A Barrier-Terrain Methodology for Global Optimization

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Abstract

It is shown that all stationary and singular points to optimization problems do not necessarily need to lie in the same valley and that valleys in the residual error space are not necessarily smoothly connected. Logarithmic barrier functions are shown to be an effective means to create a smooth connection between distinct valleys for some set of barrier parameter values bounded away from zero, so that the resulting terrain method is guaranteed to explore the entire feasible region. Once valleys are connected at ‘intermediate’ values of the barrier parameter, different stationary and singular points in separate regions of the feasible space can be calculated and identified by the terrain method and sequentially tracked as the barrier parameter is further reduced. A simple barrier-terrain algorithm is presented and considerable details are presented for a small example to make the underlying ideas clear. The proposed barrier-terrain methodology is then used to successfully find all physically meaningful solutions to a collocation model for a spherical catalyst pellet problem with 20 variables. The key contribution of this work is the discovery of a fundamental property of barrier methods that provides connections between valleys of the residual error space containing stationary points for some set of intermediate values of the barrier parameter under mild conditions on the underlying model equations.
1. Introduction. Many important models of chemical engineering applications have multiple solutions that are sometimes difficult to find in the absence of prior knowledge. Examples include equations of state such as the Statistical Associating Fluid Theory (SAFT) equations, phase stability/equilibrium problems and problems in chemical kinetics. One way to find multiple solutions is to formulate the underlying problem in the form of a global mathematical program and use a global optimization methodology such as an interval method (Schnepper & Stadtherr, 1995), continuation method (Sun & Seider, 1992), a branch and bound algorithm (Maranas & Floudas, 1995), simulated annealing (Kirkpatrick et al., 1983), genetic algorithms (Holland, 1992), a terrain following method or some other strategy. In this article, we use the terrain method of Lucia and co-workers (Lucia & Yang, 2003; Lucia, DiMaggio & Depa, 2004).

Barrier methods of nonlinear programming are old techniques that were developed in the 1950’s and are similar to penalty function methods. See Frisch (1955) and Fiacco and McCormick (1968). In particular, logarithmic-barrier methods form the backbone of an entire class of methods called interior-point methods. The main objective of logarithmic barrier methods is to enforce feasibility on iterates in equation-solving methods like quasi-Newton and Newton methods. Barrier methods force iterates to lie in the interior of the feasible region by constructing a function that tends to infinity at the boundaries of the feasible region. The typical functional form of a logarithmic barrier function for the simple bound \( x > 0 \) is \(-\mu \log(x)\), where \( \mu \) is called a barrier parameter. Barrier functions can also be used with upper bounds on variables and general inequality constraints in a straightforward manner. The key aspects of any barrier approach are to

1) Create an augmented objective function consisting of the given objective function and the barrier function.
2) Start with a large value of the barrier parameter so that the augmented objective function is convex and has a unique minimum.
3) Reduce the value of the barrier parameter and use a solution from the previous barrier sub-problem, \( x^*(\mu_k) \), to find a solution to the current barrier sub-problem, \( x^*(\mu_{k+1}) \).
4) Terminate the optimization calculations when \( \mu \) is sufficiently close to 0, where the values of the augmented objective function and given objective function coincide.

Note that the barrier function ensures iterates are always in the interior of the feasible region and the barrier parameter serves as a continuation parameter.

Barrier methods are powerful techniques; however, they are not without disadvantages. In particular, if there are active inequality constraints at the solution for \( \mu \approx 0 \), then it is well known that the Hessian matrix of the augmented objective function becomes increasingly ill-conditioned and this ill-conditioning cannot be avoided. See, for example, Luenberger (1973). If no inequalities are active at the solution, then the eigen-structure of the Hessian matrix at the desired solution is that of the given objective function.

In this article, we discover that barrier functions can be an effective tool to identify all solutions for global optimization with terrain methods in cases where some solutions belong to separate disconnected regions in the feasible space. To the best of our knowledge, this use of barrier functions beyond their classical purpose is reported for the first time in the open literature.