Variational Inference

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 - Introduction
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Inference is NP-hard!

Variational Inference

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Other Topics

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ELBO

Evidence Lower Bound Objective (ELBO)

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Introduction

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Univariate Gaussian

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- m_p , s_p^2 , α_p and β_p are hyper-parameters

Other Topics

Univariate Gaussian (Cont.)

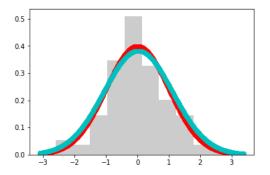


Figure 1: True (red) vs Approximated (blue) Distribution

Univariate Gaussian (Cont.)

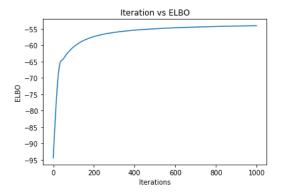


Figure 2: ELBO(q) vs Iterations

Gaussian Mixture Model

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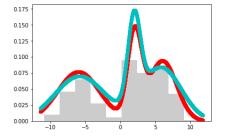


Figure 3: True (red) vs Approximated (blue) Distribution

Gaussian Mixture Model (Cont.)

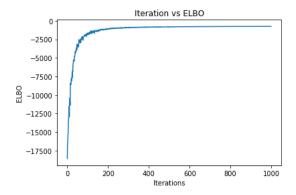


Figure 4: ELBO(q) vs Iterations

Introduction

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- \bullet and ϕ : Neural networks

Optimize ϕ and θ using variational inference Core Idea:

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Motivation

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This highlights the usual trade-off between prior and observations

Results on MNIST

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Figure 5: Generated Images

Results on CIFAR-10



Figure 6: Generated Images

Comparison with maximum likelihood estimation for univariate Gaussian

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Tutorials and other resources are available at:

https://github.com/sh-gupta/VariationalInference

References

- D. M. Blei, A. Kucukelbir, and J. D. McAuliffe, *Variational Inference: A Review for Statisticians*, ArXiv e-prints (2016).
- David M. Blei, Andrew Y. Ng, and Michael I. Jordan, *Latent dirichlet allocation*, J. Mach. Learn. Res. **3** (2003), 993–1022.
- D. P Kingma and M. Welling, *Auto-Encoding Variational Bayes*, ArXiv e-prints (2013).

Thank You!