UNIVERSITY OF CALIFORNIA SANTA CRUZ

IDENTIFYING CONVERGENCE IN GAUSSIAN PROCESS SURROGATE MODEL OPTIMIZATION, VIA STATISTICAL PROCESS CONTROL

A document submitted in partial satisfaction of the requirements for the degree of

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in

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by

Nicholas R. Grunloh

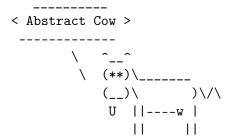
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Approv	eu by:
	Professor Herbie Lee
	ociate Professor John Musacchio

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Abstract



1 Introduction

- Identify convergence problem
- Define properties of convergence
- A taste of my stuff
- Explicate road-map

1.1 General

- Optimization: Background and our Philosophy
 - gradient free [5]
 - GA [5], Simulated Annealing [5], Pattern Search [5], Trust Regions [5]
 - benefits of a model based approach (ie. uncertain measures) (i.e. General/No GP)
 - uncertainty measures as convergence criteria
- Statistical process control for monitoring convergence
 - General [4] (ie. no EWMA)
 - tease EWMA

1.2 Gaussian Process Models

- Gaussian Process Surrogate Model
- How does a Gaussian process work? [1]
- Add Flexibility through treed Partitioning [2]

1.3 Convergence Criteria

- Measures?
- Choose $\mathbb{E}[I(\boldsymbol{x})]$, why? [8], [3]
- some characteristics [bounded at 0], decreasing.
- which $\mathbb{E}[I^g(\boldsymbol{x})]$, ie. which g? [8]
- maximum $\mathbb{E}[I(x)]$ (i.e. the mean at the predictive location that achieves the maximum mean of the samples at that location)

1.4 Optimization

- Optimization Procedure [3]
 - code appendix, using tgp
- advantages of model based approach for convergence sake
- $\mathbb{E}[I(x)]$ Behavior for convergence

1.5 Statistical Process Control

1.5.1 Shewhart's \bar{x} Chart

- the notion of control (draw similarities to convergence). [4]
- how the typical charts work
- philosophy.
 - establish control (herbies book)
 - control \rightarrow out-of-control
- stumbling blocks of convergence for me.
 - out-of-control \rightarrow control
 - the notion of a sliding average (i.e. convergence)
 - normal assumptions are very strong for an application that strongly desired robustness in varied applications

1.5.2 Exponentially Weighted Moving Average Chart

- EWMA philosophy (Robustness) [7].
- How it works (derivation cite).
- look at the statistics and bounds
- Tracking slight changes (general scale and behavior of $\mathbb{E}[I(x)]$)
- weight recent data more heavily to handle the sliding average (also mention later about the window; maybe set-up here)

2 Identifying Convergence

- tie this stuff together and motivate the coolness factor.
- use optimization procedure outlined [3] also above and in appendix.
- recall that the maximum $\mathbb{E}[I(x)]$ each iteration is the mean at the predictive location that achieves the highest mean value.
- SPC is based on normality assumptions of the underlying sampling distribution.
- a thesis statement for the research that I did: SPC, EWMA, empirical predictive MCMC control limits, Log-Normal → model based limits.

2.1 The Control Window

- convergence formulated in the context of statistical process control has unique challenges since almost by definition max $\mathbb{E}\left[\ \mathbf{I}(\boldsymbol{x})\ \right]$ starts in an out-of-control state then moves into a state of control the optimization routine approaches a state of convergence
- typical SPC goes through an initialization process, in which, initially out-of-control observation are investigated and systematically accounted for to establish an initial state of control.
- introduce the window to automate this process and thus set the current control state at a window of the most recently observed values.
- window of size w, tuning parameter, thus partitioning the observations into points in the control window(i.e. control training set) and points outside of the control window(i.e. control test set)
- convergence rules: out-of-control in control test set and in-control in control training set.
- choosing w for difficulty of problem.

2.2 \bar{x} Chart

- basic shewhart chart
- issues with robustness since you often see linear trends toward the lower control limit as $\max \mathbb{E} [I(x)]$ seems to converge in probability to 0 from the positive direction.

2.3 Model-Based Transformation

- Transformation
- \bar{x} Chart
- equally weighted observations leads to false positive in identifying convergence since initial $\mathbb{E}[I(x)]$ may be very large.

2.4 EWMA Chart

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Example pictures above?, or keep most of the figures that I made in the below sections?, start Rosenbrok example early?:

• $\max \mathbb{E}[I(\boldsymbol{x})]$, General Behavior (3 stages, not-converged(inital exploration), converging(pre-convergence) and converged(converged))

•

3 Test Functions

use each example as an excuse to look at different things?

3.1 Rosenbrock

- write the general function down, focus on the 2-D case, code appendix (cite?)
- get a good looking window
- plot what function looks like in this window, perspective and heat plot,
- gaussian process fit perspective and heat plot (movie?), thumbnail:first converged picture
- Simple $\mathbb{E}[I(x)]$ Pictures
 - $max\mathbb{E}[I(\boldsymbol{x})]/best Z$ (tell three stages convergence story)
 - hist of $max\mathbb{E}[I(\boldsymbol{x})]$ samples

- Q-Q plot?
- $-\bar{x}$ Chart
- Transformed Pictures
 - $max\mathbb{E} [I(\boldsymbol{x})]/best Z$
 - hist of $max\mathbb{E}[I(\boldsymbol{x})]$ samples
 - Q-Q plot?
- discussion of results

3.2 Rastringin

- write down function cite)
- several mode window
- plot what function looks like in this window, perspective and heat plot,
- gaussian process fit perspective and heat plot (movie?), thumbnail:first converged picture
- Transformed Picture $max\mathbb{E}[I(\boldsymbol{x})]/\text{best Z}$
- ullet discussion of results

3.3 Easom

- write down function cite
- Get reasonably flat window
- plot what function looks like in this window, perspective and heat plot,
- gaussian process fit perspective and heat plot (movie?), thumbnail:first converged picture
- Transformed Picture $max\mathbb{E}[I(\boldsymbol{x})]/\text{best Z}$
- discussion of results

3.4 Real Data

- explore this data cite
- get good lookin picture of objective function
- gaussian process fit perspective and heat plot (movie?), thumbnail:first converged picture
- Transformed Picture $max\mathbb{E}[I(\boldsymbol{x})]/\text{best Z}$
- discussion of results

4 Discussion

- argument for a convergence criteria based on above results
- Robustness of EWMA [7]
- further research partitioned model idea.

5 Code Appendix

- tgp optimization [3]
- qcc EWMA SPC [6]
- example implimentation (cite data)

References

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