The solution of polynomial equations in interval arithmetic

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A two-stage method for use in interval arithmetic is given for the solution of algebraic equations. A particular adaptation for finding bounds on the roots of general polynomials with interval coefficients is described.

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1. Introduction

In the last few years, several generalised Newton-Raphson methods have been developed for use in interval arithmetic (Dargel *et al.*, 1966, Hanson, 1970). These have been implemented to produce algorithms giving information about the real roots of polynomials with real coefficients. In the following an account is given of an extension of these algorithms to the complex plane (though only real interval arithmetic is used), the aim being to produce regions which do not contain any root of the given polynomial, regions which may contain at most one root and regions which may contain more than one root.

The proposed method consists of two stages. In the first, a simple search is performed to isolate regions which may contain at most one root. During this stage, certain regions which do not contain roots or which may contain more than one root will also be isolated. In the second stage, the regions which may contain a root are examined using a generalisation of the Newton-Raphson process in an attempt to refine them by interval contraction. The theory developed below is derived for any regular function, a polynomial having either real or complex coefficients being a particular case.

The terminology of the interval analysis and arithmetic is that of Moore (1966).

2. Theory of the initial search

Let

$$f(z) = f(x + iy) = R(x, y) + iJ(x, y) \qquad (1)$$

be any regular function. The problem of finding the zeros of equation (1) can be regarded as the problem of solving the pair of simultaneous equations

$$R(x, y) = 0 \quad J(x, y) = 0 \qquad (2)$$

and it is supposed that it is required to find those zeros of equation (1) lying in a region D of the complex plane. Attention is restricted to rectangular regions with sides parallel to the co-ordinate axes when D may be represented by the interval vector (X, Y). (Upper case characters for variables denote intervals.) Let $R^*(X, Y)$ denote an interval extension of $R(x, y)$ over D, which is to say that

$$R^*(X, Y) \supset \{R(x, y) \mid x \in X, y \in Y\}\,. \qquad (3)$$

Similarly $J^*(X, Y)$ is defined to be an interval extension of $J(x, y)$ over D. Clearly a necessary condition for D to contain a zero of equation (1) is that

$$R^*(X, Y) \supset 0 \text{ and } J^*(X, Y) \supset 0\,. \qquad (4)$$

In order to examine whether D may contain more than one zero, use can be made of the following theorem.

Theorem:
Given a closed convex region D and a regular function $f(z) = R(x, y) + iJ(x, y)$, if $f(z)$ has two or more zeros in D then the partial derivatives R_x, R_y, J_x and J_y all take the value zero somewhere in D, though not necessarily simultaneously.

Proof:
Since $f(z)$ is regular, $R_x = J_y$ and $R_y = -J_x$ and so it is sufficient to show that both R_x and R_y take the value zero somewhere in D. If $f(z)$ has a repeated zero, say z_1, then $f(z_1) = f'(z_1) = 0$. But $f'(z) = R_x + iJ_x = R_x - iR_y$ and the required result is immediate.

Assume then that $f(z)$ has two isolated zeros in D, say z_1 and z_2, where $z_1 = x_1 + iy_1$ and $z_2 = x_2 + iy_2$. Let $\tan\theta = (y_1 - y_2)/(x_1 - x_2)$ be the gradient of the line joining z_1 and z_2. Since D is convex, the line segment $(1 - t)z_1 + tz_2$, $0 \leqslant t \leqslant 1$, is contained in D.

Then

$$\frac{d}{dt} R = R_x \cos\theta + R_y \sin\theta$$

$$\frac{d}{dt} J = J_x \cos\theta + J_y \sin\theta$$

$$= -R_y \cos\theta + R_x \sin\theta$$

whence

$$\frac{d}{dt}(R\cos\theta + J\sin\theta) = R_x$$

and

$$\frac{d}{dt}(R\sin\theta - J\cos\theta) = R_y\,.$$

Now $R\cos\theta + J\sin\theta$ may be considered as a real valued function of the variable t and is such that it takes the value zero when $t = 0$ or 1. Thus, by applying Rolle's Theorem, $\frac{d}{dt}(R\cos\theta + J\sin\theta)$ must take the value zero for some t, $0 < t < 1$. Hence R_x, and similarly R_y, takes the value zero at some point on the line (z_1, z_2). Thus R_x and R_y, and hence J_x and J_y, both vanish somewhere in D. Thus a necessary condition for D to contain at most one zero of equation (1) is that $R^*_x(X, Y)$, where $R^*_x(X, Y)$ is an interval extension of $R_x(x, y)$ over (X, Y), etc., and $R^*_y(X, Y)$ do not both contain zero. Using this condition and equation (4) it is possible to examine D and isolate subregions which contain at most one zero of equation (1). An account of one possible approach is given in Section 4.

3. The generalised Newton-Raphson process

Consider a general system of k equations in k unknowns

$$\mathbf{p}(\mathbf{x}) = \mathbf{0}\,. \qquad (5)$$

Let $\mathbf{X} = (X_1, X_2, \ldots, X_k)^T$ denote a k-dimensional interval vector.

Let $\mathbf{P}$ represent an interval extension of $\mathbf{p}$ over $\mathbf{X}$, which is to say that $\mathbf{P}(\mathbf{X}) = \mathbf{P}(X_1, X_2, \ldots, X_k) \supset \{\mathbf{p}(x_1, \ldots, x_k) \mid x_i \in X_i, i = 1, 2, \ldots, k\}$. Let $\mathbf{X}$ be an interval vector containing a solution of equation (5), $\mathbf{r}$ say, and let $\mathbf{t}$ be any other vector belonging to $\mathbf{X}$. Then, using the mean value theorem

$$0 = p_i(\mathbf{r}) = p_i(\mathbf{t}) + \mathbf{G}_i(\mathbf{t} + \theta_i(\mathbf{r} - \mathbf{t}))\,.\,(\mathbf{r} - \qquad 0 < \theta_i < 1, i = 1, 2, \ldots, k \qquad (6)$$

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where $\mathbf{G}_i$ is the i-th row of $\mathbf{G}$, the matrix of first derivatives of $\mathbf{p}$.

From this it follows immediately that

$$\mathbf{r} \in \mathbf{t} - \mathbf{V}(\mathbf{X})\,\mathbf{p}(\mathbf{t}) \qquad (7)$$

where $\mathbf{V}(\mathbf{X})$ is an interval matrix containing the inverses of all the matrices in $\mathbf{G}^*$, the interval extension of $\mathbf{G}$ defined over $\mathbf{X}$. For the interval vector $\mathbf{X}$ let

$$\mathbf{m}(\mathbf{X}) = (m(X_1), m(X_2), \ldots, m(X_k))^T$$

where $m(X_i)$ denotes the mid-point of X_i. We can then define

$$\mathbf{N}(\mathbf{X}) = \mathbf{m}(\mathbf{X}) - \mathbf{V}(\mathbf{X})\,\mathbf{P}(\mathbf{m}(\mathbf{X})) \qquad (8)$$

as the basis for a refinement algorithm in interval arithmetic. The full algorithm consists of starting from some $\mathbf{X}_0$ and determining a sequence of intervals $\{\mathbf{X}_i\}$ by the relation

$$\mathbf{X}_{i+1} = \mathbf{X}_i \cap \mathbf{N}(\mathbf{X}_i) \quad i = 0, 1, 2, \ldots \qquad (9)$$

A necessary condition for the existence of $\mathbf{V}(\mathbf{X}_0)$ is that $\mathbf{G}^*(\mathbf{X}_0)$ does not contain a singular matrix. Assuming that this is so, then since $\mathbf{Y} \subset \mathbf{X}$ implies $\mathbf{G}^*(\mathbf{Y}) \subset \mathbf{G}^*(\mathbf{X})$, $\mathbf{V}(\mathbf{X}_i)$ is defined for all $i > 0$. Further, if $\mathbf{r} \in \mathbf{X}_0$ then $\mathbf{r} \in \mathbf{N}(\mathbf{X}_0)$ using equations (7) and (8), and hence to $\mathbf{X}_1$ from equation (9) and, by induction,

$$\mathbf{r} \in \mathbf{X}_i \; \forall_i \qquad (10)$$

Starting from an interval $\mathbf{X}_0$ which may contain a zero (for which it is clearly necessary that $\mathbf{P}(\mathbf{X}_0) \supset \mathbf{0}$) and assuming that $\mathbf{V}(\mathbf{X}_0)$ exists, application of the algorithm defined by equations (8) and (9) leads to two possibilities. Firstly, the sequence may terminate due to either the intersection of equation (9) becoming empty or $\mathbf{P}(\mathbf{X}_i)$ not containing $\mathbf{0}$ for some i. Such a termination, due to either reason, indicates that $\mathbf{X}_0$ did not contain a solution. The second possibility is that the interval vectors given by the algorithm converge to some interval which may contain one or more zeros of the function.

Few results are known about sufficient conditions for ensuring the presence of a solution. One, due to Kahan (Hansen, 1969) is that if for some i,

$$\mathbf{N}(\mathbf{X}_i) \subset \mathbf{X}_i \qquad (11)$$

then $\mathbf{X}_i$ definitely contains a solution of equation (5).

Returning to the problem of finding the zeros of a regular function,

$$\mathbf{p} = \begin{pmatrix} R(x, y) \\ J(x, y) \end{pmatrix} \text{ and } \mathbf{G} = \begin{pmatrix} R_x & J_x \\ R_y & J_y \end{pmatrix}.$$

Using the Cauchy–Riemann relations, it is readily shown that

$$\mathbf{G}^{-1} = \frac{1}{R_x^2 + J_x^2} \begin{pmatrix} R_x & J_x \\ -J_x & R_x \end{pmatrix}$$

and hence the interval matrix $\mathbf{V}$ of equation (7) is given by

$$\frac{1}{R_x^{*2}(X, Y) + J_x^{*2}(X, Y)} \begin{pmatrix} R_x^*(X, Y) & J_x^*(X, Y) \\ -J_x^*(X, Y) & R_x^*(X, Y) \end{pmatrix}.$$

It is thus seen that $\mathbf{V}$ is not defined if $R_x^{*2}(X, Y) + J_x^{*2}(X, Y)$ contains zero. This will be the case only if $R_x^*(X, Y)$ and $J_x^*(X, Y)$ both contain zero, and this is just one of the criteria used in the initial search in deciding that an interval may contain at most one zero.

4. Computational details

A polynomial solver has been developed using the above theory and with the following strategy:

1. Assuming that a complete solution is required, the polynomial is normalised to have all its roots lying in some rectangular region with sides parallel to the co-ordinate areas. (The simplest normalisations lead to all the roots lying in the unit circle which lies within the square with sides of length 2 units, centre the origin. Note that if the polynomial has real coefficients, a complete solution can be found by considering only the top half of this square.) Alternatively, it may be required to find only those roots lying within some given rectangular region.
2. The interval extensions R^* and J^* are evaluated over the rectangular region under consideration. If $0 \notin R^*$ or $0 \notin J^*$, then there is no root in the given region. In general there will be a list of sub-intervals requiring investigation with the current interval at the end of the list. If it is found that there is no root in the interval, the interval is removed from the list and a return is made to 2 with the new current interval.
3. The interval extensions R_x^* and J_x^* are evaluated over the interval under consideration. If $0 \in R_x^*$ and $0 \in J_x^*$ the refinement process cannot be applied. The interval is divided into four sub-intervals by bisection in both the x- and y-components and these sub-intervals are added to the list of intervals requiring investigation and a return is made to 2. An exit may be forced at this stage if the size of the intervals falls below a certain tolerance when an interval which may contain more than one root will have been isolated.
4. The refinement process is applied to the interval under consideration leading to one of the following results:
   (*a*) convergence to an interval containing at most one root and definitely known to contain a root if equation (11) holds. Convergence here is taken to mean that, for some i, $\mathbf{X}_{i+1} = \mathbf{X}_i$. From the form of equation (9) it is seen that this situation must arise eventually, but, due to the possibility of ultimate first order convergence, it has been found desirable to use a test for convergence based on changes in the limits defining the interval. In practice, it has been found that convergence can be established misleadingly at an early stage in the iterations if $\mathbf{N}(\mathbf{X}_i) \supset \mathbf{X}_i$ and hence $\mathbf{X}_{i+1} = \mathbf{X}_i$. Although this has only been found to happen on the first iteration, it is perhaps advisable to include a check on this occurrence for the first few iterations, its detection leading to the subdivision of the interval followed by a return to 2;
   (*b*) the interval is shown to contain no root.

On a satisfactory conclusion to the refinement stage, the interval is removed from the list and a return is made to 2, the whole process being completed when the list of subintervals is exhausted. In practice, it has been found that about eight applications of the refinement stage lead to convergence for polynomials of fairly low order. To safeguard against slow convergence, it is suggested that for well-conditioned polynomials an upper bound, say 12, should be set on the number of applications of the refinement stage. If this limit is reached before convergence occurs, the interval is subdivided and a return is made to 2.

On completion of the whole search and refinement process, it is possible that more than n (the degree of the polynomial) intervals will have been isolated. This could be the case, for example, if the polynomial has a root close to or on a line of sub-division, when one could expect to obtain overlapping or abutting intervals. Should this occur, it is possible to specify the union of such intervals as the input for the polynomial solver. In this way, a more detailed examination may indicate the definite presence of a single root if equation (11) holds; alternatively, it may not be possible to resolve the uncertainty.

The interval extensions R^*, J^*, R_x^* and J_x^* are evaluated many times during the execution of the algorithms and efficient methods for doing this are required. Two criteria are important, the cost of each evaluation and the width of the extension produced. In order to decrease the number of interval splittings, this being the likely limiting factor in any computation, it is necessary to evaluate the interval extensions with minimum

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width so as to exclude regions not containing a root as rapidly as possible and this should be the decisive criterion.

Consider the function $R(x, y)$. Two methods are available for its evaluation. Firstly it is readily shown that

$$R(x, y) = f(x) - y^2 \frac{f^{(2)}(x)}{2!} + y^4 \frac{f^{(4)}(x)}{4!} - \dots$$

with the series terminating after a finite number of terms since $f(x)$ is a polynomial. Numerical values for $f^{(r)}(x)/r!$ can be obtained by a process of repeated synthetic division which can be re-formulated in interval arithmetic to lead to the interval extensions

$$[F^{(r)}(X)/r!]$$

and hence

$$\begin{aligned} R^*(X, Y) &= F(X) - Y^2[F^{(2)}(X)/2!] + Y^4[F^{(4)}(X)/4!] - \dots \\ &= F(X) - L[F^{(2)}(X)/2!] + L^2[F^{(4)}(X)/4!] - \dots \quad (12) \end{aligned}$$

where $L = Y^2$. Similarly

$$J^*(X, Y) = Y\{F^{(1)}(X) - L[F^{(3)}(X)/3!] + L^2[F^{(5)}(X)/5!] - \dots\}$$

$$R_x^*(X, Y) = F^{(1)}(X) - 3L[F^{(3)}(X)/3!] + 5L^2[F^{(5)}(X)/5!] - \dots$$

and

$$J_x^*(X, Y) = Y\{2[F^{(2)}(X)/2!] - 4L[F^{(4)}(X)/4!] + 6L^2[F^{(6)}(X)/6!] - \dots\}.$$

These polynomials in L can be evaluated in interval arithmetic either by the direct use of nested multiplication or with the initial re-formulation in centred form (Moore, 1966). In practice, it seems (Hitchins, 1971) that the centred form does produce the more satisfactory results, but some advantage may be gained by performing both evaluations and then taking the intersection of the two extensions.

An alternative method for evaluating $R(x, y)$ would appear to be the standard algorithm for division of a polynomial by the complex number $x + iy$. Experimental evidence (Hitchins, 1971) indicates that while this is computationally faster, the interval extensions obtained are wider than those obtained from equation (12) and the corresponding expressions.

5. Examples

The complete algorithm described above has been used successfully to solve many low order interval polynomials with real coefficients. Each polynomial was normalised so as to have all its roots lying within the unit circle, centre the origin. The initial rectangle examined was taken to be ([−1·01, 1·00], [−0·01, 1·00]), the perturbations being introduced to lessen the likelihood of a root lying exactly on the boundary of a subrectangle when dealing with the test examples.

Some typical results for polynomials with well-separated roots are given in **Table 1.** The degree of the polynomial is denoted

Table 1

NO	n	COEFFICIENTS	ϵ	A	N_R	N_N	N_F	INITIAL	N_C	N_K	CALCULATED ROOT	EXACT ROOT
1	3	(1, 1, 1, 1)	10^{-4}	2·00	53	15	7	[−0·51, −0·38] + i[−0·01, 0·06]	6	2	[−1·00020043, −0·99979957]	1
								[−0·01, 0·25] + i[0·49, 0·63]	8	5	[−0·00010017, −0·00010066] + i[0·99989983, 1·00010017]	i
2	4	(1, −8, 39, −62, 1)	10^{-3}	8·00	361	86	63	[0·37, 0·44] + i[0·49, 0·53]	9	5	[2·98563613, 3·01436658] + i[3·98564064, 4·01431042]	3 + 4i
								[0·12, 0·25] + i[0·11, 0·18]	8	4	[0·99953425, 1·00046575] + i[0·99951429, 1·00048571]	1 + i
3	5	(1, −6, 14, −16, −7, −30)	10^{-4}	6·00	549	95	76	[−0·14, −0·06] + i[0·14, 0·18]	8	4	[−0·49592257, −0·49589203] + i[0·90228483, 0·90231578]	−0·49590730 + i0·90230031
								[0·56, 0·63] + i[−0·01, 0·01]	7	2	[3·68073213, 3·68186044]	3·68129628
								[0·24, 0·31] + i[0·36, 0·41]	9	4	[1·65460315, 1·65591516] + i[2·22367129, 2·22498344]	1·65525916 + i2·22432737
4	6	(1, 0, 0, 0, 0, 0, −1)	10^{-6}	2·00	1,021	191	161	[0·49, 0·63] + i[−0·01, 0·06]	8	5	[0·99999883, 1·00000117]	1
								[0·24, 0·28] + i[0·43, 0·45]	7	3	[0·49999757, 0·50000243] + i[0·86602293, 0·86602788]	0·5 + i0·86602540
								[−0·51, −0·44] + i[−0·01, 0·03]	6	2	[−1·00000117, −0·99999883]	−1
								[−0·26, −0·19] + i[0·43, 0·47]	8	5	[−0·50000243, −0·49999757] + i[0·86602293, 0·86602788]	−0·5 + i0·86602540
5	7	(1, 4·87, −0·67, −0·15430003, −0·4265, −1·02113, −2·48608, −6·2771496)	10^{-6}	5·87	2,421	336	306	[−0·89, −0·82] + i[−0·01, 0·01]	5	1	[−5·00000610, −4·99999390]	−5
								[0·07, 0·09] + i[0·15, 0·17]	9	3	[0·49999936, 0·50000063] + i[0·92195380, 0·92195507]	0·5 + i0·92195444
								[−0·10, −0·08] + i[0·14, 0·16]	7	3	[−0·50000062, −0·49999938] + i[0·87177914, 0·87178041]	−0·5 + i0·87177978
								[0·18, 0·22] + i[−0·01, 0·01]	8	2	[1·12999976, 1·13000023]	1·13
								[−0·20, −0·16] + i[−0·01, 0 01	6	2	[−1·00000029, −0·99999968]	−1

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by n and the unperturbed coefficients are given in order of decreasing powers, the coefficients of the interval polynomials being obtained by perturbing each exact coefficient by $[\epsilon, -\epsilon]$ before the roots of the polynomial are normalised by the factor A. N_R indicates the number of rectangles examined during the initial search. For N_N of them, an entry is made into the Newton refinement stage and in N_F cases the refinement stage is left after one iteration. The regions of the normalised plane which converge to roots are given to two decimal places. N_C iterations are required before convergence occurs (a tolerance of $5_{10}{}^{-11}$ was used) and after N_K of these iterations, equation (11) holds indicating the definite presence of a root. Finally, the calculated interval root is given to eight decimal places together with the corresponding root of the unperturbed polynomial. (In these cases where no imaginary part is given, it was found to be less than the machine tolerance.)

As an example of a problem with equal roots, consider the polynomial

$$z^4 - 6z^3 + 9z^2 + 4z - 12$$

which has exact roots -1, 2, 2 and 3. The coefficients were each perturbed by $[-10^{-3}, 10^{-3}]$ and a normalisation factor of 3·5 was used. In the initial search, after examining 325 subintervals, three were isolated as containing at most one root. The first can be represented by the interval vector ([−0·51, −0·25], [−0·01, 0·12]) and this was refined to the real interval root [−1·00013912, −0·99986088] after nine applications of the Newton process, equation (11) being established after five of them. The other two regions were refined to the real interval roots [2·96086884, 3·00535157] and [3·00535156, 3·03104179] in 24 and 15 iterations respectively and for neither interval was equation (11) established. During the search, the minimum width of subdivision permitted was taken to be $5_{10}{}^{-3}$ and 56 intervals were then isolated as containing one or more roots. Their union indicated the possibility of one or more roots of the original polynomial in the cross-shape region which is the union of the two intervals ([1·906133, 2·125977], [−0·000479, 0·006426]) and ([1·988574, 2·016055], [−0·109990, 0·109990]) which correspond to perturbations of the double root along the real axis and off the real axis respectively. Similar behaviour is noted when the exact polynomial is solved using interval arithmetic, though, of course, the induced perturbations are much less.

As a final example of the use of the algorithm, consider the fifteenth order polynomial first given by Henrici and Watkins (1965)

$$\begin{aligned} z^{15} &+ 39{\cdot}247z^{14} - 20{\cdot}573z^{13} - 8{\cdot}3243z^{12} + 22{\cdot}834z^{11} \\ &- 0{\cdot}78440z^{10} - 4{\cdot}2754z^9 + 504{\cdot}15z^8 - 21{\cdot}134z^7 \\ &+ 72{\cdot}874z^6 + 2{\cdot}9240z^5 - 94{\cdot}501z^4 + 5{\cdot}5945z^3 \\ &+ 4{\cdot}0532z^2 + 2549{\cdot}3z + 21{\cdot}129. \end{aligned}$$

The implementation of the full algorithm available proves too slow to permit the complete solution of higher order polynomials. It can, however, be used to obtain interval bounds from known estimates of the roots. Among the roots of the polynomial as given by Henrici and Watkins are $-0{\cdot}0082883$ and $-0{\cdot}70578 + 0{\cdot}96858i$. In order to obtain interval bounds for these roots, the Newton process was started from the intervals ([−0·5075, −0·0050], [−0·0100, 0·2425]) and ([−0·710, −0·705], [0·960, 0·970]) respectively, taking the given coefficients as being exact. The process converged after four and six iterations to the interval roots [−0·00828827, −0·00828826] and [−0·70578427, −0·70578426] + i[0·96858404, 0·96858405] and for both equation (11) held. The non-feasibility of the complete algorithm is due, generally, to the large number of interval splittings required to obtain regions in which the Newton process can be applied. For well-separated roots, this may not be a problem, and, in fact, the starting interval used for the real root in this example is obtained from the standard search routine as used in the examples of Table 1.

6. Discussion

The main difficulty in the practical implementation of the algorithm lies in the initial bisection-type search (with its first-order convergence) for a region in which the Newton process can be applied. This renders the solution of even fairly low order polynomials possibly prohibitively time-consuming, particularly in regions of close roots.

Some overall improvement in efficiency would be possible through changes in the interval arithmetic package. The current implementation, developed for the ICL KDF9 computer at the University of Leeds, is written in ALGOL in the form of a single-address, low-level language with a pseudo-accumulator. A full description is available in Hitchins (1972).

Improvements in the search routine could be obtained by several means. Firstly, if the interval extensions required could be evaluated so as to have narrower widths, the earlier exclusion of intervals definitely containing no root would be possible. Secondly, some improvement may result from an extension of the algorithm to include additional exclusion criteria. A further possibility would be the use of a more refined interval splitting algorithm making use of the calculated function and derivative values.

An alternative approach would be to find initial estimates for the roots using a polynomial solver in real arithmetic (see, for example, Grant and Hitchins, 1971), followed by the determination of error bounds on these estimates using a method such as that given by Fekete (Hansen, 1969). The resulting intervals could then be used as data for the interval polynomial solver.

It is claimed, however, that in spite of the difficulties mentioned above, the algorithm does provide a means of extending some of the ideas of interval arithmetic to the solution of polynomial equations in the complex plane.

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