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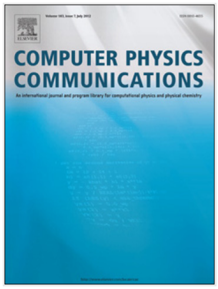


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Qing-Xiao Li, Rong-Qiang He, Zhong-Yi Lu

PII: S0010-4655(16)30060-1
DOI: http://dx.doi.org/10.1016/j.cpc.2016.03.002
Reference: COMPHY 5894

To appear in: *Computer Physics Communications*

Received date: 20 August 2015
Revised date: 13 December 2015
Accepted date: 6 March 2016

Please cite this article as: Q.-X. Li, R.-Q. He, Z.-Y. Lu, Accelerating optimization by tracing valley, *Computer Physics Communications* (2016), http://dx.doi.org/10.1016/j.cpc.2016.03.002

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# Accelerating optimization by tracing valley

Qing-Xiao Li[a], Rong-Qiang He[b,a,*], Zhong-Yi Lu[a]

[a] *Department of Physics, Renmin University of China, Beijing 100872, China*
[b] *Institute for Advanced Study, Tsinghua University, Beijing 100084, China*

## Abstract

We propose an algorithm to accelerate optimization when an objective function locally resembles a long narrow valley. In such a case, a conventional optimization algorithm usually wanders with too many tiny steps in the valley. The new algorithm approximates the valley bottom locally by a parabola that is obtained by fitting a set of successive points generated recently by a conventional optimization method. Then large steps are taken along the parabola, accompanied by fine adjustment to trace the valley bottom. The effectiveness of the new algorithm has been demonstrated by accelerating the Newton trust-region minimization method and the Levenberg–Marquardt method on the nonlinear fitting problem in exact diagonalization dynamical mean-field theory and on the classic minimization problem of the Rosenbrock's function. Many times speedup has been achieved for both problems, showing the high efficiency of the new algorithm.

*Keywords:* accelerate optimization, long narrow valley, nonlinear fitting, Newton trust-region minimization, Levenberg–Marquardt method

## 1. Introduction

The dynamical mean-field theory [1] is one of the most important approaches for studying strongly correlated electronic systems in condensed matter physics. A nonlinear fitting problem appears in dynamical mean-field theory with exact diagonalization as impurity solver (ED-DMFT) [2]. As the number of fitting parameters increases, the fitting becomes exponentially difficult. This difficulty represents one of the most challenging scenarios for optimization. In such a scenario, the optimum lies inside a long narrow valley (ravine) of the surface of an objective function. Sometimes, it is also called "poor scaling" [3] or "pathological curvature" [4]. In the valley, the function is insensitive to changes of its variables in some direction, i.e., along the valley bottom, and is very sensitive to changes in other directions. A simple example is $f(x, y) = 10^4x^4 + y^4$. The "long narrow valley" scenario is frequently encountered in a variety of research fields such as machine learning [4–8], engineering [9–16], physics [17–19], etc. [20–22]

This difficulty is the severest for curvature-blind methods such as steepest descent and simplex method, while it is considerably reduced by (quasi-) second-order methods like conjugate gradient and quasi-Newton. Constant effort has been being devoted to this issue [3–6, 11, 13, 19, 21, 23–43]. Generally, improvement is made case by case because each method has its own underlying logic and best applicable situation. For example, a trust-region method can be improved by an elliptic trust-region method [3] or by a nonmonotone method [8, 34, 39–42].

In this paper, we propose a relatively universal acceleration algorithm that can be used to accelerate all iterative optimization methods whose successive steps can roughly follow the valley bottom of the surface of the objective function. Our observation is that although the profile of an objective function surface may be very complicated and the curvatures may differ enormously in different directions, the profile of the valley bottom is much simpler, usually just a smooth curve in multi-dimensional space. The new algorithm identifies the valley bottom trend by fitting the points of the recent successive steps — "footprints" — generated by a regular iterative optimization method to a parabola and moves with large steps along the fitted parabola, accompanied with fine adjustment to prevent from getting out of the valley. We test the new algorithm against the Newton trust-region (NTR) [3, 44] minimization method and the Levenberg–Marquardt (LM) [24] method upon the nonlinear fitting problem in ED-DMFT and the classic minimization problem of the Rosenbrock's function. Significant speedup is observed, especially for higher spatial dimensions.

This paper is organized as follows. To make the discussion self-contained, we briefly review the NTR and LM methods in Sections 2 and 3, respectively. Used in our new algorithm, the methods for fitting points to a straight line and to a parabola in multi-dimensional space are developed in Sections 4 and 5, respectively. The long-narrow-

*Corresponding author
*Email addresses:* rqhe@ruc.edu.cn (Rong-Qiang He), zlu@ruc.edu.cn (Zhong-Yi Lu)

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