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A simple algorithm for the fast calculation of higher order derivatives of the inverse function

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ABSTRACT

The paper deals with the calculation of higher order derivatives of the inverse function. A simple and fast recursive procedure is presented and compared with other methods known in literature both with respect to the computation time and memory usage.

1. Introduction

Let $y(x) = f(x)$ be a function which can be represented by the Taylor power series around a point x_0 as

$$y(x_0 + \xi) = \sum_{i=0}^{\infty} \frac{\xi^i}{i!} y_i(x_0), \quad y_i(x_0) = \left.\frac{d^i y}{dx^i}\right|_{x_0}, \quad i = 1, 2, \ldots \tag{1}$$

According to the Lagrange inversion theorem this function can be inverted if $y_1(x_0) \neq 0$. Then, the series expansion of the inverse function $x = f^{-1}(y)$ around $y_0 = y(x_0)$ is given by

$$x(y_0 + \eta) = \sum_{i=0}^{\infty} \frac{\eta^i}{i!} x_i(y_0), \quad x_i(y_0) = \left.\frac{d^i x}{dy^i}\right|_{y_0}, \quad i = 1, 2, \ldots \tag{2}$$

For the case $x_0 = y_0 = 0$ the derivatives of the inverse function are expressed by the Lagrange inversion formula as [11]

$$x_i = \left.\frac{d^{i-1}}{dx^{i-1}} \left(\frac{x}{f(x)}\right)^i\right|_{x=x_0}, \quad i = 1, 2, \ldots. \tag{3}$$

Accordingly, the first few derivatives take the form

$$\begin{aligned} &x_1 = \frac{1}{y_1}, \quad x_2 = -\frac{y_2}{y_1^3}, \quad x_3 = 3\frac{y_2^2}{y_1^5} - \frac{y_3}{y_1^4}, \quad x_4 = -15\frac{y_2^3}{y_1^7} + 10\frac{y_2 y_3}{y_1^6} - \frac{y_4}{y_1^5}, \\ &x_5 = 105\frac{y_2^4}{y_1^9} - 105\frac{y_2^2 y_3}{y_1^8} + 10\frac{y_3^2}{y_1^7} + 15\frac{y_2 y_4}{y_1^7} - \frac{y_5}{y_1^6}. \end{aligned} \tag{4}$$

The calculation of higher order derivatives becomes excessively difficult and time consuming since it requires multiple differentiation of the term $\left(\frac{x}{f(x)}\right)^i$. For this reason, alternative methods for the calculation of higher order derivatives of the inverse functions have always been the subject of interest [3,4].

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Thus, Faà die Bruno proposed a formula [5] for the n-th derivative of a composed function which can also be applied to the inverse function. Despite of the simple implementation, the formulation becomes extremely complicated for higher order derivatives. Later, Chernoff [2] introduced a movable strip method to approximate coefficients of the inverse series. The main idea was to reduce the computational efforts by rewriting the differentiation rules in a systematical order.

Following the approach of Ostrowski [13], Traub [15] derived a compact explicit formulation for the derivatives of the inverse function. Recently, Floater [6] presented the same formulation by expanding the Johnson's combinatoric approach [9]. Accordingly,

$$x_n = \sum_i \frac{(-1)^{k_i}}{y_1^{n+k_i}} \frac{(n+k_i-1)!}{b_{i,2}!\dots b_{i,n}!} \left(\frac{y_2}{2!}\right)^{b_{i,2}} \cdots \left(\frac{y_n}{n!}\right)^{b_{i,n}}, \tag{5}$$

where $b_{i,2},\ b_{i,3}\dots,b_{i,n},\ i=1,2\dots$ denote non-negative integer solutions of the Diophantine equation

$$b_{i,2} + 2b_{i,3} + \cdots + (n-1)b_{i,n} = n-1. \tag{6}$$

For each of the solutions $i,\ k_i$ is given by

$$k_i = \sum_{j=2}^{n} b_{i,j}. \tag{7}$$

Thus, for every order n a system of additional equalities and inequalities should be solved. Nevertheless, the Traub method is considerably faster than the classical Lagrange approach but still slow for higher order derivatives.

Apostol [1] further proposed the following simple expression

$$x_n = \frac{P_n}{y_1^{2n-1}}, \tag{8}$$

where

$$P_{n+1} = y_1 P'_n - (2n-1) y_2 P_n. \tag{9}$$

Here, $P_1 = 1$ while P'_n is the derivative of P_n with respect to x. Accordingly, the formulation requires a recursive differentiation of P_i which represent polynomials in y_j, $(j=1,2,\dots,i)$ with integer coefficients. Explicit expressions of these polynomials grow up and increase in complexity as n increases. Thus, the calculation of higher order derivatives becomes numerically expensive and extremely time consuming.

Johnson further simplified this approach by introducing a combinatorial argument for the representation of x_n [9]. Accordingly

$$x_{n+1} = \sum_{k=0}^{n} y_1^{-n-k-1} (-1)^k \mathbf{R}_{n,k}(y_2,\dots,y_{n-k+2}), \tag{10}$$

where

$$\mathbf{R}_{n,k}(y_2,\dots,y_{n-k+2}) = \frac{1}{k!} \sum_i \binom{n+k}{b_{i,1},\dots,b_{i,k}} y_{b_{i,1}} y_{b_{i,2}} \dots y_{b_{i,k}}. \tag{11}$$

The summation is carried out over each set of integer solutions $b_{i,1},\ b_{i,1},\dots,b_{i,k},\ i=1,2\dots$ of the following Diophantine equation

$$b_{i,1} + \cdots + b_{i,k} = n+k, \quad b_{i,j} \geqslant 2. \tag{12}$$

Recently, Liptaj [12] proposed a solution for derivatives of the inverse function in a recursive limit form as

$$x_n = \lim_{\Delta x \to 0} n! \frac{\Delta x - \sum_{i=1}^{n-1} \frac{x_i}{i!} \left(\sum_{j=1}^{n} \frac{x_j (\Delta x)^j}{j!} \right)^i}{\left(\sum_{i=1}^{n} \frac{y_i (\Delta x)^i}{i!} \right)^n}, \quad x_1 = \frac{1}{y_1}, \quad n = 2,3,\dots. \tag{13}$$

Unlike the conventional methods the procedure of Liptaj does not require the successive differentiation and is relatively fast for lower order derivatives. For higher orders, however, the calculation of limits becomes very difficult and time consuming.

We further developed the procedure by Liptaj and proposed a simple recursive formula for the calculation of Taylor coefficients of the inverse function [8]. In this contribution, we shortly present this formula and additionally provide more insight into the computational aspects of the calculation. The advantages and capabilities of the proposed formulation are then illustrated in comparison with the procedures by Traub/Floater, Apostol, Johnson and Liptaj discussed above.

2. Proposed formulation

In view of (1) and (2) we can write