Direct event location techniques based on Adams multistep methods for discontinuous ODEs

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Abstract

In this paper we consider numerical techniques to locate the event points of the differential system $x' = f(x)$, where f is a discontinuous vector field along an event surface $\Sigma = \{x \in \mathbb{R}^n | \ h(x) = 0\}$ splitting the state space into two different regions R_1 and R_2 and $f(x) = f_i(x)$ when $x \in R_i$, for $i = 1, 2$ while $f_1(x) \neq f_2(x)$ when $x \in \Sigma$. Methods based on Adams multistep schemes which approach the event surface Σ from one side only and in a finite number of steps are proposed. Particularly, these techniques do not require the evaluation of the vector field f_1 (respectively, f_2) in the region R_2 (respectively R_1) and are based on the computation – at each step – of a new time step τ reducing the value of the event function $h(x)$ by a fixed quantity.

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1. Introduction

Several theoretical aspects on differential systems with discontinuous right-hand sides have been studied in past years (see for instance [16, 11, 10, 9]) while, more recently, discontinuous systems appeared pervasively in several applications (see [1, 3, 4, 19, 17, 20, 21, 23, 8]). From a computational point of view, the detection of event points, that is points at which the solution trajectories of a piecewise-smooth dynamical (PWS) system hit the discontinuity surfaces, is an important task when PWS are studied (see [2, 14, 15, 12, 13, 25, 24]).

Consider a differential system in $\mathbb{R}^n$ of the form:

$$x' = f(x) = \begin{cases} f_1(x) & x \in R_1 \\ f_2(x) & x \in R_2 \end{cases} \tag{1}$$

where $\mathbb{R}^n$ is (locally) split into two regions R_1 and R_2 by a surface Σ such that $\mathbb{R}^n = R_1 \cup \Sigma \cup R_2$. Σ is called **event surface** and points $x \in \Sigma$ are called **event points**. Let $h : \mathbb{R}^n \to \mathbb{R}$ be a scalar **event** function such that $h \in C^k$, $k \geq 2$ with $h_x(x) \neq 0$ for all $x \in \Sigma$, where $h_x(x)$ indicates the gradient vector of h. Event function h implicitly characterizes the separated regions R_1 and R_2 and Σ as

$$\Sigma = \{x \in \mathbb{R}^n | \ h(x) = 0\}, \ R_1 = \{x \in \mathbb{R}^n | \ h(x) < 0\}, \ R_2 = \{x \in \mathbb{R}^n | \ h(x) > 0\}; \tag{2}$$

moreover, in many real applications, it is a linear function so that Σ is a (hyper-)plane.

The right-hand side $f(x)$ in (1) can be assumed to be smooth in R_1 and R_2 separately, but it is usually discontinuous across Σ, that is $f_1(x) \neq f_2(x)$, for $x \in \Sigma$.

Without loss of generality, suppose that $x(t_0) = x_0 \in R_1$ (that is $h(x_0) < 0$), the trajectory $x(t)$ of (1) starting from x_0 is directed towards Σ and reaches it in a finite time, $\bar{t}$, not tangentially at a event point $x(\bar{t})$ on Σ (that is $x(\bar{t}) \in \Sigma$ and $h_x(x(\bar{t}))^\top f(x(\bar{t})) \neq 0$). Let us assume that there exists a strictly positive constant δ, such that, for all $x \in R_1 \cup \Sigma$ (sufficiently close to Σ)

$$h_x^\top(x) f_1(x) \geq \delta \tag{3}$$

Observe that for a trajectory $x(t) \in R_1$, it results

$$\frac{d}{dt} h(x(t)) = h_x^\top(x(t)) x'(t) = h_x^\top(x(t)) f_1(x(t)), \quad \forall t \in (t_0, \bar{t}). \tag{4}$$

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The condition (3) implies that the function h monotonically increases along a solution trajectory $x(t) \in R_1$ (and close to Σ), until eventually this trajectory hits Σ non-tangentially.

Frequently in literature, f_1 and f_2 are defined smoothly everywhere in an open neighborhood of Σ. However, this occurrence represents a strong restriction from both theoretical and practical points of view (see for instance [6, 5, 15, 22, 7]). In this paper we consider event location procedures which do not need to compute the vector field f_1 outside $R_1 \cup \Sigma$ (respectively f_2 outside $R_2 \cup \Sigma$). Particularly, we study **one-sided direct event location procedures**, that is numerical procedures which approach the discontinuity surface from one side when the numerical trajectory reaches Σ, at an event point, in a finite number of steps. One-sided direct event location techniques based on Runge-Kutta schemes have been recently proposed in [13], while in [2, 14, 15, 18] Adams multistep formulas have been used in some way for the event location task. We propose event location procedures based on the Adams-Bashforth method which arrive on Σ from one side only and in a finite number of steps.

2. One-sided Adams-Bashforth methods

Since we are going to approach the discontinuity surface Σ only from one side, values of a numerical trajectory in R_1 are used and, for the sake of simplicity, the vector field f_1 will be denoted by f. Let us consider a numerical trajectory starting from $x_0 \in R_1$ obtained by an explicit m-step Adams-Bashforth method (of order m) with variable stepsize:

$$x_{k+1} = x_k + \tau_{k+1} \sum_{j=1}^{m} \beta_j f_{k+1-j} \ , \qquad k = 0, 1, \ldots , \tag{5}$$

where $f_{k+1-j} = f(x_{k+1-j})$ and β_j is rational function of $\tau_{k+1}, \tau_k, \ldots, \tau_{k-(m-2)}$ for each $j = 1, \ldots, m$. Adams-Bashforth methods are particularly advantageous because –in case of linear or quadratic $h(x)$– allow to compute the new step size τ_{k+1} as a root of an algebraic equation of degree 2 (as shown in the following).

Since $h(x_0) < 0$, we impose that the function $h(x)$ increases by a positive quantity η at each step k, that is the numerical method in (5) satisfies the condition:

$$h(x_{k+1}) = h(x_k) + \eta, \qquad k = 0, \ldots, K-1 \ , \tag{6}$$

where $\eta > 0$ is a sufficiently small constant and $K > 0$ is such that $K\eta = -h(x_0)$ (this implies that $h(x_K) = 0$). K is assumed to be a positive integer, otherwise, the relation (6) will hold for $k = 0, \ldots, K-2$, and

$$h(x_K) = h(x_{K-1}) + \hat{\eta} \Leftrightarrow \hat{\eta} = -h(x_{K-1}) = -h(x_0) - (K-1)\eta \tag{7}$$

for any $\hat{\eta} < \eta$. Let us observe that the parameter η has to be small enough to preserve the accuracy of the numerical method.

To guarantee that condition (6) holds, the new step size τ_{k+1} has to satisfy:

$$h\left(x_k + \tau_{k+1} \sum_{j=1}^{m} \beta_j f_{k+1-j} \right) = h(x_k) + \eta \tag{8}$$

Equation (8) represents a scalar nonlinear equation in τ_{k+1}, whose smallest positive root is a possible choice for τ_{k+1}. The new step-size has to overcome also a local truncation error test providing τ_{k+1}^{err}, hence it should be chosen as $\min(\tau_{k+1}, \tau_{k+1}^{err})$. If no positive real roots of (8) exist, we set $\tau_{k+1} = \infty$, and the new step size is chosen by the local error control device, that is τ_{k+1}^{err}.

For general event function $h(x)$, roots of (8) are difficult to be computed; however when $h(x)$ has a polynomial form (i.e. it is linear or quadratic w.r.t x) simple explicit formulas for τ_{k+1} can be obtained.

Case of $h(x)$ linear. Let $h(x)$ be a linear function, i.e. $h(x) = d^\top x + e$, with $d \in \mathbb{R}^n$ and $e \in \mathbb{R}$, then

$$\tau_{k+1} = \frac{\eta_k}{\sum_{j=1}^{m} \beta_j d^\top f_{k+1-j}} \ , \quad k = 0, \ldots, K-1 \ , \tag{9}$$

where $\eta_k = \eta$ for $k = 0, \ldots, K-2$, while $\eta_{K-1} = \hat{\eta}$.

To have a positive value of τ_{k+1}, the denominator of (9) has to be positive. In this case, the smallest positive root of the polynomial equation (9) of degree m in τ_{k+1} is the time size satisfying (8).

When a two-step, second order, Adams-Bashforth method is considered, equation (9) becomes:

$$\tau_{k+1} = \frac{\eta_k}{d^\top [\beta_1 f_k + \beta_2 f_{k-1}]} \ , \quad k = 0, \ldots, K-1 \ , \tag{10}$$

with $\beta_1 = 1 + \frac{\tau_{k+1}}{2\tau_k}$, and $\beta_2 = -\frac{\tau_{k+1}}{2\tau_k}$. The denominator of (10) is positive when the monotonicity condition $d^\top f_k \geq d^\top f_{k-1}$ holds. Thus (10) becomes the quadratic algebraic equation:

$$a_2\tau_{k+1}^2 + a_1\tau_{k+1} - \eta_k = 0 \ , \tag{11}$$

with $a_2 = \frac{1}{2\tau_k} d^\top [f_k - f_{k-1}] \geq 0$, and $a_1 = d^\top f_k > 0$; the smallest positive root of which is the sought time step.

Case of $h(x)$ quadratic. Let $h(x) = \frac{1}{2}x^\top Ax + d^\top x + c$, and consider the expansion

$$h(x_{k+1}(\tau)) = h(x_k) + \tau h_x^\top(x_k)[x'_{k+1}(0) + \frac{\tau}{2}x''_{k+1}(0)] + \frac{\tau^2}{2}[x'_{k+1}(0)]^\top A[x'_{k+1}(0)] \tag{12}$$

where $x_{k+1}(\tau)$ is the numerical solution (5) for $m = 2$ written as function of the new step size τ, that is:

$$x_{k+1}(\tau) = x_k + \tau[\beta_1(\tau) f_k + \beta_2(\tau) f_{k-1}] = x_k + \tau f_k + \frac{\tau^2}{2\tau_k}[f_k - f_{k-1}] \ . \tag{13}$$

Requiring that condition (6) holds, we derive the following quadratic equation (similar to (11))

$$\frac{\tau^2}{2}\left\{[x'_{k+1}(0)]^\top A[x'_{k+1}(0)] + h_x^\top(x_k)x''_{k+1}(0)\right\} + \tau h_x^\top(x_k)x'_{k+1}(0) - \eta \ = 0 \ , \tag{14}$$

with coefficient given by $a_1 = \frac{1}{2\tau_k}h_x^\top(x_k)[f_k - f_{k-1}] + \frac{1}{2}f_k^\top Af_k$ and $a_2 = h_x^\top(x_k)f_k$.

Thus for event functions, $h(x)$, being both linear and quadratic w.r.t.x, the new time step τ_{k+1} for the 2-step Adams-Bashforth method, is the smallest positive root of a quadratic scalar equation, and it may be computed by using an explicit formula. Instead, in case of Adams-Bashforth methods with $m > 2$, the quadratic polynomial equation is replaced by a polynomial equation of degree greater than 2.

Remark 2.1. *Since, the step size τ_{k+1} for $k = 0, \ldots, K-1$ is computed as a root of a polynomial equation, the condition (6) could not be satisfied within an high accuracy and a correction of τ_{k+1} could be necessary. This is particularly useful at the last step (when $k = K-1$) where a correction of τ_K is usually required otherwise $h(x_K) \neq 0$. Then, we can assume, as τ_K, the zero of $h(x_K(\tau)) = 0$, given by the Newton iteration $\{\tau_K^m\}_m$ starting with $\tau_K^0 = \tau_{K-1}$. Alternatively, the last time step τ_K can be computed by the Adams-Bashforth formula with constant step-size starting from x_{K-1}, that is by (10) where $\beta_1 = 3/2$ and $\beta_2 = -1/2$.*

3. Predictor-Corrector methods and selection of η

The parameter η has to be small enough to guarantee both that $h(x_{k+1}) \leq 0$, for each $k = 0, 1, \ldots, K-1$, and the local truncation error of the numerical method is less than a fixed tolerance ϵ. Thus, to control the local truncation error a predictor-corrector Adams method can be used. Consider the explicit $m-$step Adams-Bashforth method denoted by the index P:

$$x_{k+1}^P = x_k + \tau_{k+1}^P \sum_{j=1}^{m} \beta_j^P f_{k+1-j} \ , \qquad k = 0, 1, \ldots, K-1, \tag{15}$$

where $\beta_j^P = \beta_j^P(\tau_{k+1}^P)$, for $j = 1, \ldots, m$, are the coefficients of the predictor formula and the step size τ_{k+1}^P has been derived to have $h(x_{k+1}^P) = h(x_k) + \eta$. Then the corrector formula can be applied:

$$x_{k+1} = x_k + \tau_{k+1}^P [\sum_{j=1}^{m} \beta_j^C f_{k+1-j} + \beta_0^C f(x_{k+1}^P)] \ , \qquad k = 0, 1, \ldots \tag{16}$$

where β_j^C, for $j = 1, \ldots, m$, denote the coefficients of the corrector. Let us notice that, when the numerical solution is close to Σ, the corrector x_{k+1} could be on the right side of Σ. If $h(x_{k+1}) > 0$, we reject τ_{k+1}^P, reduce η (for istance take $\frac{\eta}{2}$), recompute (15)-(16) with the new step size given by the condition $h(x_{k+1}^P) = h(x_k) + \frac{\eta}{2}$, until $h(x_{k+1}) \leq 0$. We have to observe that a reduction of η implies a reduction of τ; this can be easily proved when τ_{k+1}^P is the smallest positive root of equations of the form $a_2\tau^2 + a_1\tau - \eta = 0$ (see (11)), where a_2 and a_1 are coefficients independent on η, with $a_1, \eta > 0$. A reduction of the step size can also be suggested by the truncation control device. The local error Err of the numerical method at t_{k+1}, can be estimated by Milne's method:

$$Err \cong \rho \| x_{k+1}^P - x_{k+1} \| \ , \tag{17}$$

where ρ is a constant which depends on the particular predictor-corrector used. Let ϵ a known tolerance, if $Err \leq \epsilon$ then the step size τ_{k+1}^P will be accepted. On the other hand, if $Err > \epsilon$, we reduce η and recompute (15)-(16) with the reduced step size. Denote by τ_{k+1}^{err} the time step which overcomes the local truncation error test, thus we will assume $\tau_{k+1} = \min\left\{\tau_{k+1}^P, \tau_{k+1}^{err}\right\}$.

A different way to apply the predictor-corrector formula consists in the application of the correction (16) where the time step τ_{k+1} of the corrector is unknown and determined in order to obtain $h(x_{k+1}) = h(x_{k+1}^P)$, which guarantees that $h(x_{k+1}) \leq 0$ being $h(x_{k+1}^P) \leq 0$. In this way there is no need to reduce η, because $h(x_{k+1}) \leq 0$.

For instance, if $h(x)$ is linear, τ_{k+1}^P and τ_{k+1} are the roots of the following equations:

$$\tau_{k+1}^P = \frac{\eta}{d^\top \sum_{j=1}^m \beta_j^P(\tau_{k+1}) f_{k+1-j}}\ , \tag{18}$$

$$\tau_{k+1} = \frac{\eta}{d^\top [\sum_{j=1}^m \beta_j^C(\tau_{k+1}) f_{k+1-j} + \beta_0^C(\tau_{k+1}) f(x_{k+1}^P)]}, \tag{19}$$

then the Milne's device (17) may be applied.

Remark 3.1. *We observe that if the local truncation mechanism requires a reduction of η, then we will get the discontinuity surface in a number of step greater than K. For instance if at the step $k = K_1$ a reduction of η in $\eta/2^i$ is required then we will get Σ in $K_1 + 2^i(K - K_1)$ steps.*

4. Numerical tests

In this section we report some numerical experiments obtained integrating (1) by the second order Adams-Bashforth scheme. In the numerical test below, we take the initial condition x_0 so that condition (3) is satisfied for all $x(t)$ on the solution trajectory starting from x_0 for all $t \in (0, \bar{t}]$, where $x(\bar{t})$ denotes the event point on the discontinuity surface Σ.

Example 1. (See [12]). As first example we consider the discontinuous system (1) with vector fields

$$f_1(x_1, x_2) = \begin{pmatrix} x_1(1-x_2)^{\frac{2r+1}{2}} \\ 1 \end{pmatrix}, \quad f_2(x_1, x_2) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\ , \tag{20}$$

and initial conditions $(x_1(0), x_2(0)) = (0.5, 0)$. The function f_1 cannot be computed when $x_2 > 1$, and the event surface is given by the linear function $h(x_1, x_2) = x_2 - 1 = 0$, separating the two regions $R_1 = \{x : x_2 < 1\}$ and $R_2 = \{x : x_2 > 1\}$. The exact solution of the differential system at $x_2 = 1$ is given by $x_1(1) = x_1(0)\exp(\frac{2}{2r+3})$.

Table 1 reports the global error between the numerical solution provided by the second order Adams-Bashforth method and the exact solution at the event point on the discontinuity surface while halving η, when different values of the parameter r are used for the vector field (20). The second and the last column of the table report the number of steps performed and the absolute value of $h(x)$ at the event point x_K, respectively. As it can be observed, the numerical solution approaches the event surface $x_2 = 1$ in a finite number K of steps with a machine precision accuracy. In this example the sequences of steps τ_k generated by the proposed procedure is constant during the integration because $d^\top f_1(x) = 1$ and is given by $\tau_k = \eta$, for all k. Moreover, for a fixed value of r, observing the reduction behavior of the global error, we may conclude that the theoretical order of the numerical method is preserved when $r = 2$, while is lost when $r = 0$. This is due to the different smoothness of f_1 and the event point for these two values of the parameter r.

Example 2. (See [22]). Let us consider the discontinuous neural network in $\mathbb{R}^3$ with nonlinear growth activation:

$$x'(t) = -Ax(t) + Bg + I(t) \tag{21}$$

with $A = \mathrm{diag}(2, 2.4, 2.8)$, $B = \begin{pmatrix} -0.25 & -0.1 & 0.15 \\ 0.1 & -0.25 & 0 \\ 0 & 0.2 & -0.25 \end{pmatrix}$, $I(t) = \begin{pmatrix} \sin t \\ -\cos t \\ \sin t \end{pmatrix}$, $g(x) = [g_1(x_1), g_2(x_2), g_3(x_3)]^\top$ being $g_i(x_i) = \begin{cases} \sqrt{x_i} + 1 & \text{when } x_i > 0, \\ 0.5\cos x_i - 0.25 & \text{when } x_i < 0 \end{cases}$ and initial point $x_0 = [1, -1, 1]^\top$. Table 2 reports the sequence $\{\tau_k\}$ of the (variable) time steps and the sequence of increasing value of $h(x_k)$, provided by the second order Adams-Bashforth method applied from the initial point x_0 to the event point on the surface $\Sigma : x_2 = 0$. In particular τ_k is given by (11) where $\eta = 0.1$. Instead, Table 3 reports, for different values of the tolerance ϵ, the

Table 1: Error behavior at the event point for different values of r.

		$r = 0$	$r = 1$	$r = 2$	
$\eta = 0.1$	K	Error	Error	Error	$\|h(x_K)\|$
η	9	0.0106	2.1064e-4	0.0031	1.1102e-16
$\eta/2$	19	0.0037	1.1996e-5	7.8008e-4	0
$\eta/4$	39	0.0013	6.0163e-6	1.9480e-4	4.4409e-16
$\eta/8$	79	4.3373e-4	3.3620e-6	4.8594e-5	1.5543e-15
$\eta/16$	159	1.4983e-4	1.2042e-6	1.2129e-5	2.5535e-15
$\eta/32$	319	5.2042e-5	3.6987e-7	3.0293e-6	0
$\eta/64$	639	1.8162e-5	1.0521e-7	7.5692e-7	9.9920e-15

minimum and the maximum values of η selected by the Predictor-Corrector method (based on the second order Adams-Bashforth scheme) together with the total number of the required reduction for η and the number K of steps used to approximate the solution from x_0 to the event point on Σ. Figure 1 plots the sequence of the variable time steps τ_k when the tolerance for the local truncation error (LTE) is $\epsilon = 0.01$. On this plot each iteration point in which the mechanism of reduction of η is called has been denoted by a circle mark. As it can be observed, the value of η was reduced at the first step (i.e., $k = 1$ for two times) and at $k = 23$ (for one time).

Table 2: Sequence of steps for the two-step Adams-Bashforth method.

k	τ_k	$h(x_k)$
1	0.1	-0.8609
2	0.09275	-0.7620
3	0.11785	-0.6582
4	0.16809	-0.5497
5	0.25797	-0.4350
6	0.30945	-0.3306
7	0.25777	-0.2309
8	0.25706	-0.1309
9	0.24370	-0.0308
10	0.07607	-1.73447e-18

Table 3: Predictor Corrector based on Adams-Bashforth method.

ϵ	η_{max}	η_{min}	$N(\epsilon)$	K
0.01	0.1	0.1/8	3	60
0.001	0.1	0.1/64	6	641
0.0001	0.1	0.1/512	9	5221

5. Conclusion

One-sided Adams-Bashforth methods locating event points on Σ in a finite number of steps are proposed either for linear and quadratic function $h(x)$ together with a predictor-corrector Adams method which guarantees that $h(x_{k+1}) < 0$ and the local truncation error of the method is less than a fixed tolerance. The proposed techniques enrich the literature panorama and can be useful for treating PWS where the discontinuity manifold is a plane.

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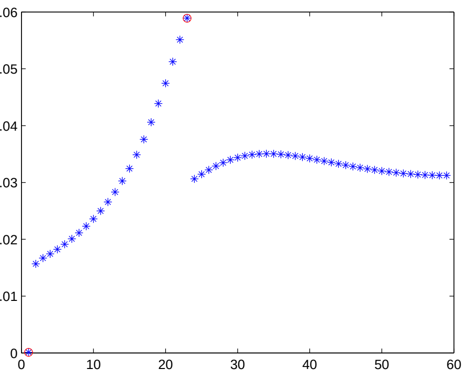
Figure 1: Plot of the sequence of the variable time steps τ_k provided by the Predictor-Corrector method (with tolerance $\epsilon = 0.01$) when integrating (21) on the time interval $[0, \bar{t}]$.



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