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From Differential to Difference Equations for First Order ODEs

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Abstract

When constructing an algorithm for the numerical integration of a differential equation, one should first convert the known ordinary *differential* equation (ODE) into an ordinary *difference* equation (OΔE). Given this difference equation, one can then develop an appropriate numerical algorithm. This technical note describes the derivation of two such OΔEs applicable to a first order ODE. The implicit OΔE has the same asymptotic expansion as the ODE itself; whereas, the explicit OΔE has an asymptotic expansion that is similar in structure but different in value when compared with that of the ODE.

Many physical processes can be represented by systems of first order ODEs of the form

$$\dot{\boldsymbol{X}}_\alpha + P_\alpha \boldsymbol{X}_\alpha = \boldsymbol{Q}_\alpha \qquad (\text{for } \alpha = 1, 2, \ldots, N)\,, \tag{1}$$

or equivalently as

$$\begin{aligned} \dot{\boldsymbol{X}}_\alpha &= \boldsymbol{F}_\alpha[\boldsymbol{X}_\beta, t] \\ &\equiv \boldsymbol{Q}_\alpha[\boldsymbol{X}_\beta, t] - P_\alpha[\boldsymbol{X}_\beta, t]\, \boldsymbol{X}_\alpha \qquad (\text{for } \alpha, \beta = 1, 2, \ldots, N)\,, \end{aligned} \tag{2}$$

where the $\boldsymbol{X}_\alpha$ are the N independent variables to be solved for, which may be scalar, vector or tensor valued in applications. The parameters P_α (a scalar), and $\boldsymbol{F}_\alpha$ and $\boldsymbol{Q}_\alpha$ (of the same rank/type as $\boldsymbol{X}_\alpha$), are functions of the variables $\boldsymbol{X}_\beta$ and t, in general. If neither P_α or $\boldsymbol{Q}_\alpha$ depends on $\boldsymbol{X}_\beta$ for all α, β, then the system of equations is said to be linear; otherwise, it is nonlinear. The dot '˙' is used to denote differentiation with respect to time, t. We choose time to be the dependent variable for illustrative purposes, as it so often is in physical applications; however, this is not a necessary restriction on the theory presented herein.

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The ODE of equations (1) and (2) is a point function in time. Numerical integration algorithms, however, are based on functions evaluated over an interval in time. We therefore introduce the first order OΔE

$$\frac{\Delta \boldsymbol{X}_\alpha}{\Delta t} = \boldsymbol{\mathcal{F}}_\alpha[\boldsymbol{X}_\beta, \Delta t, \tau] , \tag{3}$$

where

$$\Delta \boldsymbol{X}_\alpha = \boldsymbol{X}_\alpha[t+\Delta t] - \boldsymbol{X}_\alpha[t] , \tag{4}$$

and therefore

$$\boldsymbol{X}_\alpha[t+\Delta t] = \boldsymbol{X}_\alpha[t] + \boldsymbol{\mathcal{F}}_\alpha[\boldsymbol{X}_\beta, \Delta t, \tau]\cdot \Delta t . \tag{5}$$

The OΔE represents the ODE in numerical integration algorithms. The formulation is implicit when $\tau = t + \Delta t$; whereas, it is explicit when $\tau = t$. The development of existing algorithms begins with the tacit assumption that $\boldsymbol{\mathcal{F}}_\alpha \equiv \boldsymbol{F}_\alpha$. We shall now show that this assumption is in error. This is accomplished by analytically integrating the ODE of (1) in a recursive manner, which permits the difference function $\boldsymbol{\mathcal{F}}_\alpha$ in (3) to be determined for the OΔE.

One can introduce an integrating factor into the differential equation (1) and thereby obtain the recursive integral equation [1]

$$\begin{aligned} \boldsymbol{X}_\alpha[t+\Delta t] &= \exp\left[-\int_{\xi=t}^{t+\Delta t} P_\alpha[\boldsymbol{X}_\beta, \xi]\, d\xi\right] \boldsymbol{X}_\alpha[t] \\ &+ \int_{\xi=t}^{t+\Delta t} \exp\left[-\int_{\zeta=\xi}^{t+\Delta t} P_\alpha[\boldsymbol{X}_\beta, \zeta]\, d\zeta\right] \boldsymbol{Q}_\alpha[\boldsymbol{X}_\beta, \xi]\, d\xi , \end{aligned} \tag{6}$$

which is an exact solution to this first order ODE. John Bernoulli [2] developed a nonrecursive solution similar to (6) in 1697 for the equation $\dot{X} = aX + bX^n$, whose solution was sought by Jacob Bernoulli [3] in 1695. John's solution was expressed as a quadrature because the integral of dz/z in the form of a logarithm was not generally known until later that same year [4].

The authors have obtained a variety of approximate and exact solutions to (6) by representing the parameters P_α and $\boldsymbol{Q}_\alpha$ with series expansions, and integrating them term by term. The resulting linear approximation, which was acquired by using Taylor series expansions, is given by [1]

$$\boldsymbol{X}_\alpha[t+\Delta t] = e^{-P_\alpha[\boldsymbol{X}_\beta,\tau]\cdot\Delta t}\, \boldsymbol{X}_\alpha[t] + \left(1 - e^{-P_\alpha[\boldsymbol{X}_\beta,\tau]\cdot\Delta t}\right) \frac{\boldsymbol{Q}_\alpha[\boldsymbol{X}_\beta,\tau]}{P_\alpha[\boldsymbol{X}_\beta,\tau]} + O\left[\frac{\partial}{\partial \tau} \frac{\boldsymbol{Q}_\alpha[\boldsymbol{X}_\beta,\tau]}{P_\alpha[\boldsymbol{X}_\beta,\tau]}\right] . \tag{7}$$

This approximation becomes exact whenever P_α and $\boldsymbol{Q}_\alpha$ are both constants, *i.e.* whenever the ODE is linear.

Rearranging the recursive solution (7) into a difference equation, one obtains two new relationships; they are, for the implicit case,

$$\begin{aligned} \boldsymbol{\mathcal{F}}_\alpha[\boldsymbol{X}_\beta, \Delta t, t+\Delta t] &= \left(\frac{1 - e^{-P_\alpha[\boldsymbol{X}_\beta, t+\Delta t]\cdot\Delta t}}{P_\alpha[\boldsymbol{X}_\beta, t+\Delta t]\cdot \Delta t}\right) \left(P_\alpha[\boldsymbol{X}_\beta, t+\Delta t]\cdot\Delta \boldsymbol{X}_\alpha + \boldsymbol{F}_\alpha[\boldsymbol{X}_\beta, t+\Delta t]\right) \\ &+ O\left[\frac{\partial}{\partial(t+\Delta t)} \frac{\boldsymbol{Q}_\alpha[\boldsymbol{X}_\beta, t+\Delta t]}{P_\alpha[\boldsymbol{X}_\beta, t+\Delta t]}\right] , \end{aligned} \tag{8}$$

and for the explicit case,

$$\mathcal{F}_\alpha[X_\beta, \Delta t, t] = \left(\frac{1 - e^{-P_\alpha[X_\beta,t]\cdot\Delta t}}{P_\alpha[X_\beta,t]\cdot\Delta t}\right) F_\alpha[X_\beta,t] + O\left[\frac{\partial}{\partial t}\frac{Q_\alpha[X_\beta,t]}{P_\alpha[X_\beta,t]}\right] . \tag{9}$$

Notice the presence of an extra ΔX_α term in the implicit relation (8), which acts as a correction to the derivative F_α, and which is not present in the explicit relation (9).

The coefficient $(1 - e^{-P_\alpha[X_\beta,\tau]\cdot\Delta t})/P_\alpha[X_\beta,\tau]\cdot\Delta t$ is a correction factor of the first order that results from taking the differential function F_α at time τ and converting it into a difference function $\mathcal{F}_\alpha$ at time τ taken over the interval $(t, t+\Delta t)$. (Higher order solutions for the difference function $\mathcal{F}_\alpha$ will be given in a future paper.) This coefficient goes to 1 in the limit as Δt goes to 0, as it must so as to recover the differential; in other words,

$$\lim_{\Delta t\to 0} \mathcal{F}_\alpha[X_\beta, \Delta t, \tau] = F_\alpha[X_\beta, \tau] \tag{10}$$

for both the implicit and explicit cases. A note of caution when writing computer code. In the neighborhood of $P_\alpha[X_\beta,\tau]\cdot\Delta t \approx 0$, one needs to expand $(1-e^{-P_\alpha[X_\beta,\tau]\cdot\Delta t})/P_\alpha[X_\beta,\tau]\cdot\Delta t$ into a power series to secure a sound computational algorithm.

The presence of the coefficient $(1-e^{-P_\alpha[X_\beta,\tau]\cdot\Delta t})/P_\alpha[X_\beta,\tau]\cdot\Delta t$ also introduces desirable asymptotic characteristics into our numerical approximations. In particular, for the implicit case where $\tau = t + \Delta t$, the asymptotic expansion for the OΔE (3 with 8) is given by

$$\lim_{\substack{\Delta t\to \text{large} \\ P_\alpha>0}} X_\alpha[t+\Delta t] \asymp \frac{Q_\alpha[X_\beta, t+\Delta t]}{P_\alpha[X_\beta, t+\Delta t]} , \tag{11}$$

which is also the asymptotic expansion of the ODE (1 & 2). In contrast, for the explicit case where $\tau = t$, the asymptotic expansion for the OΔE (3 with 9) is given by

$$\lim_{\substack{\Delta t\to \text{large} \\ P_\alpha>0}} X_\alpha[t+\Delta t] \asymp \frac{Q_\alpha[X_\beta, t]}{P_\alpha[X_\beta, t]} . \tag{12}$$

These two asymptotic expansions differ only in when their parameters P_α and Q_α are evaluated. For large time steps, the implicit case is asymptotically accurate and stable for exponentially decaying solutions, *i.e.* when $P_\alpha[X_\beta,t] > 0 \ \forall \ t$. Stability becomes an issue only when $P_\alpha < 0$. In constrast, the explicit case will oscillate around the true solution for large time steps, but with much less potential of becoming unbounded when compared with equivalent algorithms constructed without our correction coefficient. These oscillations can be mitigated only by choosing smaller time steps.

The second integral in (6) is a Laplace [5] integral where the integrand has its largest value at the upper limit, $t+\Delta t$, and possesses an evanescent memory of the forcing function, $Q_\alpha[X_\beta,\xi]$, provided that $P_\alpha[X_\beta,\zeta] > 0$ over the interval $(t, t+\Delta t)$. This fading memory means that the solution will depend mainly on the recent values of the forcing function, and that by concentrating the accuracy on the recent past we obtain accurate asymptotic representations of the solution.

In the implicit solution, the integrands in (6) were expanded in Taylor series about their upper limits [1], where each integrand has its largest value and contributes the most to the integral. By retaining but a single term in the Taylor series expansions the integrands are accurately approximated where they are largest, and the neglect of the higher order terms is only felt near the lower limits where each integrand contributes only a small amount to the integral because of its exponential decay from the upper limit. The neglect of the higher order terms in the Taylor series thus results in an algorithm that is asymptotically correct at the upper limit. Normally, when treating asymptotic expansions, the exponential decay of the integrand allows the lower limit to be replaced with zero or minus infinity to ease the integration. This was not done in the present case, however, so that by retaining the lower limit as t, we obtain a uniformly valid asymptotic algorithm in the implicit approximation provided that $P_\alpha[\boldsymbol{X}_\beta, \zeta] > 0$ over the interval $(t, t+\Delta t)$.

In the explicit solution, the integrands in (6) were expanded in Taylor series about their lower limits [1], where the neglect of the higher order terms in the Taylor series results in integrands that become progressively more inaccurate as they approach their upper limits where the contribution from each integrand is most important. The explicit approximation is not, therefore, a valid asymptotic representation of the integral when the Taylor series is truncated at a finite number of terms. However, when $P_\alpha[\boldsymbol{X}_\beta, \zeta] < 0$ over the interval $(t, t+\Delta t)$, the reverse situation occurs. In this case the asymptotic solution is now obtained by expanding the integrands about their lower limits, where this region of each integrand now contributes the most to the integral. Here the implicit method, obtained by expanding about the upper limit, does not give a valid asymptotic representation of the integral.

In conclusion, one only needs to replace the *differential* function $\boldsymbol{F}_\alpha[\boldsymbol{X}_\beta, \tau]$ with the appropriate *difference* function $\boldsymbol{\mathcal{F}}_\alpha[\boldsymbol{X}_\beta, \Delta t, \tau]$ in many existing numerical integration methods (*e.g.* Euler and Runge-Kutta) to construct an appropriate OΔE for the numerical integration of a given ODE, and thereby obtain substantial improvements in their performance. We have demonstrated this in references [1, 6].

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