Master's Thesis

Bridging Optimization and Sampling: The Role of Warmstarts and Mass Matrix Adaptation in SG-MCMC

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Abstract

This is my new abstract.

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1 Introduction

1.1 Motivation

1.2 Problem

- in high dimensional, complex posteriors we are often confronted with ill-conditioned modes
- this might lead to slow convergence when the sampler is not able to adapt to the local curvature of the posterior
- we can show this effect on some simple gaussian (mixture) examples

Note: the visualizations show the true density in the background, while compute the steps of the MCMC sampler on samples of the log density.

1.3 Research Objective

- preconditioning the MCMC sampler to accord to the local curvature of the posterior
- investigate whether this leads to better uncertainty quantification and convergence properties
- investigate whether this leads to better exploration of the posterior (detect multi-modality)

This contributes to the fields in the way, that overall less samples/shorter chains are needed to achieve resonably good results.

1.4 Outline

2 Background

3 Related Work

4 Method

4.1 General Idea

- best case would be to compute the inverse Fisher Information Matrix in each step as preconditioning to apply to local geometry of the current position
- cannot be done in our MCMC preconditioning context since it is much to expensive to estimate the FIM in every step from scratch
- we cannot do a Hessian approximation like RmsProp or Adam, since they utilize values depending which depend on previous steps. This does then not meet meet the markov property (MCMC theory breaks)
- this is why we optimize first obtaining a high likelihood soultion and a rough estimation of the local geometry (via Adam like Hessia approximation or IVON)
- using this information might help shorten the warmup/burnin phase without hurting the performance
- during sampling we then want to efficiently sample the a local subspace of the high dimensional posterior where the optimizer landed
- multimodality is tackled through ensembling and lengthy markov chains

5 Experiments

6 Conclusion

A Appendix

B Electronic appendix

Data, code and figures are provided in electronic form.

Declaration of authorship

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