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THE "PEGASUS" METHOD FOR COMPUTING THE ROOT OF AN EQUATION

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Abstract.

A modified Regula Falsi method is described which is appropriate for use when an interval bracketing of the root is known. The algorithm appears to exhibit superior asymptotic convergence properties to other modified linear methods.

1. Introduction.

In the Regula Falsi method for computing a root of the equation

$$f(x) = 0 \tag{1.1}$$

starting values x_{i-1} and x_i are chosen such that $f_{i-1}f_i < 0$. A new value x_{i+1} is computed by linear interpolation and f_{i+1} evaluated. The estimates used for the next iteration are x_{i+1} and whichever of x_{i-1} and x_i give a function value of opposite sign to f_{i+1}. A recent paper (Dowell and Jarratt, 1971) described a modification of the Regula Falsi algorithm which led to a process with efficiency 1.442. In the present work an alternative modification is given which appears to show superior properties. The technique seems first to have been used in a library subroutine for the Pegasus computer but its authorship is not known to us. We give here a theoretical analysis of its behaviour together with a report on our numerical experience with it.

2. The 'Pegasus' Algorithm.

The method follows the Regula Falsi, with the variation that the approximations for the next iteration are chosen as follows:

i) if $f_{i+1}f_i < 0$, then (x_{i-1}, f_{i-1}) is replaced by (x_i, f_i).
ii) if $f_{i+1}f_i > 0$, then (x_{i-1}, f_{i-1}) is replaced by $(x_{i-1}, f_{i-1}f_i/(f_i+f_{i+1}))$.

In either case (x_{i+1}, f_{i+1}) replaces (x_i, f_i) and this choice ensures that the function values used at each iteration will always have opposite signs.

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The philosophy of the method is to scale down the value f_{i-1} by the factor $f_i/(f_i+f_{i+1})$, in order to prevent the retention of an end-point. The importance of the modification, however, is that in this form it leads, as we shall show, to an order of convergence which is superior to that of the Secant Iteration while still retaining the advantage of bracketing the zero sought. It is therefore clearly to be preferred to the Illinois method (Dowell and Jarratt, 1971) and also, in particular, to the various hybrid algorithms obtained by combining the Secant method with the bisection rule.

3. Analysis of Asymptotic Convergence.

We begin by defining the error in the rth approximation to a root, θ, of (1.1) by $\varepsilon_r = x_r-\theta$ and using the Taylor expansion of f_r about θ we find

$$f_r = \sum_{j=1}^{\infty} c_j \varepsilon_r^{\,j}, \quad \text{where } c_j = f^{(j)}(\theta)/j!\,,$$

and $c_0 = f(\theta) = 0$.

If now we assume that x_{i-1} and x_i are both close to θ, then by substituting in the iterative formula

$$x_{i+1} = \frac{x_i f_{i-1} - x_{i-1} f_i}{f_{i-1}-f_i},$$

it is easy to show that for a simple root the errors satisfy

$$\varepsilon_{i+1} \cong \left(\frac{c_2}{c_1}\right) \varepsilon_i \varepsilon_{i-1}\,, \tag{3.1}$$

this result being the normal Secant error relation.

The subsequent error behaviour now depends on the sign of $f_i f_{i+1}$.

In the unmodified case, we can again apply (3.1) to obtain

$$\varepsilon_{i+2} \cong \left(\frac{c_2}{c_1}\right) \varepsilon_{i+1} \varepsilon_i\,,$$

while for the modified case, in which $f_i f_{i+1}$ is positive, lengthy analysis gives

$$\varepsilon_{i+2} \cong \left(\frac{c_2}{c_1}\right)^2 \varepsilon_{i+1} \varepsilon_{i-1}^2\,. \tag{3.2}$$

The solution of this difference equation is readily shown to be $\varepsilon_{i+2} = c\varepsilon_{i+1}^{d_1}$, where c is constant and d_1 is the real root of the equation $x^3-x^2-2 = 0$. We find $d_1 = 1.69562\ldots$. From (3.2) it is clear that asymptotically

ε_{i+1} and ε_{i+2} will take the same sign and we therefore deduce that a modified iteration (M_1) must always be followed by a second modified iteration (M_2). Further analysis now shows that ε_{i+3} satisfies

$$\varepsilon_{i+3} \cong \left(\frac{c_2}{c_1}\right) \varepsilon_{i+2}\varepsilon_{i+1} ,$$

a result identical with the Secant error relation (3.1).

By using the error relations derived above, it is possible to examine the asymptotic iterating pattern of the Pegasus method. Assuming that ε_{i-1} is negative and ε_i positive, and taking the constant (c_2/c_1) positive, we find a sequence of values calculated from modified (M_1 and M_2) and unmodified (U) iterations in the order UUM_1M_2, $UUM_1M_2, \ldots$. For (c_2/c_1) negative the behaviour is the same.

This gives a complete cycle of four substeps and a relationship of the form $\varepsilon_{i+8} \cong (c_2/c_1)^8\varepsilon_i^2\varepsilon_{i+4}^7$, leading to a process of order 7.275 at a cost of four function evaluations. Hence using Traub's (1964, Appendix C) Efficiency Index, we find that the computational efficiency for the Pegasus method is

$$E = (7.275)^{\frac{1}{4}} = 1.642\ldots .$$

4. Numerical Illustrations.

For the purpose of checking the theoretical analysis, we show first in Table 1 the behavior of the method for the simple equation $x^3+1 = 0$.

The root is $\theta = -1$, for which $c_2/c_1 = -1$, and we start with initial estimates $x_0 = 0, x_1 = -2$.

Table 1.

i	ε_i	Iteration
2	0.750	U
3	0.534	U
4	0.232	M_1
5	-0.682×10^{-2}	M_2
6	0.184×10^{-2}	U
7	0.125×10^{-4}	U
8	0.480×10^{-9}	M_1
9	0.593×10^{-14}	M_2

The asymptotic error formulae predict $\varepsilon_8 \simeq 0.581\times10^{-9}$, $\varepsilon_9 \simeq 0.595\times10^{-14}$, which gives good agreement with the tabular values.

The Pegasus method has been extensively tested over a wide range of problems arising in a University environment and we have found no cases where it has failed to converge in a reasonable number of iterations. Our experience shows that it is very considerably faster than the Illinois method. This improvement is clearly important in cases where f is expensive to evaluate.

We now give four illustrative examples showing a numerical comparison of the Pegasus, Illinois and Regula Falsi methods.

PROBLEM 1.

$$f(x) \equiv (Nx-1)/((N-1)x)$$

We choose a 'difficult' function, designed to display the very slow convergence of the Regula Falsi in certain cases. The starting values used were $x_0 = 0.01$, $x_1 = 1.0$.

N	Number of Iterations ($\lvert f(x)\rvert < 0.5 \times 10^{-17}$)		
	Pegasus Method	Illinois Method	Regula Falsi
2	13	14	2008
10	13	16	446
20	11	15	192

PROBLEM 2.

$$f(x) \equiv J_0(K)Y_1(Kx)-J_1(Kx)Y_0(K)\,,$$

K being a given constant.

This practical problem which arises in nuclear reactor theory, again displays the possibility of slow convergence with the unmodified Regula Falsi.

The starting values were $x_0 = 0.1$, $x_1 = 1.0$.

K	Number of Iterations ($\lvert f(x)\rvert < 0.5 \times 10^{-19}$)			θ
	Pegasus Metod	Illinois Method	Regula Falsi	
2.5	12	13	1483	0.149436
3.0	5	6	7	0.370989

PROBLEM 3.

$$f(x) \equiv \sum_{-\infty}^{\infty} (-1)^n x^{(3n^2+n)/2} - 1, \quad (-1 < x < 1).$$

$\theta = -0.679334$. Starting values $x_0 = -0.0001, x_1 = -0.9999$.

We take here a 'well-behaved' mathematical function to give some idea of normal relative performance.

Number of Iterations ($\lvert f(x)\rvert < 0.5 \times 10^{-19}$)		
Pegasus Method	Illinois Method	Regula Falsi
16	18	51

PROBLEM 4.

Finally we show the performances of the three methods in solving an interesting practical root-finding problem which arises in the Statistical Theory of Double Sampling (Chambers and Jarratt (1964)).

We take

$$f(x) = \int_{-\infty}^{\infty} \varphi(u)[1-\Phi(v)]^{K-1} du - P^*$$

where

$$\varphi(u) = e^{-u^2/2}/\sqrt{2\pi}, \quad \Phi(v) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{v} e^{-t^2/2}\, dt, \quad v = \frac{u-x}{c},$$

and c, K and P^* are given constants.

For a given x, the integral was computed using Gauss-Hermite roots and weights.

c	K	P^*	Number of Iterations ($\lvert f(x)\rvert < 0.5 \times 10^{-17}$)			φ
			Pegasus Method	Illinois Method	Regula Falsi	
1	4	0.8	5	7	10	0.205528
1	3	0.5	4	5	7	0.106712

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