A COMPARISON BETWEEN EQUIDISTANT PWL APPROXIMATIONS AND FUZZY CLUSTERING APPLIED TO THE INITIAL VALUE PROBLEM FOR ODES

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Abstract

This paper document several experiments and improvements made on the basis of an ODE solver using Piecewise Linear Approximations and the impact when Fuzzy Clustering is used to decide the allocation of the simplex divisions. A comparison is analyzed in order to compare the potential applicability of the Fuzzy clustering for a stable and unstable ODEs using different number of simplices and number of points to produce the Piecewise Linear (PWL) approximation. The case with stable ODEs is considered first focusing in the reduction of a predefined global error when decreasing vector fields are used. The less smooth nature of the Fuzzy approximations when compared to the classic Equidistant basis is researched using two different number of points and analyzing the changes into the PWL slopes from simplex to simplex. The asymptotic behavior of the error bounds in the case of stable ODEs is also considered showing the tightness of the bounds as t goes to infinity. This is of crucial collaborative importance for existent techniques like validated interval methods, etc. Unstable ODEs can be also integrated with the methodology in this paper but the analysis of the required predefined domain and number of points for the PWL approximate vector field is not so straight as in the case of stable ones. Finally some conclusions and future directions for further improvements in such a methodologies applying PWL approximations for ODEs are depicted.

Keywords: Nonlinear Vector Fields; ODE system, ODE solver, Interval Methods, Validated Methods.

Presenting Author's Biography

Osvaldo Enrique Agamennoni was born in Bahía Blanca, Argentina on December 21, 1953. He received the Electrical Engineering degree and the Doctorate in Control System both from the Universidad Nacional del Sur (UNS), Bahía Blanca, Argentina, in 1979 and 1991 respectively. His research interest include nonlinear system modeling, identification and control, piecewise linear approximation and robust control of nonlinear systems.

1 Introduction

Solutions to Ordinary Differential Equations (ODEs) has been always a topic of interest since they are the heart of many modelling processes. In the particular case of Initial Value problems, let say when an ODE system and an initial condition are given and a solution must be provided, the available tools nowadays are all based on Taylor series (see [1] for a complete survey).

One of the problems arising in these methodologies based on Taylor series is the calculation of the Taylor's coefficients, either for first approximations like the classical Euler's method or whit bigger degrees like Runge-Kutta ([1], pp. 297 and references therein). On the other hand is well known that for these classical numerical methods using Taylor series is not possible to write an explicit expression for the error of truncation neither an explicit bound.

This is one of the reasons why Interval Methods was introduced by Moore in 1966 [2] and improved by Krückeberg [3], Eijgenraam [4], Lohner [5], Berz [6], Nedialkov [7] and many others (see the survey by Corliss in [8]) where instead of using an approximate solution to the true one and then try to guess a bound for the error committed, intervals are calculated for approximate solution and error. Between these techniques we can find one using piecewise approximations minimizing the size of the interval for the approximate solutions whit respect to the initial conditions, in other words we are looking for an appropriate initial conditions for each instant of time where the solutions have to be approximated (this idea regarding the initial condition selection is known as *shadowing*, see the survey in [9]).

On the other hand all of the methodologies surveyed up to now are explicit providing an approximation to the true solution in discrete instants of time, besides, there exists implicit methods where algebraic formulas has to be resolved on line to obtain approximate trajectories (see [10], [11]). Is worth to notice that all of these methodologies only ensures bounds of the solutions for a certain period of time and just a few articles addressed algorithms allowing valid bounds for large intervals (see for instance [12], [13], [14] and [15]).

As a last detail in these existent tools for numerically approximation of ODEs, we notice that in general the improvements regarding error bounding requires the consideration of higher order Taylor coefficients (see [10] and [16]). This is computationally expensive and for large systems could be difficult to solve for on-line applications of real-time tools. In this way, if instead an approximation of a vector field with any desired degree of accuracy is considered using a Piecewise Linear Vector fields (from now on called as PWL), then is possible to easily implement in a computer or even faster in a chip (see [17]).

Only a few results were addressed in this direction (see [18], [19]) showing some results using an equidistant simplex division for the considered State-Space Domain for smooth vector fields. Even when the cases in both papers ([18]) and ([19]) are using different method for generating the PWL approximation the idea of an equidistant simplicial division it seems not be so appealing.

In this paper the concept of Fuzzy Simplicial Division is introduced providing a unequal spaced simplices but using *Fuzzy Clustering* theory to stress the zones of the domain where the vector field is more nonlinear. We expect with this idea to improve the errors in the approximation in such a way that the proposed ODE solver can be tested with some benchmark ODE system while with the approximation in the works up to now is not possible due to the increasing errors with time.

Several simulations are presented in order to compare the present work with the one in [19] using two classes of ODEs: one stable (whit one half-stable equilibrium point) and one Unstable whit no equilibrium points.

This paper is organized as follows: Section 2 presents the formal statement of the problem addressed here, Section 3 is the heart of the paper introducing the idea of Fuzzy simplicial division applied to ODEs and making a deep comparison between classic equidistant PWL technique and this new idea of clustering. Section 4 is stressing the impact on inappropriate domain to consider for the evolution of the ODE trajectories and the effect of Curvature Changes into the errors, finally Section 5 presents some conclusions and future directions for research.

2 Problem Statement

The problem considered in this paper is known as Initial Value Problem (IVP) for ODEs and can be written as follows:

$$\begin{cases} \dot{X} = f(X) \\ X(0) = X_0; \end{cases} \tag{1}$$

where $f(X)$ is a smooth vector field in $\Re^n$ and X is the state vector with initial condition given by $X(0)$. Then the request is to provide a vector function of t, let' say $X(t, X_0)$.

Since is not possible in general for any nonlinear vector field $f(X)$ to obtain a closed-form expression for $X(t, X_0)$, only approximate solution are to be expected in practice. In this way the proposed methodology in this report make use of PWL approximations to approximate the nonlinear vector field $f(X)$ with one linear by simplices.

As reported in [18] and later in [19] this kind of techniques for ODEs only provide enough accuracy for sufficient smooth vector fields while many benchmarks for ODEs are not of this class (consider for example the Van der Pol system).

It seems that this limitations are due to the equidistant simplicial division used to produce the PWL approximation because this "a priori" constant grid of the consider domain in state space is not capturing the main nonlinearities of the vector field $f(X)$. In this regard, is an appealing idea to use Fuzzy Clustering to decide where the divisions of the domain should be placed.

On the other hand in the case of [19] a PWL basis in the spirit of [20] was used taking advantage of the continuous characteristic of this basis and its computational efficiency. However, this showed to be not so effective when applied for nonlinear vector fields with different velocities for each state space variable (that means the directions of the local linear approximation are very different).

A possible explanation for this failing can be provided noticing that even when a reduction of the grid size should relies on more accurate results, this reduction is moving the PWL basis components for the whole domain improving the zone where we were experiencing problems but may be worsening other zones where the approximation was good enough before.

This lack of flexibility can be relaxed in a very natural way which concentrates a good grid size for those zones whit more nonlinearities and leaving a less accurate approximation for other more linear. This technique is the well known *Fuzzy Clustering*, in this way the algorithm is then defined to decide using this fuzzy technique the allocation of the simplex divisions and after based on this division to produce a PWL vector field.

Once the setup of the problem addressed in this paper was presented, next section is showing some results using fuzzy clustering and a brief overview of this method.

3 Improving the Simplex Domain Division using Fuzzy Clustering

The theory of Clustering was built in the heart of identification data, in fact was developed to separate a set of data point into ”clusters” of classes where point belongs differently, this subdivides de complete set of data into subsets classified according to some rules of identification. (see [21] and [22] for a nice tutorial about clustering in general and Fig. 1 for a visual scheme).

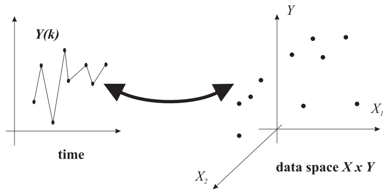

Fig. 1 General Idea of Clustering

On the other hand Fuzzy clustering is a particular case of clustering where the separation into classes is made according to a least squares criterion and in particular Gustafson-Kessel algorithm is forming the clusters using ellipsoids (se Fig. 2).

Since now we are in a fuzzy context one of the outcomes of the Gustafson-Kessel algorithm are the membership functions for identification of the different clusters, in this way is possible to apply this theory of clustering for a set of points coming from our nonlinear vector field in Eq. (1) in order to identify a possible simplex division using some predefined amount of clusters.

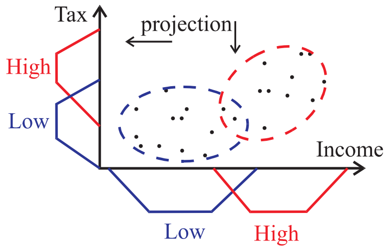

Fig. 2 Gustafson-Kessel clustering.

In what follows we are going to settle experiments using a scalar ODE taken from [23] and [1], which is of the form:

$$\dot{x} = f(x) = -x(t)^2 \tag{2}$$

A posterior analysis will be focused on non-increasing ODEs possesing no equilibrium points in order to conclude about the error and error bounds in unstable systems. The considered ODE for this unstable case is:

$$\dot{x} = f(x) = \frac{1}{x(t)^2 + 1} \tag{3}$$

3.1 A comparison whit the classic equidistant simplicial division

Given the ODE system whose solution has to be approximated, the PWL approximation technique introduced in [18] and [19] need a simplicial division of the state-space with some specified amount of simplices and providing also the limits for the working domain (the case of [19] made use of the basis developed in [20]).

In this way let's start by considering 2 simplices and a total amount of 500 points to produce the approximation. It turns out that the traditional PWL basis is compared whit this new clustering idea where a PWL basis is used in the Fuzzy case but shifting the elements of the basis (see for instance [24] to visualize how this shifting is carried out). In Fig. 3 and 4 we see the trajectories and the PWL approximation for both: Equidistant and Fuzzy basis, then is clear that for such a few amount of simplices the classic equidistant method is working better than the new version using Fuzzy clustering (in the sense of absolute error and error bounds), since the number of simplices (clusters in the context of Fuzzy clustering) is too scanty then the separation in clusters is also too poor and we will expect that for some reasonable bigger amount of simplices the situation turns the other way around (as we will see for 8 simplices).

We present also the membership functions arising in the G-K algorithm applied to this vector field $f(x) = -x^2$ in Fig. 5, notice that the simplex changing is moved

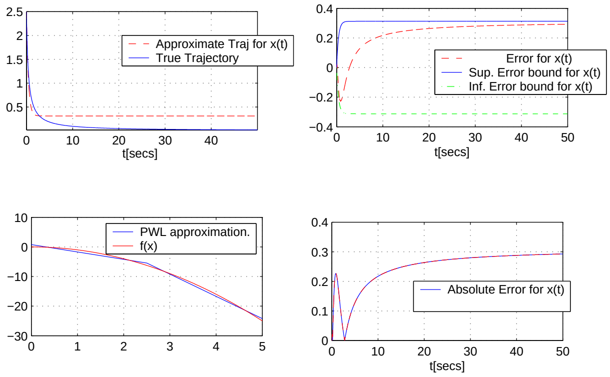

Fig. 3 Equidistant simplicial Division using 2 simplices whit 500 points.

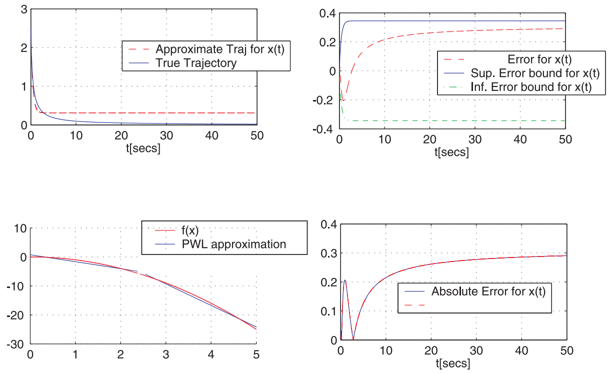

Fig. 4 Fuzzy Clustering simplicial Division using 2 simplices whit 500 points.

from 2.5 in the case of equidistant division to 2.6 in the Fuzzy case. It turns out that in order to decide automatically where the change of the simplices have to be allocated a curve fitting is carried out of the membership functions resulting in the G-K algorithm using Gaussian curves. In this sense the simplex division is decided using the crossing point of the Gaussian fitting curves.

If we perform several experiments for different amount of simplices keeping the number of points (500) to produce the approximation of the vector field, then we get the results summarized in Fig. 6. In this figure is presented the values of the Steady-State errors since this ODE posses a half-stable equilibrium point at $x = 0$ (see [25] for a formal definition of half equilibrium points). We clearly see that there exists a lower limit (in the number of simplices) where the classic PWL exhibits less steady-state error, after this value (7 simplices) the Fuzzy clustering systematically exhibits lower values than the classic equidistant PWL basis.

The important partial conclusion up to now is that the Fuzzy idea improves the steady-state errors when a sufficiently big number of simplices is used, this is the case from a practical point of view because even when we are requiring a bigger number of simplices when compared whit the classic equidistant PWL case, then the

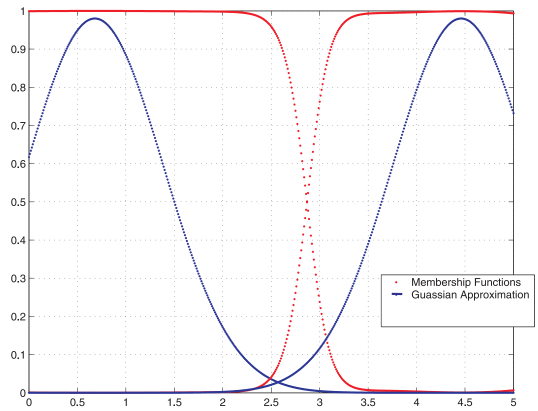

Fig. 5 Membership Functions using 2 simplices and 500 points.

steady-state error is reducing more and more according to the increase of the number of simplices used.

In other words for low number of simplices the classic equidistant simplex division is working better (from a steady-state point of view) but then to the time we want a reduction of the errors an increasing of the number of simplices is required turning the Fuzzy clustering more appropriate. On the other hand taking into account that the G-K algorithm is working on the basis of points, we know that the bigger number of points is used, the better cluster separation is obtained. In this way the question is: Does the clustering technique produce better steady-state errors using bigger number of points for the vector field approximation?.

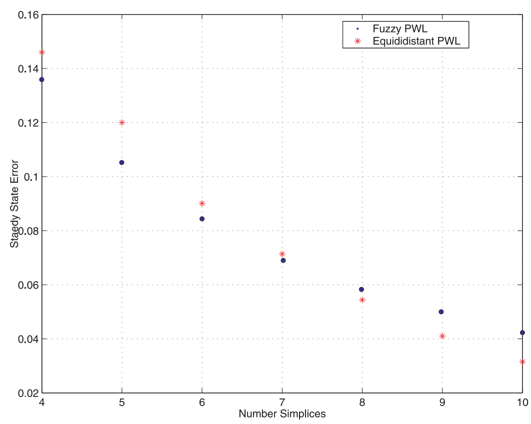

Fig. 6 Steady-State errors using 500 points for several number of simplices.

In order to answer this question and extract more conclusions, we run more experiments but this time using only Fuzzy clustering for 500, 1000, 2000 and 5000 points to produce the vector field approximation and then the separation into clusters keeping fixed the number of clusters (simplices) into 6. The results can be summarized in Tab. 1.

where λ is the maximum error committed in the PWL

Tab. 1 Different Number of Points using 6 simplices and Fuzzy clustering.

Number Points	λ	Steady-State Errors
500	0.1568	0.0897
1000	0.1568	0.0904
2000	0.1549	0.0909
5000	0.1548	0.092

approximation of the vector field, i.e:

$$\lambda = max_{x \in D} |(f(x) - f_{PWL}(x))| \qquad (4)$$

where D is the whole domain for the approximation of the vector field. In this way in the view of Tab. 1, we see that while the number of points to produce the approximation is augmented (yielding a more accurate approximation in the vector field) the parameter λ is decreasing but the steady-state error increases (2 and 6 percent respectively), this is telling that in the Fuzzy case the relation between number of points and accuracy in steady-state present an inverse behavior when compared whit the case of fixed number of points and increasing the number of simplices.

The reason for this "inverse" behavior lies into the clustering technique which in fact produces a better approximation (in the sense of λ quantity) but also a less smooth approximate vector field, that is, the slopes from one simplex to another suffer a bigger change when less amount of points is used. To see this effect see Fig. 7 where the number of simplices was fixed in 6 but two approximations are shown for 500 and 1000 Points in the first and second simplices using Fuzzy clustering.

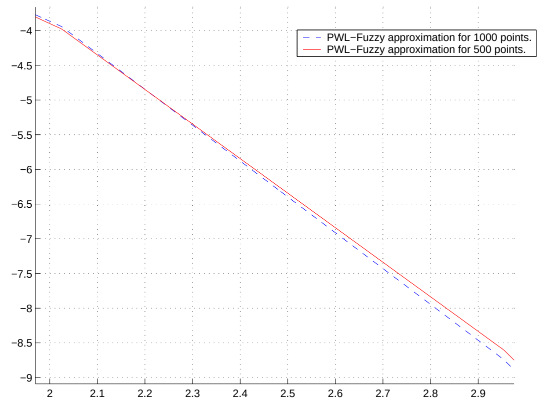

Fig. 7 Two PWL approximations using Fuzzy clustering for 500 and 1000 points.

It worth to mention that this behavior is not observed if the same set of experiment as in Table 1 using the equidistant PWL basis, this is clear because the borders (delimiters) for each simplex are fix anytime for any number of points to produce the vector field approximation. Also notice that even when the Fuzzy technique is improving a lot the results for a big enough number of simplices the error bounds are more tighter in the classic equidistant case, this is a trade-off we should made to the time we decide which of these methodologies is suitable for a particular application (see Figs. 8 and 9)

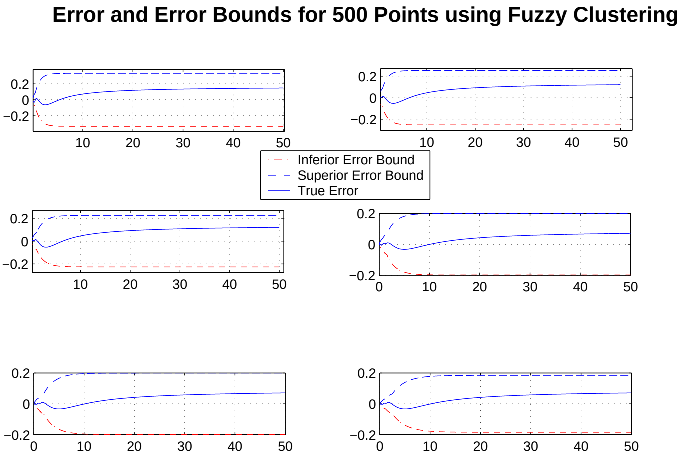

Fig. 8 Fuzzy clustering and 500 points.

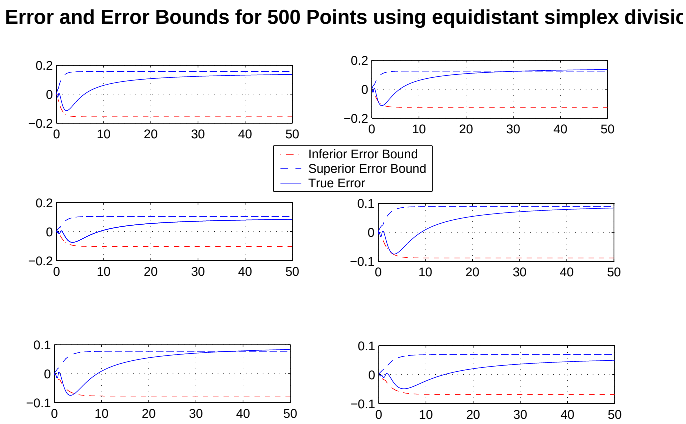

Fig. 9 Equidistant division and 500 points.

Next subsection is providing a further analysis using the ODE introduced in Eq. (3) to contrast results whit the present case (see the ODE in Eq. (2)) and showing that the Fuzzy idea also works and improves results for unstable systems.

3.2 Analysis for Unstable ODEs

The ODE in Eq. (2) posses a half-stable equilibrium point in $x = 0$, however the accurate results obtained in previous section are due to the fact that the system is non-increasing in the considered domain (that is $x \in [0, 5]$). Now the point is to make more clear this idea by providing experiments whit a similar system (in the sense that is non-increasing in $x \in [0, \infty]$) but whit the particularity of possessing no equilibrium points.

In this way the considered ODE will be in this case the one in Eq. (3) in a domain $x \in [0, 5]$, the focus will be in experimenting for the same number of simplices as in previous section (let's say 4 to 10) and the same number of points for the approximation (500 to 5000). One of the most desirable properties using PWL approximations is a decreasing error whit an increment in the number of simplices.

Let's run a simulation using 500 points to produce the PWL approximation whit 2 simplices and a classic equidistant simplicial division (this time the initial condition $X(0)$ will be 0.1, since the ODE is unstable and increasing values as t goes to infinity). The results are shown in Fig. 10, clearly the accuracy is not as good as it was for 2 simplices in the case of the ODE in Eq.(2), however the error is decreasing after 40 seconds and we expect that the error (and error bounds) will suffer a sudden decrease as the number of simplices increases.

In order to conclude about the Fuzzy method, we run a simulation whit the same setup for the Fuzzy clustering method. The results shown in Fig. 11 tells that even when the peak of the absolute error is bigger (1 for Fuzzy and 0.8 for the classic case), the error is not all the time bigger (see Fig. 12). Moreover the interval of time $t \in [45secs, 50secs]$ shows that the error decays much faster for the Fuzzy technique.

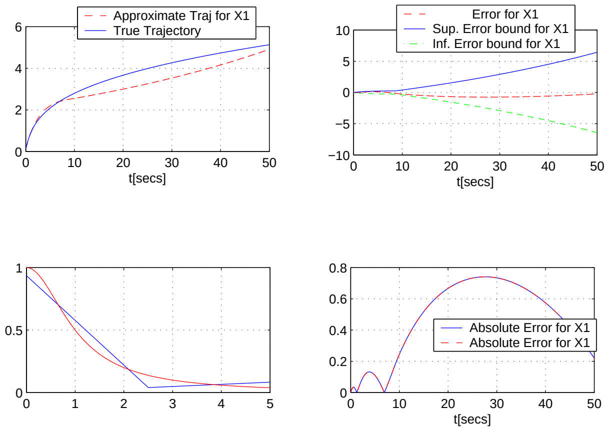

Fig. 10 Equidistant simplicial Division using 2 simplices whit 500 points.

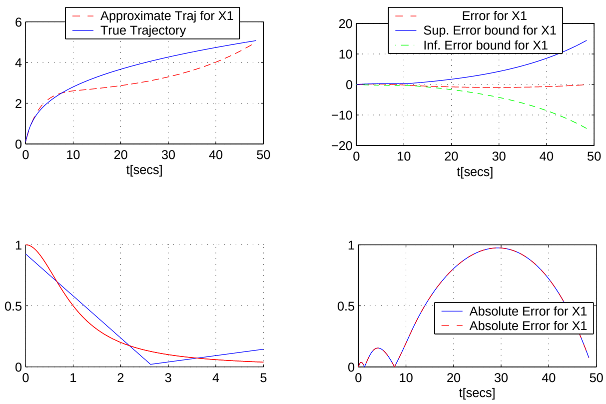

Fig. 11 Fuzzy simplicial Division using 2 simplices whit 500 points.

In order to observe precise conclusions for the present unstable case about the errors several experiments were run for 4 to 10 simplices keeping the number of points

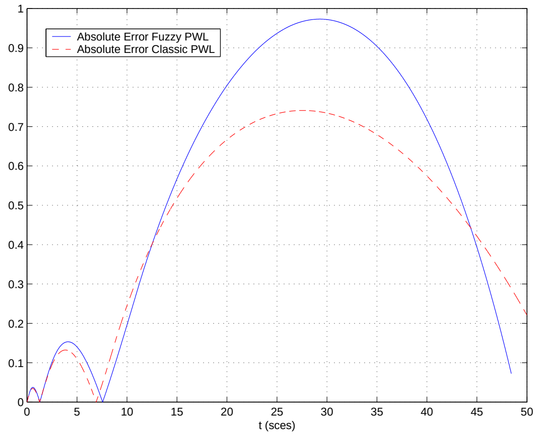

Fig. 12 Comparison between classic and Fuzzy clustering using 2 simplices whit 500 points.

in the approximation in 500, the results are shown in Figs. 13 and 14 for the classic case while Figs. 15 and 16 show the results for the Fuzzy one.

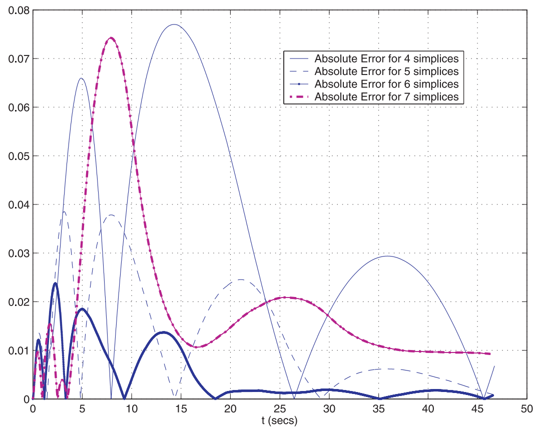

Fig. 13 Absolute Errors using 500 points and equidistant simplicial division.

The conclusion when unstable ODEs have to be integrated whit a PWL simplicial division technique (classical or Fuzzy) is that the error is not following the strict reducing path as in the stable case (Compare Fig. 13 and 9 for instance). The point is to realize that even when the on-propose ODE in Eq. (3) was chosen in such a way that is monotonically decreasing in $x \in [0, \infty]$, is unstable (in fact posses no any equilibrium points) amplifying any small error into the approximation of the trajectories. However as shown in Figs. 13 to 16 we encounter several points where the error coincide in zero yielding the clue that the error bound for a non-increasing vector field is tight.

Incidentally notice that the bounds in Figs. 10 and 11 are blowing up due to the bad approximation observed for only 2 simplices, while we are expecting a stable error bound this is not the case for 2 simplices. Instead in Fig. 17 the error and error bounds for Equidistant and Fuzzy are shown where the expected stable bounds

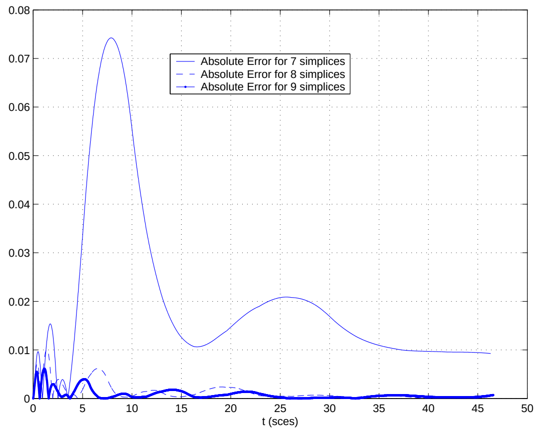

Fig. 14 Absolute Errors using 500 points and equidistant simplicial division.

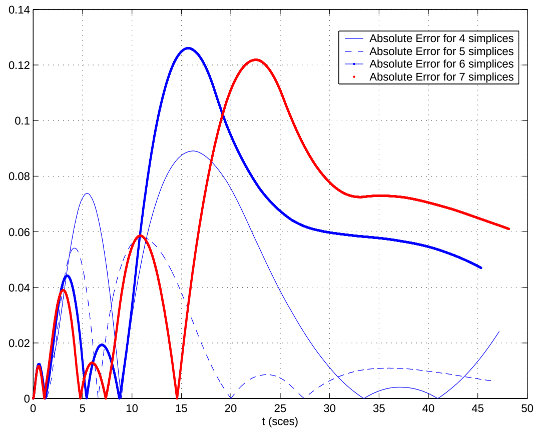

Fig. 15 Absolute Errors using 500 points and Fuzzy clustering.

can be depicted. This is important in the sense that also for unstable ODEs (decreasing) the bounds also tend to a constant value as t goes to infinity.

4 Curvature changes affect the approximate trajectories behavior

As it was introduced in [19] the considered domain for the vector field approximation has to be predefined by the user in advanced, in this way one can decide for the former ODE considered in this paper in Eq. (2) in an initial domain $x \in [-5, 5]$.

Since the vector field approximation is improving whit the increment of the number of simplices used (see [20]) then is natural to expect that increasing the number of simplices the error into the approximate trajectories for the PWL ODE is also reduced in accordance. Unfortunately as we will see in the next set of experiments this is not happening either for the classical equidistant PWL basis or the new Fuzzy clustering idea.

In order to get a flavor of this phenomenon let's start using 3 simplices and 500 points to produce the ap-

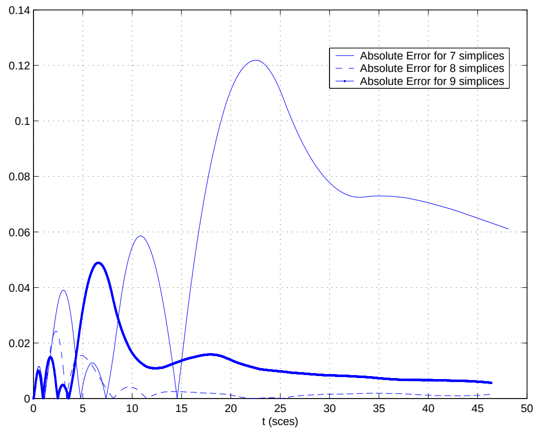

Fig. 16 Absolute Errors using 500 points and Fuzzy clustering.

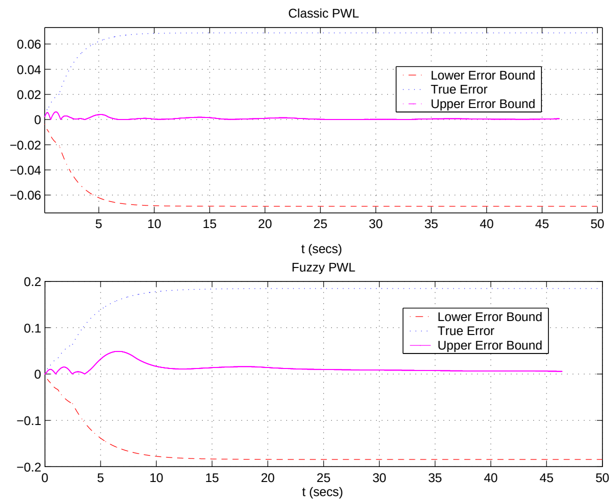

Fig. 17 Error and Error Bound using 9 simplices and 500 points.

proximation, the results are shown in Fig. 18 for the equidistant case and Fig. 19 for the Fuzzy one. Notice that even when the true nonlinear ODE is stable, the approximate solution we obtain whit the classic equidistant PWL method is blowing up.

The point to investigate here is that the changes into the curvature of the given nonlinear ODE is affecting the PWL approximation even when this ODE is stable. In this way and to verify that the error in trajectories is not reduced by an increasing of the number of simplices let's run a simulation using 4 simplices. The results are shown in Fig. 20 and 21, this time the situation is reversed yielding a more accurate approximation for the equidistant classical case. As we can see there is no a uniform pattern to follow in deciding which is an appropriate number of simplices to use when the vector field of the ODE is not *monotonically* decreasing (stable or unstable).

The general conclusion here can be depicted saying that the case of ODEs possessing changes in its curvature

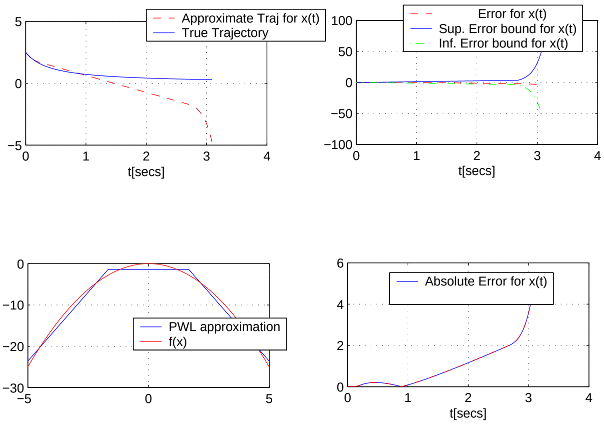

Fig. 18 Equidistant Domain division using 500 points.

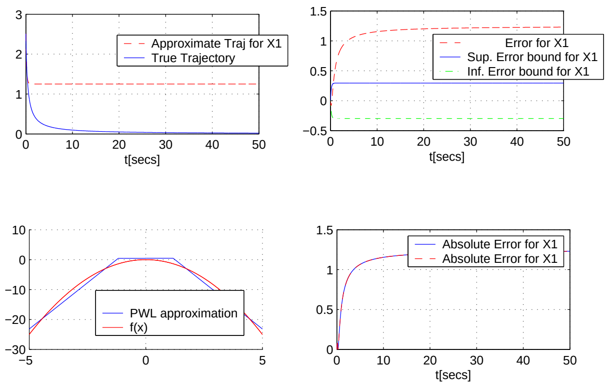

Fig. 19 Fuzzy Clustering Domain division using 500 points.

should be integrated whit PWL techniques in several steps, let's say isolating regions where no any change of the curvature is observed.

5 Conclusions and Future Work

An alternative to the classic equidistant simplicial division applied to the approximation of ODE trajectories was presented. The set of experiments carried out using two ODEs (Eq. (2) and Eq.(3)) showed the advantages of using Fuzzy clustering in deciding the allocation of the simplex division once the number of simplices and the domain of the state-space is decided.

However as reported in subsection 3.2, the case of Unstable decreasing ODEs presents a different behavior, the error is not monotonically tending to any fixed value but oscillating and touching the zero several times. When compared whit the classic PWL basis the conclusion is not so straight except for the faster decaying to zero in some intervals of time.

Moreover even when the focus of this paper is a comparison between classic equidistant PWL and Fuzzy clustering, is also possible in these experiments to make clear that the case of vector fields (ODEs) whit a decreasing behavior in the state-space is suitable for being integrated whit PWL techniques since the error and error bounds tends to constant values when t goes to infinity. On the other hand the error bounds (introduced in [19]) showed to be tight for the cases analyzed in this paper and it is expected to be the case for many ODEs presenting a decreasing structure.

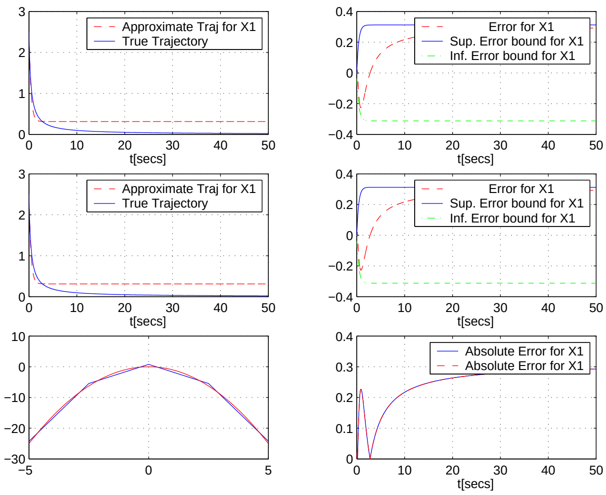

Fig. 20 Equidistant Domain division using 500 points.

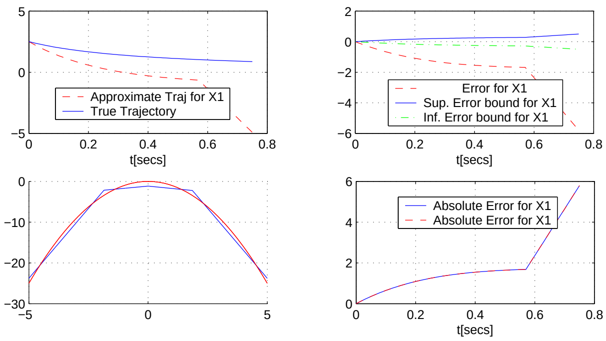

Fig. 21 Fuzzy Clustering Domain division using 500 points.

It turns out that the improvements observed whit the Fuzzy idea introduced in this work is contributing and not opposite to the algorithms in use in Interval methods for ODEs, for instance can be applied to develop an "a priori" bound needed in "Algorithm I" of the method of Nedialkov (see [7]). Finally notice that this kind of methods applying PWL techniques provides not only an interval where the true solution belongs but also an approximate trajectory to be considered as real if the error bounds are tight.

Future directions could bring light in several regions of the theory and practice of PWL basis applied to the integration of ODEs, some of them are:

1. Improvements of clustering for multivariate systems stressing the regions of nonlinearities keeping a predefined degree of smoothness.

2. Improvements of the error bounds for systems possessing positive eigenvalues in its PWL approximation allowing a constant asymptotic behavior (as opposed to the present case where the bound tend to infinity)

3. The possibility of including equilibrium points into the approximation in a such a way that both: PWL and real systems share the same set of equilibrium points

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