$\begin{aligned} c_0 = f_2(z_0) \quad c_1 = f_2'(z_0) \\ c_{i+2} = -(F_i + G_i) / z_0^2 (i + 2)(i + 1) \quad i = 0, 1, 2, \dots \end{aligned} \tag{2.15}$$

where F_i are the same as in the formula after (2.6).

3. Examples

3.1. Coulomb wavefunctions

The DE for the Coulomb wavefunction of order L in normal Forbenius form is

$$z^2 u'' + [-L(L+1) - 2\eta z + z^2]u = 0. \tag{3.1}$$

The expansion about zero is (for the regular solution)

$$F_L(\eta, z) = \sum a_i z^{i+r} \quad r = L + 1 \tag{3.2}$$

where

$$\begin{aligned} a_i &= (2\eta a_{i-1} - a_{i-2}) / i(i + 2L + 1) \\ a_0 &= 2^L \exp(-\pi\eta/2) |\Gamma(L + 1 + i\eta)| / \Gamma(2L + 2). \end{aligned} \tag{3.3}$$

The expansion about z_0 is

$$F_L(\eta, z) = \sum c_i (z - z_0)^i \tag{3.4}$$

where

$$\begin{aligned} c_i &= 0 \quad \text{for } i < 0 \\ c_0 &= u(z_0) \\ c_1 &= u'(z_0) \end{aligned} \tag{3.5}$$

$$\begin{aligned} c_{i+2} &= -\{2z_0 i(i+1)c_{i+1} + [(i-1)i - L(L+1) - 2\eta z_0 + z_0^2]c_i \\ &\quad + 2(z_0 - \eta)c_{i-1} + c_{i-2}\} / z_0^2(i+1)(i+2) \quad i = 0, 1, 2, \dots \end{aligned}$$

The results for $L = 0, \eta = z = 1$ are shown in table 1. For simplicity we put $n = N$, where n is the number of points on $[0, 1]$ and N is the degree of Taylor polynomial.

Note that only correct digits are shown. Thus we see from table 1 that for $n = N = 17$ we have achieved the accuracy of Barnett (1982). His algorithm, based on the original work by Steed (1967), computes the logarithmic derivative F'_L/F_L from continued fractions. This algorithm which is efficient if $x_L \ll x$, where $x_L = \eta + [\eta^2 + L(L+1)]^{1/2}$ is the classical turning point, needs hundreds of terms if $x \leq x_L$ and does not work for

Table 1. Results for the Coulomb wavefunction $F_0(1, 1)$ (i.e. $L = 0, \eta = z = 1$). N is the degree of the Taylor polynomial used and is also the number of points in $[0, 1]$.

N	$F_0(1, 1)$
11	0.227 526 210 510 560 0
12	0.227 526 210 510 560 029 23
13	0.227 526 210 510 560 029 239
14	0.227 526 210 510 560 029 239 295
15	0.227 526 210 510 560 029 239 295 890
16	0.227 526 210 510 560 029 239 295 890 88
17	0.227 526 210 510 560 029 239 295 890 889 14
18	0.227 526 210 510 560 029 239 295 890 889 146
19	0.227 526 210 510 560 029 239 295 890 889 146
20	0.227 526 210 510 560 029 239 295 890 889 146
Barnett (1982)	0.227 526 210 510 560 029 239 295 890 889 1

$x \ll x_L$. On the other hand, our Taylor series algorithm works on the whole interval with the same efficiency.

In figure 1 we compare the speed of our Taylor series method with that of the Numerov method for this same function.

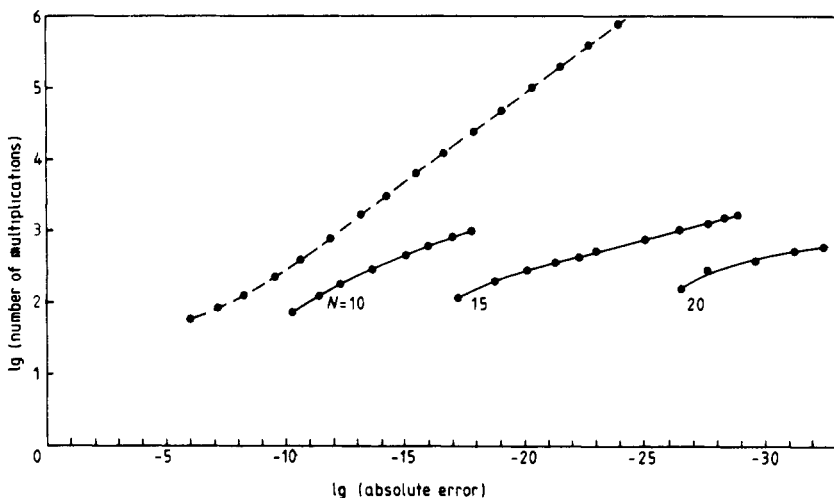


Figure 1. Number of multiplications required for calculation of $F_0(1,1)$ to the accuracy shown. ---, solution by Numerov's method; —, solution by present method. N denotes the order of the Taylor polynomial.

3.2. Confluent hypergeometric functions

Kummer's equation is

$$zu'' + (b - z)u' - au = 0 \tag{3.6}$$

with regular solution

$$M(a, b, z) = \sum c_i(z - z_0)^i \tag{3.7}$$

where

$$c_0 = M(a, b, z_0) \quad c_1 = M'(a, b, z_0) \tag{3.8}$$

$$c_{i+2} = [(z_0 - i - b)(i + 1)c_{i+1} + (i + a)c_i] / z_0(i + 2)(i + 1)$$

and irregular solution $U(a, b, z)$ which, for $a = b = 1$, for which case $r_1 = r_2 = 0$, can be written

$$U(1, 1, z) = -\exp(z) \ln(z) + zf_2(z) \tag{3.9}$$

where

$$f_2(z) = \sum c_i(z - z_0)^i \tag{3.10}$$

and

$$c_0 = f_2(z_0) \quad c_1 = f_2'(z_0) \quad c_i = 0 \quad \text{for } i < 0 \tag{3.11}$$

$$c_{i+2} = -\{z_0(i + 1)(2i + 3 - z_0)c_{i+1} + [(i + 1)^2 - 2z_0(i + 1)]c_i - (i + 1)c_{i-1} \exp z_0/i!\} / z_0^2(i + 2)(i + 1)$$

are found from direct substitution of (3.9) into (3.6). We integrated (3.6) along the ray $z = r \exp i(17/30)$ ($1 \leq r \leq 7$) in the second quadrant with the step size $h = \frac{1}{16} \exp i(17/30)$ and a Taylor polynomial of degree $N = 25$.

Because tables of $U(1, 1, z)$ of comparable accuracy are not available we have checked our values using the algorithm of Beam (1960) which is based on the well known continued fraction representation of $U(1, 1, z)$. This continued fraction algorithm (CFA) which is efficient if $|z| \gg T$, where $T = 2^{1/2} - 1$ is the classical turning point, needs thousands of terms if $|z| \leq T$ and does not work for $|z| \ll T$. Thus the situation is very similar to that of the Coulomb wavefunction which we discussed above. The results for our algorithm are shown in table 2. The computation of successive convergents of the CFA was stopped when they differed by less than 10^{-30} . (This, of course, does not imply that the error is less than 10^{-30}). Note that the CFA is more efficient only for very large $|z|$ and only for the first point in a given region. In the present method storing the values of the coefficients of the Taylor polynomials for given a region enables us to calculate $U(1, 1, z)$ at any point within the region with at most 25 multiplications.

Table 2. Results for the confluent hypergeometric function $U(1, 1, z)$ using a Taylor polynomial of degree 25 for $z = r \exp i(17/30)$. Here n is the number of terms in the CFA required to get comparable accuracy.

r	Re U	Im U	n
1	0.265 140 373 591 172 527 085 689 417 226 693E + 00	-0.699 914 570 363 053 710 739 591 235 609 459E + 00	1623
2	0.790 476 820 526 539 385 287 739 720 110 070E - 01	-0.438 591 626 614 630 913 524 543 913 543 972E + 00	819
3	0.258 451 523 285 909 629 858 367 889 673 286E - 01	-0.314 763 918 480 468 468 171 503 430 628 676E + 00	548
4	0.542 272 001 458 179 742 971 758 644 531 812E - 02	-0.243 462 234 697 021 961 596 538 284 522 224E + 00	412
5	-0.357 263 158 526 021 190 204 549 759 002 152E - 02	-0.197 585 636 738 600 911 244 633 704 818 831E + 00	330
6	-0.780 223 375 633 228 686 260 875 533 211 722E - 02	-0.165 809 415 196 983 651 085 002 821 795 384E + 00	275
7	-0.981 063 377 977 311 618 253 562 227 697 801E - 02	-0.142 602 773 767 741 852 565 186 933 206 512E + 00	236

3.3. Zeros of $J_\nu(x)$

In this example we illustrate another of the advantages of our method. Here we have used the Taylor series method to find an approximation to $J_\nu(x)$ and then used the approximate function to evaluate its zeros. Since we can calculate $u''(z)$ during the integration process with very little additional effort, zeros have been computed iteratively using Laguerre's method (Laguerre 1880, Parlett 1964). This method converges cubically and we have never needed more than four iterations to get 32S accuracy.

Let $f(z)$ be a Taylor polynomial of degree p . (In our calculations $20 \leq p \leq 25$.) Then the Laguerre iterate for z which is a zero of $f(z)$ is given by

$$z \leftarrow z - \frac{pf(z)}{f'(z) + \text{sgn}(f'(z))[(p-1)^2 f'(z)^2 - p(p-1)f(z)f''(z)]^{1/2}} \tag{3.12}$$

The first five zeros of $J_{1/3}(x)$ have been calculated using (3.12) where f is defined by (2.8) with $r = \frac{1}{3}$. These were calculated using step size $h = \frac{1}{16}$ and are shown in table 3. In fact we have calculated the first 100 zeros of $J_\nu(x)$ and $F_L(\eta, x)$ for different values of ν, η and L . These calculations confirm the results of Gerber (1964), who

calculated the first one hundred zeros of $J_0(x)$ to 19 digits accuracy and Ikebe (1975) (first five zeros of $F_L(\eta, x)$, $L = 0, 1$; $\eta = 0, 1, 2, 4, 8, 16$; 10 digit accuracy). We believe the minimum accuracy of the calculated zeros to be 30 significant digits. The tables are freely available from the authors to any interested persons.

Table 3. Zeros of $J_{1/3}(x)$ where x_n denotes the n th zero.

n	x_n
1	0.290 258 624 841 695 248 022 426 195 312 381E + 01
2	0.603 274 705 726 584 195 936 781 151 263 709E + 01
3	0.917 050 666 946 388 776 809 000 306 821 929E + 01
4	0.123 101 937 716 449 286 113 022 899 742 393E + 02
5	0.154 506 489 678 171 220 193 971 281 331 899E + 02

3.4. Phaseshifts

Here we show that the present method works for more general $P(z)$ and $Q(z)$ than finite polynomials. The radial scattering equation for electron scattering from the static potential of hydrogen, $V(r) = -(2 + 2/r) \exp(-2r)$, in normal Forbenius form is given by

$$z^2 u'' + Q(z)u = 0 \tag{3.13}$$

where

$$Q(z) = -L(L + 1) + k^2 z^2 + (2z^2 + 2z) \exp(-2z) \tag{3.14}$$

(Brandsen 1970), or

$$Q(z) = \sum Q_i z^i = \sum \tilde{Q}_i (z - z_0)^i \tag{3.15}$$

where

$$\begin{aligned} Q_0 &= -L(L + 1) & Q_1 &= 2 & Q_2 &= k^2 - 2 \\ Q_i &= 2(-2)^{i-2}(i-3)/(i-1)! & & & & i \geq 3 \end{aligned} \tag{3.16}$$

and

$$\begin{aligned} \tilde{Q}_0 &= -L(L + 1) + k^2 z_0^2 + 2z_0(1 + z_0) \exp(-2z_0) \\ \tilde{Q}_1 &= 2k^2 z_0 + (2 - 4z_0^2) \exp(-2z_0) \\ \tilde{Q}_2 &= k^2 + (-2 - 4z_0 + 4z_0^2) \exp(-2z_0) \end{aligned} \tag{3.17}$$

$$\tilde{Q}_i = [(-2)^{i-2}/i!][8z_0(1 + z_0) - 4i(1 + 2z_0) + 2(i - 1)i] \exp(-2z_0) \quad i \geq 3$$

where L represents the angular momentum of the electron and k its linear momentum.

Values of the phaseshift $\delta_0(k)$, $k = 0.1(0.1)1$, are shown in table 4 and agree with those given in Brandsen (1970). This test shows only the absence of gross errors, since Brandsen's results are given to at most four digits. From the analysis of the convergence with respect to both h and N we expect at least 30 digits accuracy.

Table 4. Phaseshift of electrons scattered from the static potential of hydrogen with zero angular momentum and linear momentum k .

k	$\delta_0(k)$
0.1	0.722 219 884 989 656 960 042 797 268 119 351E + 00
0.2	0.972 521 479 187 175 394 865 553 553 455 166E + 00
0.3	0.104 555 247 629 390 166 893 343 512 251 309E + 01
0.4	0.105 749 666 553 219 405 253 251 065 370 165E + 01
0.5	0.104 465 983 029 150 347 277 794 358 101 542E + 01
0.6	0.102 103 193 307 384 370 493 627 394 278 586E + 01
0.7	0.992 902 121 194 692 056 913 379 991 328 390E + 00
0.8	0.963 356 548 302 217 764 398 546 682 942 943E + 00
0.9	0.933 965 895 184 333 182 027 747 689 153 385E + 00
1.0	0.905 522 948 301 231 414 580 770 433 067 187E + 00

Appendix. Solution near the regular singular point

It is convenient to write the DE with regular singularity at $z = 0$ in the Frobenius normal form

$$z^2 u'' + zP(z)u' + Q(z)u = 0 \tag{A1}$$

where

$$P(z) = \sum P_i z^i \quad Q(z) = \sum Q_i z^i \tag{A2}$$

We assume $P_0^2 + Q_0^2 \neq 0$. (If $P_0 = Q_0 = 0$ we can divide (A1) by z and proceed similarly.) Then a solution to (A1) is of the form

$$u = z^r \sum a_i z^i \quad r \in \{r_1, r_2\} \tag{A3}$$

where r_1 and r_2 are roots of the indicial equation

$$r(r-1) + P_0 r + Q_0 = 0 \quad \text{Re } r_1 \geq \text{Re } r_2 \tag{A4}$$

and the a_i are given by

$$a_i = \frac{-\sum_{j=0}^{i-1} [(r+j)P_{i-j} + Q_{i-j}]a_j}{(r+i)(r+i-1) + (r+i)P_0 + Q_0} \quad a_0 = 1 \tag{A5}$$

where $r \in \{r_1, r_2\}$.

If $r_1 - r_2 = n$ is an integer and $n > 0$, then the second independent solution is of the form

$$u_2 = Cu_1 \ln(z) + \sum b_i z^{i+r_2} \tag{A6}$$

where $b_0 = 1$ and

$$b_i = \frac{-\sum_{j=1}^i (r_2 + i - j)P_j + Q_j}{(r_2 + i)(r_2 + i - 1) + (r_2 + i)P_0 + Q_0} b_{i-1} \quad 0 < i < n \tag{A7}$$

$$C = -\frac{1}{n} \sum_{j=1}^n [(r_1 - j)P_j + Q_j] b_{n-j} \tag{A8}$$

$$\begin{aligned}
 b_i = - & \left(C[2(r_2 + i) - 1]a_{i-n} + C \sum_{j=0}^{i-n} P_j a_{i-n-j} \right. \\
 & \left. + \sum_{j=1}^i [(r_2 + i - j)P_j + Q_j]b_{i-j} \right) [(r_2 + i)(r_2 + i - 1) \\
 & + (r_2 + i)P_0 + Q_0]^{-1} \quad i > n, \quad b_n = 0.
 \end{aligned} \tag{A9}$$

Lastly if $n = 0$ then $r_1 = r_2 = r$, say, and we have

$$u_2 = Cu_1 \ln(z) + \sum b_i z^{i+r+1} \tag{A10}$$

with

$$C = 1/(2Q_1 - P_0P_1) \tag{A11}$$

and

$$\begin{aligned}
 b_i = & \left[- \sum_{j=1}^i [(i-j+r+1)P_j + Q_j]b_{i-j} + C \left(\sum_{j=0}^i P_{j+1}a_{i-j} + 2(i+1)a_{i+1} \right) \right] (i+1)^{-1} \\
 & i = 1, 2, 3, \dots
 \end{aligned} \tag{A12}$$

$$b_0 = 1.$$

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