Adjoint Function as Bisection Heuristic for Guaranteed Global Optimization with Nonlinear Ordinary Differential Equations

Julien Alexandre Dit Sandretto

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Abstract

We focus on interval algorithms for computing guaranteed enclosures of the solutions of constrained global optimization problems where differential constraints occur. To solve such a problem of global optimization with nonlinear ordinary differential equations, a branch and bound algorithm can be used based on guaranteed numerical integration methods. Nevertheless, this kind of algorithms is expensive in term of computation. Defining new methods to reduce the number of branches is still a challenge. Bisection based on the smear value is known to be often the most efficient heuristic for branching algorithms. This heuristic consists in bisecting in the coordinate direction for which the values of the considered function change the most "rapidly".

We propose to define a smear-like function using the adjoint (or sensitivity) function obtained from the differentiation of ordinary differential equation with respect to parameters. The adjoint has been already used in validated simulation for local optimization but not as a bisection heuristic. We implement this heuristic in a branch and bound algorithm to solve a problem of global optimization with nonlinear ordinary differential equations. Experiments show that the gain in term of number of branches could be up to 30%.

1 Branch and bound

1.1 Classical algo

version jaulin

1.2 Smear heuristic

this mode is based on the smear function as defined by Kearfott [7]: let $J = ((J_{ij}))$ be the Jacobian matrix of the system and let define for the variable x_i the smear value $s_i = \text{Max}(|\underline{J_{ij}[\underline{x_i},\overline{x_i}]}|, |\overline{J_{ij}[\underline{x_i},\overline{x_i}]}|\ \forall j \in [1,n]$ where n is the total number of functions. The variable that will be bisected will be the one having the largest s_i. There is however a drawback f the smear function: let consider for example the equation $F = f^2b^3 - 1 = 0$ where f,b are large identical intervals centered at 0. The derivative of F with respect to f is $2fb^3$ and with respect to b $3f^2b^2$: multiplied by the width of the interval we get $2f^2b^3$ and $3f^2b^3$. Hence the smear function for b will be in general larger than for f and b will always be bisected until its width is lower than the desired accuracy.

Another example in which the smear function is not the best choice is presented in section 2.4.3.4. However the smear function is very often the most efficient mode and should be privileged.

2 Adjoint

2.1 Sensitivity analysis

Sensitivity has been used in a different manner in [**?**]. It consists to simultaneously simulate an ODE described by

$$\dot{s} = \frac{\partial f}{\partial y} \times s + \frac{\partial f}{\partial p}. \tag{1}$$

to obtain the adjoint function $s(t) = \frac{\partial y}{\partial p}$, which is the evolution of state w.r.t. parameters.

adjoint used locally, etc..

2.2 Adjoint based smear

3 Experiments

3.1 Problem

3.2 Results

largest first nb bissection : 16864 hull of solutions : ([0.95, 0.950274658203125] ; [0.999920654296875, 1] ; [0.99996337890625, 1]) nb bissection : 16867 cout min : 0.718753753324554 real 1573m24.041s

smear nb bissection : 12146 hull of solutions : ([0.95, 0.950274658203125] ; [0.999920654296875, 1] ; [0.99996337890625, 1]) nb bissection : 12154 cout min : 0.718753753324554 real 7536m16.196s