Generalise to systems of ordinary differential equations

CONVERGENCE BEHAVIOUR OF THE NEWTON ITERATION FOR FIRST ORDER DIFFERENTIAL EQUATIONS*

K.O. Geddes
University of Waterloo, Waterloo, Ontario, Canada

ABSTRACT

In a typical application of the Newton iteration in a power series domain (e.g. to compute an algebraic function), the number of correct power series coefficients in the k-th iterate is exactly double the number of correct coefficients in the preceding iterate. This paper considers the application of the Newton iteration to compute the power series solution of a first-order nonlinear differential equation. It is proved that in one iteration the number of correct coefficients is more than doubled in the case of an explicit differential equation, and is less than doubled in the most general case.

1. Introduction

This paper considers the problem of computing the solution for a first-order ordinary differential equation (ODE)

$$(1)\quad G(y,y') = 0;\ y(0) = \alpha_0$$

where $G(y,y')$ is a polynomial in y and y' with coefficients which are power series in x. We consider computing the solution in the power series form

$$y = y(x) = \sum_{k=0}^{\infty} a_k x^k$$

by employing a form of the Newton iteration.

Facilities for power series manipulation are generally recognized to be an integral part of languages and systems for symbolic computation. A general treatment

*This research was supported by the Natural Sciences and Engineering Research Council of Canada under Grant A8967.

of the problem of obtaining power series exapnsions is given by Zippel [9]. Norman [6] describes a system for power series manipulation which includes, as an integral part, the power series solution of differential equations. Neither of these authors employs the concept of the Newton iteration, a concept which has the potential for a significant increase in efficiency.

Yun [7], [8] was the first to exploit the Newton iteration for power series (and polynomial) manipulation in an algebraic context. His work showed that the Newton iteration was a powerful unifying concept for the understanding of several previous algebraic algorithms and for the discovery of new algebraic algorithms. The Newton iteration has been applied very successfully to yield "fast" algorithms for the computation of algebraic functions (see [4], [5]) -- i.e. the solution of $G(y) = 0$ where $G(y)$ is a polynomial in y with power series coefficients. Brent and Kung [3] mention the application of the Newton iteration to yield "fast" algorithms for the solution of certain differential equations. In this paper we show that when the Newton iteration is applied to the ODE (1), the typical property of a Newton iteration whereby the number of correct coefficients exactly doubles at each iteration may not hold. Specifically, we identify forms of the polynomial $G(y,y')$ such that the number of correct coefficients in the k-th Newton iterate is

$$\left\{ \begin{array}{l} \text{one less than double} \\ \text{exactly double} \\ \text{one more than double} \end{array} \right\}$$

the number of correct coefficients in the preceding iterate.

When the Newton iteration is applied to the general first-order nonlinear ODE (1), each step of the iteration requires that a first-order <u>linear</u> ODE be solved for the correction term. The general solution of a first-order linear ODE can be expressed in closed form (see Lemma 1) in terms of the (power series) operations of multiplication, division, integration, and exponentiation. We consider these to be basic power series operations and hence the solution of a first-order linear ODE may be considered to be a basic operation. (See [2] for the exponentiation of a power series.)

2. Notation and Terminology

We consider the first-order ODE (1) to be such that $G(y,y') \in D[y,y']$, where $D[y,y']$ denotes the set of bivariate polynomials in y and y' with coefficients lying in a power series domain $D = F[[x]]$ over some field F. (Typically, F is the field $\underline{Q}$ of rational numbers or else a field $\underline{Q}(\underline{\mu})$ of rational functions in indeterminates $\underline{\mu}$.) We seek a solution $y \in F[[x]]$.

The terminology of Lipson [5] will be followed in dealing with the concepts of approximation and convergence in the power series domain F[[x]]. In particular, if

$$(2)\quad c(x) = \sum_{k=0}^{\infty} c_k x^k \in F[[x]]$$

then reduction mod x^m is defined by

$$(3)\quad c(x) \bmod x^m = \sum_{k=0}^{m-1} c_k x^k .$$

The power series (3) may be considered to be a polynomial or a truncated power series (TPS). The order ord[c(x)] of a power series $c(x) \in F[[x]]$ as in (2) is defined to be the least integer k such that $c_k \neq 0$. The power series $b(x) \in F[[x]]$ is called an $O(x^m)$ ("order x^m") approximation to $c(x) \in F[[x]]$ if

$$\text{ord}\,[c(x) - b(x)] \geq m;$$

we may also refer to b(x) as an order m approximation to c(x).

3. Derivation of the Newton Iteration

The basic formula for the Newton iteration for the ODE (1) is obtained by considering the (bivariate) Taylor series expansion of the function $G(y,y')$. If y_k is a TPS approximation to y then expanding $G(y,y')$ about the "point" (y_k,y_k') yields:

$$G(y,y') = G(y_k,y_k') + (y-y_k)G_y(y_k,y_k')$$
$$+ (y'-y_k')G_{y'}(y_k,y_k') + \ldots$$

where G_y and $G_{y'}$ denote the partial derivatives of G with respect to y and y' respectively. Ignoring terms beyond the first degree, we have that if $G(y,y') = 0$ then $G_{y'}(y'-y_k') + G_y(y-y_k) \approx -G$ (where the functions G, G_y, and $G_{y'}$ are all evaluated at (y_k,y_k')). Thus, if the linear ODE

$$(4)\quad G_{y'}\, e_k' + G_y\, e_k = -G$$

is solved for the "correction term" e_k (as a power series) then defining

$$(5)\quad y_{k+1} = y_k + e_k$$

should yield a higher-order approximation y_{k+1} to y.

The following sections prove the validity of the Newton iteration (4) - (5) and also determine the convergence behaviour of this iteration in various contexts.

4. Preliminary Results

The first result we need is the algebraic formalization of the bivariate Taylor series expansion used in the preceding section. The proof of Theorem 1 is a straightforward generalization of the proof of Lipson's Theorem 2.4 ([5], p. 264) and is omitted.

Theorem 1 (Bivariate Taylor Expansion)

Let $G(y,z)$ be a polynomial in $D[y,z]$. Then in $D[y,z]\,[\xi,\eta]$,

$$\begin{aligned} G(y+\xi,z+\eta) = G(y,z) &+ G_y(y,z)\xi \\ &+ G_z(y,z)\eta \\ &+ H_1(y,z,\xi,\eta)\xi^2 \\ &+ H_2(y,z,\xi,\eta)\xi\eta \\ &+ H_3(y,z,\xi,\eta)\eta^2 \end{aligned}$$

for some polynomials H_1, H_2, $H_3 \in D[y,z,\xi,\eta]$.

It is a familiar result that the Newton iteration is usually quadratic, which in the algebraic context means that the number of correct terms in the power series expansion exactly doubles with each successive iterate. However in the present context there are some interesting variations in the behavior of the Newton iteration. The precise nature of convergence depends on the presence or absence of the terms involving $\xi\eta$ and η^2 (see Theorem 1) in the bivariate Taylor expansion of the given function $G(y,y')$. (In applying Theorem 1 we identify z with y').

We can distinguish three separate cases.

Case 1: In the most general case of an implicit ODE

$$G(y,y') = 0,$$

all of the terms in the bivariate Taylor expansion of Theorem 1 are present and the order of approximation of a new iterate is one less than double the order of approximation of the preceding iterate.

Case 2: If the implicit ODE

$$G(y,y') = 0$$

is of degree 1 in y', then the term in η^2 in the bivariate

Taylor expansion of Theorem 1 is not present and the order of approximation of a new iterate is exactly double the order of approximation of the preceding iterate.

Case 3: If the ODE is in explicit form:

$$G(y,y') = y' + F(y) = 0,$$

then both the term in η^2 and the term in $\xi\eta$ in the bivariate Taylor expansion of Theorem 1 are absent and the order of approximation of a new iterate is one more than double the order of approximation of the preceding iterate.

These results are proved in the next section but first we formally state a corollary to Theorem 1.

Corollary 1 (to Theorem 1)

If $G(y,z)$ is as in Theorem 1 but if the degree in z is 1 then

$$\begin{aligned} G(y+\xi,z+\eta) = G(y,z) &+ G_y(y,z)\xi \\ &+ G_z(y,z)\eta \\ &+ H_1(y,z,\xi,\eta)\xi^2 \\ &+ H_2(y,z,\xi,\eta)\xi\eta \end{aligned}$$

for some polynomials H_1, $H_2 \in D[y,z,\xi,\eta]$.

If moreover

$$G(y,z) = z + F(y)$$

then

$$\begin{aligned} G(y+\xi,z+\eta) = G(y,z) &+ G_y(y,z)\xi \\ &+ G_z(y,z)\eta \\ &+ H_1(y,z,\xi,\eta)\xi^2 \end{aligned}$$

for some polynomial $H_1(y,z,\xi,\eta) \in D[y,z,\xi,\eta]$.

5. The Main Theorem

Before proceeding to the main theorem, we need the following result which gives the solution of a first-order linear ODE in closed form.

Lemma 1

The first-order linear differential equation

$$f(x)\, y' + g(x)\, y = h(x),$$

where $f(x)$, $g(x)$, $h(x) \in F[[x]]$, has a unique solution $y(x) \in F[[x]]$ satisfying

$$y(0) = \alpha_0 \text{ (a specified initial condition)}$$

if $f(0) \neq 0$. Explicitly, if we define the power series $u(x) \in F[[x]]$ by

$$u(x) = \exp \{ \int g(x)/f(x) \}$$

then the solution $y(x) \in F[[x]]$ is given by

$$y(x) = \frac{1}{u(x)} [\int u(x)\, h(x)/f(x) + \alpha_0]$$

where all operations are formal power series operations.

Proof: see Boyce and DiPrima [1], p. 19.

Theorem 2

Let the initial-value problem

$$(6) \quad G(y,y') = 0;\ y(0) = \alpha_0$$

be such that $G(y,y')$ is a bivariate polynomial in the domain $D[y,y']$ with coefficients in a power series domain $D = F[[x]]$, where $\alpha_0 \in F$. Let $\alpha_1 \in F$ be chosen such that the polynomial $y_1 = \alpha_0 + \alpha_1 x$ satisfies

$$(7) \quad G(y_1,y_1') \bmod x = 0$$

(i.e. y_1 is an $O(x^2)$ approximation to a solution y of (3.7)). Further suppose that

$$(8) \quad G_{y'}(y_1,y_1') \bmod x \neq 0.$$

Then the sequence of iterates y_2, y_3, y_4, ... defined by

$$(9) \quad y_{k+1} = y_k + e_k,$$

where $e_k \in F[[x]]$ is the solution of the linear ODE

$$(10) \quad G_{y'}(y_k,y_k')\, e_k' + G_y(y_k,y_k')\, e_k = - G(y_k,y_k')$$

(with initial condition $e_k(0) = 0$), is such that

$$\operatorname{ord}[y-y_{k+1}] \geq 2 \operatorname{ord}[y-y_k] - 1.$$

Proof: Let y_k be an $O(x_m)$ approximation to y, where $m \geq 2$. Then we have

$$\begin{aligned} &\mathrm{ord}[y-y_k] = m; \\ &\mathrm{ord}[y'-y_k'] = m-1 \end{aligned}$$

(since differentiation lowers the order of a power series by one). Applying Theorem 1 to the bivariate polynomial $G(y,y') \in D[y,y']$, we have

$$\begin{aligned} G(y+\xi,y'+\eta) = G(y,y') &+ G_y(y,y')\xi \\ &+ G_{y'}(y,y')\eta \\ &+ H_1(y,y',\xi,\eta)\xi^2 \\ &+ H_2(y,y',\xi,\eta)\xi\eta \\ &+ H_3(y,y',\xi,\eta)\eta^2 . \end{aligned}$$

Evaluating $G(y+\xi,y'+\eta)$ by substituting y_k for y, $y-y_k$ for ξ, y_k' for y', and $y'-y_k'$ for η (where all of these expressions are power series in $D = F[[x]]$), yields

$$\begin{aligned} (11) \quad 0 = G(y_k,y_k') &+ G_y(y_k,y_k')(y-y_k) \\ &+ G_{y'}(y_k,y_k')(y'-y_k') \\ &+ H_1(y-y_k)^2 \\ &+ H_2(y-y_k)(y'-y_k') \\ &+ H_3(y'-y_k')^2 \end{aligned}$$

where H_1, H_2, and H_3 are all evaluated at $(y_k,y_k',y-y_k,y'-y_k')$.

At this point we note that the linear ODE (10) has a unique solution $e_k \in F[[x]]$ for all $k \geq 1$ by Lemma 1 and condition (8). For if (8) is satisfied then

$$(12) \quad G_{y'}(y_k,y_k') \bmod x \neq 0$$

for all $k \geq 1$, since

$$\begin{aligned} &y_k \equiv y_1 \pmod{x}, \text{ and} \\ &y_k' \equiv y_1' \pmod{x} \end{aligned}$$

for all $k \geq 1$.

Now, letting $e_k \in F[[x]]$ be the unique solution of (10) and noting by (9) that $e_k = y_{k+1} - y_k$, we have the relationship (from (10))

$$G(y_k,y_k') = - G_{y'}(y_k,y_k')(y_{k+1}'-y_k') - G_y(y_k,y_k')(y_{k+1}-y_k)$$

which, when substituted into the equation (11), yields

$$(13)\quad G_{y'}(y_k,y_k')(y-y_{k+1})' + G_y(y_k,y_k')(y-y_{k+1}) = r$$

where

$$r = - H_1(y-y_k)^2 - H_2(y-y_k)(y'-y_k') - H_3(y'-y_k')^2$$

(H_1, H_2, H_3 evaluated as above). By Lemma 1, the ODE (13) can be solved explicitly to give:

$$(14)\quad y-y_{k+1} = \frac{1}{u} \int u\ r/G_{y'}(y_k,y_k')$$

where

$$u = \exp \{ \int G_y(y_k,y_k') \ / \ G_{y'}(y_k,y_k')\}.$$

It remains only to consider the orders of the power series appearing in equation (14). Now

$$\text{ord } [u] = 0$$

because the exponential of any power series has order 0, and

$$\text{ord } [G_{y'}(y_k,y_k')] = 0$$

by equation (12). (Of course, the divisions in (14) would have been invalid otherwise.) Hence

$$\text{ord } [y-y_{k+1}] = \text{ord } [r] + 1$$

since integration increases the order by 1. Considering r as defined in (13), we have

$$\begin{aligned}(15)\quad \text{ord } [r] \geq \min \{ & \text{ord } [H_1]\ (2m), \\ & \text{ord } [H_2]\ (2m-1), \\ & \text{ord } [H_3]\ (2m-2) \ \} \\ \geq 2m-2 &\end{aligned}$$

(recall that m denotes the order of $y-y_k$).
Thus,

$$\text{ord } [y-y_{k+1}] \geq 2m-1.$$

Q.E.D.

Corollary 2

If the ODE $G(y,y')$ in Theorem 2 is of degree 1 in y' then

$$\text{ord } [y-y_{k+1}] \geq 2 \text{ ord } [y-y_k].$$

In particular, the $O(x)$ approximation $y_0 = \alpha_0$ given by the initial condition is sufficient to start the iteration.

Proof: By Corollary 1, $H_3 = 0$ in the proof of Theorem 2 and hence inequality (15) becomes

$$\text{ord } [r] \geq 2m-1.$$

The result follows.

Constructive form

Corollary 3

If the ODE in Theorem 2 is in explicit form:

$$G(y,y') = y' + F(y)$$

then

$$\text{ord } [y-y_{k+1}] \geq 2 \text{ ord } [y-y_k] + 1.$$

In particular, the $O(x)$ approximation $y_0 = \alpha_0$ given by the initial condition is sufficient to start the iteration.

Proof: By Corollary 1, $H_2 \equiv 0$ and $H_3 \equiv 0$ in the proof of Theorem 2 and hence inequality (15) becomes

$$\text{ord } [r] \geq 2m.$$

The result follows.

6. Sample Application

We exhibit the "super" convergence of Corollary 3 by applying the Newton iteration to an explicit ODE.

Problem: $G(y,y') = y' - y^2 = 0; \; y(0) = \frac{2}{3}.$

Known Solution: $y(x) = \frac{2}{3-2x} = \sum_{k=0}^{\infty} (\frac{2}{3})^{k+1} x^k.$

By Corollary 3, we may take as the initial approximation $y_0 = \frac{2}{3}$. The linear ODE (10) for this problem is:

$$e_k' - (2y_k)\, e_k = -\,(y_k' - y_k^2).$$

Thus for k=0 we solve the linear ODE

$$e_0' - \frac{4}{3} e_0 = \frac{4}{9} \;;\; e_0(0) = 0$$

yielding

$$e_0 = \frac{4}{9}x + \frac{8}{27}x^2 \pmod{x^3}.$$

For the second iteration (k=1) we solve the linear ODE

$$e_1' - \left(\frac{4}{3} + \frac{8}{9}\,x + \frac{16}{27}\,x^2\right) e = \left(\frac{48}{81}\,x^2 + \frac{64}{243}\,x^3 + \frac{64}{729}\,x^4\right);$$

$$e_1(0) = 0$$

yielding

$$e_1 = \frac{16}{81}\,x^3 + \frac{32}{243}\,x^4 + \frac{64}{729}\,x^5 + \frac{128}{2187}\,x^6 \pmod{x^7}.$$

Note that after two iterations we have an $O(x^7)$ approximation rather than an $O(x^4)$ approximation which would be expected in a "typical" Newton iteration.

REFERENCES

[1] W.E. Boyce and R.C. DiPrima, Elementary Differential Equations and Boundary Value Problems, 3rd ed. John Wiley and Sons, New York, 1977.

[2] R.P. Brent, Multiple-precision zero-finding methods and the complexity of elementary function evaluation. In Analytic Computational Complexity, J.F. Traub, Ed., Academic Press, New York, 1976, pp. 151 - 176.

[3] R.P. Brent and H.T. Kung, Fast Algorithms for manipulating formal power series. J.ACM 25, 4 (Oct. 1978), pp. 581-595.

[4] H.T. Kung and J.F. Traub, All algebraic functions can be computed fast. J.ACM 25, 2 (Apr. 1978), pp. 245-260.

[5] J.D. Lipson, Newton's method: a great algebraic algorithm. In Proc. 1976 ACM Symp. on Symbolic and Algebraic Comput., R.D. Jenks, Ed., pp. 260-270.

[6] A.C. Norman, Computing with formal power series. ACM Trans. Math. Software 1, 4 (Dec. 1975), pp. 346-356.

[7] D.Y.Y. Yun, Hensel meets Newton - Algebraic constructions in an analytic setting. In Analytic Computational Complexity, J.F. Traub, Ed., Academic Press, New York, 1976, pp. 205-216.

[8] D.Y.Y. Yun, Algebraic algorithms using p-adic constructions. In Proc. 1976 ACM Symp. on Symbolic and Algebraic Comput., R.D. Jenks, Ed., pp. 248-259.

[9] R.E. Zippel, Univariate power series expansions in algebraic manipulation. In Proc. 1976 ACM Symp. on Symbolic and Algebraic Comput., R.D. Jenks, Ed., pp. 198-208.