

# Simultaneous Calculation of Gradient Enclosures and Their Use for $n$ -th Order Box Rejection

K. Makino and M. Berz

Department of Physics and Astronomy  
Michigan State University  
East Lansing, MI 48824-2320, USA  
email: makino@msu.edu

## Abstract

A method is developed that allows the efficient calculation of  $(n - 1)$ st order Taylor models (TM) for the gradient of a function in  $v$  variables simultaneously with the calculation of the Taylor model of the original function. The method is based on the well-known fact that the derivative of a Taylor polynomial of a function  $f$  equals the Taylor polynomial of the derivative of  $f$  to one less order. Thus, the knowledge of the Taylor polynomial coefficients of  $f$  to order  $n$  allows the direct determination of those of its partials by simple manipulation of the coefficients. To obtain the Taylor models for the gradient, it is hence only necessary to also accumulate  $v$  additional remainder bounds for the partials. An arithmetic is introduced that achieves this in a seamless way in parallel to conventional TM arithmetic. In typical cases of dimensions 5 to 20, the increase in computation time compared to a regular TM evaluation is less than a factor of two.

The methods are used in a simplified version of a TM-based high-order interval Newton method. This method allows the exclusion of boxes with significantly reduced dependency, and with a sharpness that scales with the  $n$ -th power of the width of the domain boxes. Examples for the practical use of the method in a verified global optimization setting are given.