Finding steady states in genome-scale biochemical reaction networks

Francisco J. Aragón Artacho[1], Phan T. Vuong[2]* (vuong.phan@uni.lu), and **Ronan M. T. Fleming**[2]

[1]Department of Statistics and Operations Research, University of Alicante, Spain; [2]Luxembourg Centre for Systems Biomedicine, University of Luxembourg, Esch-sur-Alzette, Luxembourg

http://stanford.edu/group/SOL/multiscale/

Project Goals: The problem of finding non-equilibrium steady states in genome-scale biochemical reaction networks is reformulated as an optimisation problem involving difference of convex functions (DC function). The resulted optimisation problem is then tackled by Boosted Difference of Convex function Algorithms (BDCA). Numerical tests on various biochemical models show the effiency of the implemented algorithms.

Many problems arising in science and engineering applications require the development of algorithms to minimise a nonconvex function. If a nonconvex function admits a decomposition, this may be exploited to tailor specialised optimisation algorithms. Our main focus is the following optimisation problem

$$\operatorname*{minimise}_{x\in\mathbb{R}^m} \phi(x) := f_1(x) - f_2(x),$$

where $f_1, f_2 : \mathbb{R}^m \to \mathbb{R}$ are continuously differentiable convex functions and

$$\inf_{x\in\mathbb{R}^m} \phi(x) > -\infty.$$

In biochemistry, this problem arises in the study of non-equilibrium steady states of biochemical reaction networks. We introduce two new algorithms to find stationary points of DC programs, called *Boosted Difference of Convex function Algorithms* (BDCA), which accelerate DCA [4] with a line search using an Armijo type rule. The first algorithm directly uses a backtracking technique, while the second uses a quadratic interpolation of the objective function together with backtracking. Our algorithms are based on both DCA and the proximal point algorithm approach of Fukushima–Mine [3]. We analyse the rate of convergence under the Łojasiewicz property [2] of the objective function. We discovered that the objective function arising in these biochemical reaction networks is real analytic, a class of functions which is known to satisfy the Łojasiewicz property [2]. Numerical tests on various biochemical models clearly show that our algorithm outperforms DCA, being on average more than four times faster in both computational time and the number of iterations [1]. This algorithm is guarunteed to find a non-equilibrium steady state concentration for any genome-scale biochemical network that admits one such steady state.

References

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