Assessing Convergence in Gaussian Process Surrogate Model Optimization

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Abstract

Identifying convergence in numerical optimization is an ever-present, difficult, and often subjective task. The statistical framework provided by Gaussian Process surrogate model optimization provides useful secondary measures for tracking optimization progress; however the identification of convergence via these criteria has often provided only limited success and often requires a more subjective analysis. Here we use ideas originally introduced in the field of Statistical Process Control to define convergence in the context of an robust and objective convergence heuristic. The Exponentially Weighted Moving Average (EWMA) chart provides an ideal starting point for adaptation to track convergence via the EWMA convergence chart introduced here.

Keywords: Computer Model, Derivative-free Optimization, Emulator, Expected Improvement.

1 Introduction

Black-box derivative-free optimization is an important problem with a wide variety of applications, especially in the realm of computer simulations. When dealing with computationally expensive computer models, a key question is that of convergence of the optimization. Because each function evaluation is expensive, one wants to terminate the optimization as early as possible. However for complex simluators, the response surface may be ill-behaved and optimization routines can easily become trapped in a local mode, so one needs to run the optimization sufficiently long to achieve a robust solution. In this paper, we provide an automated method for assessing convergence of Gaussian process surrogate model optimization by bringing in elements of Statistical Process Control.

Our motivating example is a hydrology application, the Lockwood pump-and-treat problem cite, discussed in more detail in Section XX, wherein contamination in the groundwater near the Yellowstone River is remediated via a set of treatment wells. The goal is to minimize the cost of running the wells while ensuring that no contamination enters the river. The contamination constraint results in a complicated boundary that is unknown in advance and requires evaluation of the simulator, and thus finding the global constrained minimum is a difficult problem and it is easy for optimization routines to at least temporarily get stuck in a local minimum. Without knowing the answer in advance, how do we know when to terminate the optimization routine?

The context of this paper is Gaussian Process surrogate model optimization, a statistical modeling approach to derivative-free numerical optimization routine that constructs a fast approximation to the expensive computer simulation using a statistical surrogate model. Analysis of the surrogate model allows for efficient exploration the objective solution space. Typically a Gaussian Process (GP) surrogate model is chosen for its robustness, relative ease of computation, and its predictive framework [?]cite. Arising naturally from the GP predictive distributioncite, the maximum Expected Improvement (EI) criterion has shown to be a valuable criterion for assessing future points of exploration on the objective function cite, and furthermore the EI shows promise for use as a convergence criterion cite.

Literature cite recommends considering the EI as a convergence criterion for GP surrogate model optimization; as of yet, little work has been done to describe what convergence of these algorithms actually looks like in the context of the EI criterion. However, the basic idea behind the use of the EI criterion, as a convergence criterion, is that convergence should occur when the GP surrogate model produces low expectations for discovering new optima; that is to say, small EI values should be associated with convergence of the algorithm. Thus, a common stopping rule, involving the EI criterion, first defines some lower EI threshold, then claims convergence upon first sight of an EI value falling below this threshold cite. This use of EI as a convergence criteria falls well within the comfort zone of the numerical optimization literature as this is certainly a reasonable approach for monitoring the convergence criteria of other routines (ex. the vanishing step sizes of Newton-Raphson, Pattern Search (PS) methods, etc.). However, this use of the EI criterion on GP surrogate model optimization has not yet been adequately justified. In fact, this use ignores the nature of the EI criterion as a random variable, and oversimplifies the stochastic nature of convergence in this setting. Thus it is no surprise that this treatment of the EI criterion results in an inconsistent stopping rule as demonstrated in Figure (1).

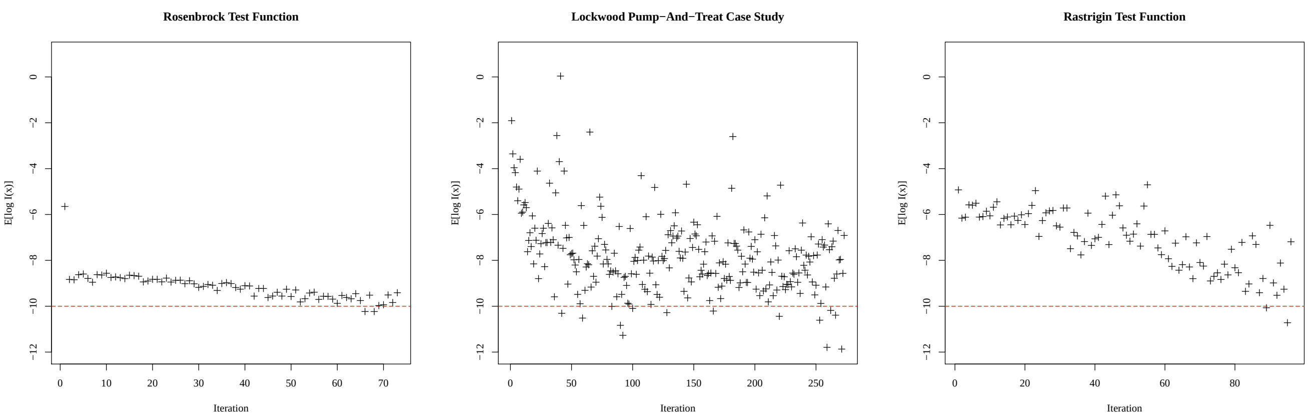

Figure 1: Three ELAI seires plotted alongside an example convergence threshold value shown as a dashed line at -10. fix ELAI y label

Because Expected Improvement is non-negative but decreasingly small, we find it more productive to work on the log scale, using a lognormal approximation to the improvement distribution, as described in more detail in Section XX. Figure (1) represents three series of the Expected Lognormal Approximation to the Improvement (ELAI) values from three different optimization problems that will be demonstrated later in this paper, where it will be shown that convergence is established near the end of each of these series. These three series demonstrate various ELAI convergence behaviors, and illustrate the difficulty in assessing convergence. In the left-most panel, optimization of the Rosenbrock test function results in a well-behaved series of ELAI values, demonstrating a case in which the simple threshold stopping rule can accuratly identify convergence. However the center panel (the Lockwood problem) demonstrates a failure of the threshold stopping rule, as this ELAI series contains much more variance, and thus small ELAI values are observed quite regularly. In the Lockwood example a simple threshold stopping rule could falsely claim convergence within the first 50 iterations of the algorithm. The large variability in ELAI with occasional large values indicates that the optimization routine is still exploring and is not yet convinced that it has found a global minimum. This optimization run appears to have converged only after the larger ELAI values stop appearing and the variability has decreased. Thus one might ask if a decrease in variability or small variability is a necessary condition for convergence. The right panel (the Rastigin test function) shows a case where convergence occurs by meeting the threshold level, but where variability has increased, demonstrating that a decrease in variability is not a necessary condition.

As the Improvement function is itself a random variable, attempting to use a threshold test oversimplifies the dynamics of convergence. Instead, we propose taking the perspective of Statistical Process Control (SPC), where a stochastic series is monitored for consistency of the distribution of the most recently observed values.