International Journal of Applied Mathematical Research, 4 (4) (2015) 513-518
www.sciencepubco.com/index.php/IJAMR
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doi: 10.14419/ijamr.v4i4.4691
Research Paper

Extending high order derivatives for special differential equations of the form $y' = f(y)$ by using monotonically labelled rooted trees

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Abstract

This paper presents a review of the role played by labelled rooted trees to obtain derivatives for numerical solution of initial value problems in special case $y' = f(y), y(x_0) = y_0$. We extend a process to find successive derivatives according to monotonically labelled rooted trees, and prove some relevant lemmas and theorems. In this regard, the k^{th} derivatives, of the monotonically labelled rooted trees with n vertices are presented by using the monotonically labelled rooted trees with $k + n$ vertices. Eventually, this process is applied to trees without labelling.

Keywords: *Labelled rooted trees; Monotonically labelled trees; Elementary differentials; Initial value problems; Derivatives.*

1. Introduction

In the numerical methods for initial value problems, the rooted trees were first used by Butcher [1-5]. Trees now play a central role in the theory of numerical methods for ordinary differential equation, and this paper surveys some aspect of this role. Throughout the paper, we will use a standard formulation for an initial value problem. That is, we will write the standard problem in autonomous form

$$y'(x) = f(y(x)), \quad y(x_0) = y_0 \tag{1}$$

where $f : R^N \to R^N$ is sufficiently differentiable. The elementary differentials are defined, using tree structures and terms of $f, f', f'', \ldots$ evaluated at y_0. There is a deep relationship between derivatives and rooted trees. One of the important usage of derivatives and rooted trees is solving the initial value problem (1) by using the Runge-Kutta methods [1-8]. By using of rooted trees, we can calculate the derivative of higher circumstances in initial value problem (1). These relationships can be generalize to monotonically labeled rooted trees.

Our main purpose is to show that the k^{th} derivatives, of the monotonically labeled rooted trees with n vertices, equal to sum on all monotonically labeled rooted trees with $k + n$ vertices.

The paper is organized as follows. First, in Section 2, we will introduce the monotonically labeled rooted trees and develop the elementary derivatives $y^{(n)}(x)$ according to rooted trees. In Section 3, we remark the lemmas and theorems on derivatives written in terms of monotonically labeled rooted trees and rooted trees without labeling and we also illustrate our ideas with some examples. Finally, some concluding remarks end the paper.

2. Labeled rooted trees and elementary differentials

Let T denote the set of all rooted trees and T_n denote the set of all rooted trees with n vertices. For a rooted tree t, the functions $r(t)$, the order of t, $\gamma(t)$, the density of t and $\sigma(t)$, the symmetry of t are introduced in [2]. Further, let $\alpha(t)$ be the number of distinct ways of labeling the vertices of t with the integers $\{1, 2, \ldots, r(t)\}$, so that if there is edge (i, j), then $i < j$. It is convenient to generalize this by writing S_n for an finite ordered set such that its cardinality is $\#S_n = n$, and count the number of trees with n vertices labeled with members of S_n such that $i < j$ for each edge (i, j). A formula for $\alpha(t)$ is given by [1,2,5,7]

$$\alpha(t) = \frac{r(t)!}{\sigma(t)\gamma(t)}. \tag{2}$$

It is appropriate that we set $S_n = \{1, 2, ..., n\}$. Denote T_n^* the set all trees with n vertices labeled in this way. Let $\mathbf{t} \in T_n^*$. We denote $\mathbf{t}u \in T_{n+k}^*(\mathbf{t})$, the subset of T_{n+k}^* such that sub-tree formed by removing vertices labeling by $n+1, n+2, ..., n+k$ from each member $\mathbf{u}$ is exactly $\mathbf{t}$. Finally $|\mathbf{t}|$ denote the member of T corresponding to $\mathbf{t} \in T_n^*$, removing the labels of the vertices. This means that $\alpha(t)$ can be interpreted as the number of members of T_n^* such that $|\cdot|$ maps them to $\mathbf{t} \in T$. For more details see [1,2,3,7].

For initial value problem (1) the second derivatives is written as

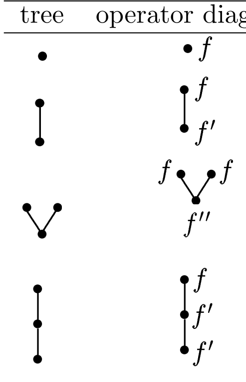
$$y''(x) = \frac{d}{dx} f(y(x)) = f'(y(x)).y'(x) = f'(y(x)).f(y(x)), \tag{3}$$

and the third derivative can be found in a similar manner, as follows

$$\begin{aligned} y'''(x) = \frac{d}{dx} y''(x) &= \frac{d}{dx}\Big(f'(y(x)).f(y(x))\Big) \\ &= f''(y(x))\Big(f(y(x)).f(y(x))\Big) + f'(y(x))\Big(f'(y(x)).f(y(x))\Big). \end{aligned} \tag{4}$$

We will generalize a visual template to show the derivatives, using the rooted trees. In each of the derivatives (1), (3) and (4), we will correspond $f(y(x))$ to each leaf, $f'(y(x))$ to each vertex with a single outward edge and $f''(y(x))$ to each vertex with two outward edges in each rooted tree. Let write f, f' and f'' as abbreviations for $f(y(x)), f'(y(x))$ and $f''(y(x))$, respectively. We will see that the operation of differentiating adds an additional vertex to an existing tree corresponding to $y^{(n)}$, in each possible way, and give the number of new rooted trees corresponding to $y^{(n+1)}$. The rooted trees of order at the most 3 and related derivatives f, f' and f'' are shown in Table 2.1.

Table 2.1. Relation between terms in y derivatives and rooted trees



tree	operator diagram	term
		$f(y(x))$
		$f'(y(x)).f(y(x))$
		$f''(y(x))\Big(f(y(x)).f(y(x))\Big)$
		$f'(y(x))\Big(f'(y(x)).f(y(x))\Big)$

Definition 2.1. *Suppose a tree t and a function $f : \mathbb{R}^N \to \mathbb{R}^N$, analytic in a neighbourhood of y are given. The elementary differential $F(t)(y)$ is defined by*

$$F(\tau)(y) = f(y), \tag{5}$$

$$F([t_1, t_2, \ldots, t_m])(y) = f^{(m)}(y)\Big(F(t_1)(y).F(t_2)(y).\ldots.F(t_m)(y)\Big). \tag{6}$$

For more details see [2-4].

3. Derivatives by monotonically labeled rooted trees

In this section we present and prove some lemmas to calculate the k-order derivative for monotonically labeled rooted trees with n vertices using monotonically labeled rooted trees with $n+k$ vertices. In fact an attempt is made that among all the monotonically labeled rooted trees with $n+k$ vertices, we consider the trees with removed the last k vertices of them, exact same labeled tree with n vertices. We put these trees in set T^{*}_{n+k} and calculated sum of all terms of this set with notation in Section 2.

Lemma 3.1. *If* $\mathbf{t} \in T^{*}_{m-1}$ *then*

$$\frac{d}{dx}F(\mathbf{t})(y(x)) = \sum_{\mathbf{u}\in T^{*}_{m}(\mathbf{t})} F(\mathbf{u})(y(x)). \tag{7}$$

Proof. For the proof we refer the reader to[2]. □

The following lemma is an extension of the Lemma 3.1.

Lemma 3.2. *If* $\mathbf{t} \in T^{*}_{m}$ *then*

$$\frac{d^k}{dx^k}F(\mathbf{t})(y(x)) = \sum_{\mathbf{u}\in T^{*}_{m+k}(\mathbf{t})} F(\mathbf{u})(y(x)). \tag{8}$$

Proof. The proof is by induction on k. When $k = 1$, applying Lemma 3.1, the result is true. Assume that the result is true for $k = n$. Therefore

$$\frac{d^n}{dx^n}F(\mathbf{t})(y(x)) = \sum_{\mathbf{u}\in T^{*}_{m+n}(\mathbf{t})} F(\mathbf{u})(y(x)).$$

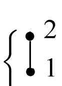
If $k = n + 1$, then

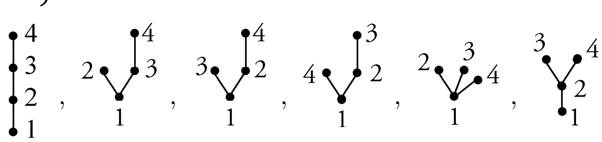
$$\begin{aligned}\frac{d^{n+1}}{dx^{n+1}}F(\mathbf{t})(y(x)) &= \frac{d}{dx}\left(\frac{d^n}{dx^n}F(\mathbf{t})(y(x))\right)\\ &= \frac{d}{dx}\left(\sum_{\mathbf{u}\in T^{*}_{m+n}(\mathbf{t})} F(\mathbf{u})(y(x))\right)\\ &= \sum_{\mathbf{u}'\in T^{*}_{m+n+1}(\mathbf{t})} F(\mathbf{u}')(y(x)).\end{aligned}$$

Where $T^{*}_{m+n+1}(\mathbf{t})$ is, the subset of T^{*}_{m+n+1} such that subtree formed by removing vertices labeling by $m+1, m+2, ..., m+n+1$ from each member is exactly $\mathbf{t}$. □

To clarify the Lemma 3.2, consider the following example.

Example 3.1. *For m=k=2, if* $S_2 = \{1, 2\}$ *and* $S_{2+2} = S_2 \cup \{3, 4\}$ *then*

$T^{*}_{2} = \{$  $\}$

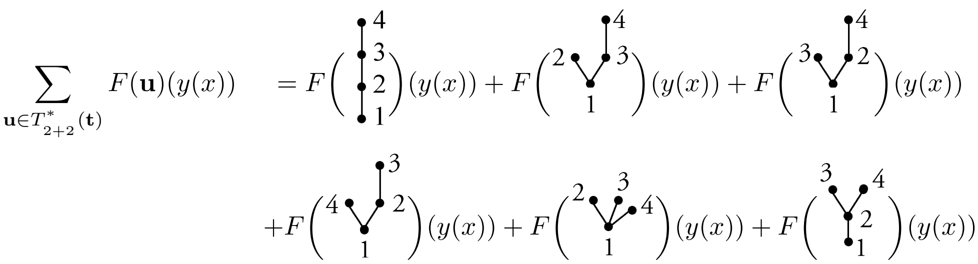
$T^{*}_{4} = \{$  $\}$.

therefore

$\dfrac{d^2}{dx^2}F($  $)(y(x)) = \dfrac{d^2}{dx^2}(f'f) = \dfrac{d}{dx}(f''ff + f'f'f)$

$= f'''fff + f''f'ff + f''ff'f + f''ff'f + f'f''ff + f'f'f'f.$

On the other hand



$$= f'f'f'f + f''ff'f + f''ff'f + f''ff'f + f'''fff + f'f''ff.$$

thus the lemma is verified.

Theorem 3.1. *Let S_m denote a finite ordered set. Then*

$$y^{(\#S_m)}(x) = \sum_{\mathbf{t}\in T^*_m} F(\mathbf{t})(y(x)). \tag{9}$$

Proof. The detailed proofs will appear in [2]. □

The following theorem is an extension of the Theorem 3.1.

Theorem 3.2. *Let S_m denote a finite ordered set. Then*

$$\frac{d^k}{dx^k}\left(y^{(\#S_m)}(x)\right) = \sum_{\mathbf{t}\in T^*_{m+k}} F(\mathbf{t})(y(x)). \tag{10}$$

Proof. The proof is by induction on k. If $k = 1$, then by applying Theorem 3.1, we have:

$$\begin{aligned}\frac{d}{dx}y^{(\#S_m)}(x) &= \frac{d}{dx}\sum_{\mathbf{t}\in T^*_m} F(\mathbf{t})(y(x))\\ &= \sum_{\mathbf{t}\in T^*_{m+1}} F(\mathbf{t})(y(x)).\end{aligned}$$

Assuming that the result of the theorem is true for $k = n-1$, this means

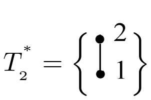
$$\frac{d^{n-1}}{dx^{n-1}}y^{(\#S_m)}(x) = \sum_{\mathbf{t}\in T^*_{m+n-1}} F(\mathbf{t})(y(x)).$$

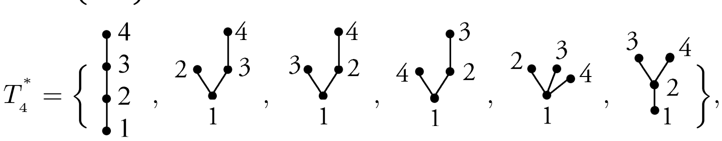
if $k = n$, then

$$\begin{aligned}\frac{d^n}{dx^n}y^{(\#S_m)}(x) &= \frac{d}{dx}\left[\frac{d^{n-1}}{dx^{n-1}}y^{(\#S_m)}(x)\right]\\ &= \frac{d}{dx}\sum_{\mathbf{t}\in T^*_{m+n-1}} F(\mathbf{t})(y(x))\\ &= \sum_{\mathbf{t}\in T^*_{m+n}} F(\mathbf{t})(y(x)).\end{aligned}$$

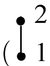
This compleat the proof. □

Example 3.2. *Let $S_2 = \{1, 2\}$ and $k = 2$, by apply Theorem 3.2, we get*



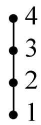
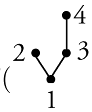
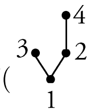


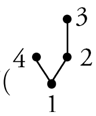
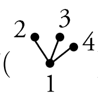
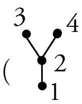
therefore,

$y^{(\#S_2)}(x) = y''(x) = F($  $)(y(x)) = f'f.$

$$\frac{d^2}{dx^2}y''(x) = \frac{d^2}{dx^2}(f'f) = \frac{d}{dx}(f''ff + f'f'f)$$
$$= f'''fff + f''f'ff + f''ff'f + f''ff'f + f'f''ff + f'f'f'f.$$

On the other hand

$\sum_{\mathbf{t}\in T_4^*} F(\mathbf{t})(y(x)) = F($  $)(y(x)) + F($  $)(y(x)) + F($  $)(y(x))$

$+ F($  $)(y(x)) + F($  $)(y(x)) + F($  $)(y(x))$

$$= f'f'f'f + f''ff'f + f''ff'f + f''ff'f + f'''fff + f'f''ff.$$

Now we rewrite this result in terms of unlabeled trees, by noting that the number of times that a tree t with order $\#S$ occurs as the unlabeled counterpart of a member of T_S^*, is exactly $\alpha(t)$.

Theorem 3.3. *The formula for the nth derivative of $y(x)$ is written as*

$$y^{(n)}(x) = \sum_{\mathbf{t}\in T_n} \alpha(t).F(|\mathbf{t}|)(y(x)). \tag{11}$$

Proof. See [2]. □

The following theorem is an extension of the Theorem 3.3.

Theorem 3.4. *The formula for the k^{th} derivative of $y^{^{(n)}}(x)$ is written as*

$$\frac{d^k}{dx^k}y^{(n)}(x) = \sum_{\mathbf{t}\in T_{n+k}} \alpha(t).F(|\mathbf{t}|)(y(x)). \tag{12}$$

Proof. The proof is by induction on k, When $k = 1$, applying Theorem 3.3

$$\frac{d}{dx}y^{(n)}(x) = \frac{d}{dx}\sum_{\mathbf{t}\in T_n} \alpha(t).F(|\mathbf{t}|)(y(x))$$
$$= \sum_{\mathbf{t}\in T_{n+1}} \alpha(t).F(|\mathbf{t}|)(y(x)).$$

We assume that the result of the theorem is true for $k = m-1$, which means

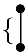
$$\frac{d^{m-1}}{dx^{m-1}}y^{(n)}(x) = \sum_{\mathbf{t}\in T_{n+m-1}} \alpha(t).F(|\mathbf{t}|)(y(x)).$$

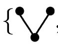
If $k = m$, then

$$\frac{d^m}{dx^m}y^{(n)}(x) = \frac{d}{dx}[\frac{d^{m-1}}{dx^{m-1}}y^{(n)}(x)]$$
$$= \frac{d}{dx}\sum_{\mathbf{t}\in T_{n+m-1}} \alpha(t).F(|\mathbf{t}|)(y(x))$$
$$= \sum_{\mathbf{t}\in T_{n+m}} \alpha(t).F(|\mathbf{t}|)(y(x)).$$

□

Example 3.3. *Let $n = 2$. If we apply Theorem 3.4, when $k = 1$ then*

$T_2 = \{$  $\}$

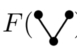
$T_{2+1} = \{$ , $\}$,

therefore

$$\frac{d}{dx} y^{''}(x) = \frac{d}{dx}(f'f) = f''ff + f'f'f.$$

On the other hand

$$\sum_{\mathbf{t} \in T_{2+1}} \alpha(t).F(|\mathbf{t}|)(y(x)) = F(\ \text{[tree]}\ )(y(x)) + F(\ \text{[tree]}\ )(y(x))$$

$$= f''ff + f'f'f.$$

4. Concluding remarks

In this paper, high order derivative of a term, using the monotonically labeled rooted trees (Lemma 3.2 and Theorem 3.2) and trees without labeling (Theorem 3.4) are obtained. The related examples have shown that the results using direct derivatives and rooted trees are equal.

5. Acknowledgment

This work was partially supported by the University of Shahrekord.
This work was partially supported by the Center of Excellence for Mathematics, Shahrekord University, Iran.

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