STOCHASTIC OPTIMIZATION IN MACHINE LEARNING

CASE STUDIES IN NONLINEAR OPTIMIZATION

F. Bauer S. Chambon R. Halbig S. Heidekrüger J. Heuke

July 10, 2015

Technische Universität München

WE'RE NOT RUNNING OUT OF DATA ANYTIME SOON. IT'S MAYBE THE ONLY RESOURCE THAT

GROWS EXPONENTIALLY.

ANDREAS WEIGEND

OUTLINE

- 1. Introduction
- 2. SQN: A Stochastic Quasi-Newton Method
- 3. Proximal Method
- 4. Logistic Regression: An Example
- 5. Dictionary Learning
- 6. Conclusion
- 7. Appendix

INTRODUCTION

INTRODUCTION: WHAT IS MACHINE LEARNING?

Implementation of autonomously learning software for:

- · Discovery of patterns and relationships in data
- · Prediction of future events

Examples:

Electroence-phalography (EEG)



Section 4

Image Denoising



Section 5

ML AND OPTIMIZATION I

Training a Machine Learning model means finding optimal parameters ω :

$$\omega^* = \operatorname{argmin}_{\omega} F(\omega, X, z)$$

ML AND OPTIMIZATION I

Training a Machine Learning model means finding optimal parameters ω :

$$\omega^* = \operatorname{argmin}_{\omega} F(\omega, X, z)$$

- F: Loss function of chosen ML-model
- X: The training data (N := #samples × #features matrix)
- · z: Training labels (only in classification models; vector of size N)

ML AND OPTIMIZATION I

Training a Machine Learning model means finding optimal parameters ω :

$$\omega^* = \operatorname{argmin}_{\omega} F(\omega, X, z)$$

- F: Loss function of chosen ML-model
- X: The training data (N := #samples × #features matrix)
- · z: Training labels (only in classification models; vector of size N)
- \cdot The dimension n of ω is model dependent, often #features+1

ML AND OPTIMIZATION II

After we have found ω^* , we can do Prediction on new data points:

$$\hat{z_i} := h(\omega^*, x_i)$$

ML AND OPTIMIZATION II

After we have found ω^* , we can do Prediction on new data points:

$$\hat{z}_i := h(\omega^*, x_i)$$

- X_i: new data point with *unknown* label Z_i
- h: hypothesis function of the ML model

CHALLENGES IN MACHINE LEARNING

- · Massive amounts of training data
- · Construction of very large models
- · Handling high memory/computational demands

CHALLENGES IN MACHINE LEARNING

- · Massive amounts of training data
- · Construction of very large models
- · Handling high memory/computational demands

Ansatz: Stochastic Methods

STOCHASTIC FRAMEWORK

$$F(\omega) := \mathbb{E}[f(\omega, \xi)]$$

STOCHASTIC FRAMEWORK

$$F(\omega) := \mathbb{E}[f(\omega, \xi)]$$

• ξ : Random variable; takes the form of an input-output-pair (x_i, z_i)

STOCHASTIC FRAMEWORK

$$F(\omega) := \mathbb{E}[f(\omega, \xi)] = \frac{1}{N} \sum_{i=1}^{N} f(\omega, x_i, z_i)$$

- ξ : Random variable; takes the form of an input-output-pair (x_i, z_i)
- f: Partial loss function corresponding to a single data point.

STOCHASTIC METHODS

Gradient Method

 $\min F(\omega)$

Stochastic Gradient Descent

 $\min \mathbb{E}\left[f(\omega,\xi)\right]$

STOCHASTIC METHODS

Gradient Method

 $\min F(\omega)$

 $\omega^{(k+1)} := \omega^{(k)} - \alpha_k \nabla F(\omega^{(k)})$

Stochastic Gradient Descent

 $\min \mathbb{E}\left[f(\omega,\xi)\right]$

STOCHASTIC METHODS

Gradient Method

 $\min F(\omega)$

$$\omega^{(k+1)} := \omega^{(k)} - \alpha_k \nabla F(\omega^{(k)})$$

Stochastic Gradient Descent

$$\min \mathbb{E}\left[f(\omega, \xi)\right]$$

$$\omega^{(k+1)} := \omega^{(k)} - \alpha_k \nabla \hat{F}(\omega^{(k)})$$
with

$$\nabla \hat{F}(\omega^{(k)}) := \frac{1}{b} \sum_{i \in \mathcal{S}_k} f(\omega, x_i, z_i)$$

where $S_k \subset [N]$, $b := |S_k| \ll N$ "Mini Batch"

SQN: A STOCHASTIC QUASI-NEWTON

METHOD

HIGGS-BOSON CLASSIFICATION PROBLEM

- · Data from Monte-Carlo simulations
- $X \in \mathbb{R}^{11.000.000 \times 29}$ Lots of samples, relatively small, dense feature set.
- · Here, we use Logistic Regression for classification.

STOCHASTIC QUASI-NEWTON METHOD (SQN)

- Stochastically use second-order information
- · Based on BFGS-method.

STOCHASTIC QUASI-NEWTON METHOD (SQN)

- Stochastically use second-order information
- · Based on BFGS-method.
- · Basic idea:

$$\omega^{(k+1)} = \omega^{(k)} - \alpha_k H_t \nabla \hat{F}(\omega^{(k)})$$

STOCHASTIC QUASI-NEWTON METHOD (SQN)

- · Stochastically use second-order information
- · Based on BFGS-method.
- · Basic idea:

$$\omega^{(k+1)} = \omega^{(k)} - \alpha_k H_t \nabla \hat{F}(\omega^{(k)})$$

- t running on slower time-scale than k.
- · H_t update in $\mathcal{O}(n)$ time and constant memory, using several tricks

BEHAVIOR

Pretty picures about the behaviour of SQN on HIGGS and comparison with traditional SGD $\,$

RESULTS

- · Can be faster than SGD on appropriate Datasets
- Requires tedious, manual tuning of hyperparameters to be efficient!

PROXIMAL METHOD

PROXIMAL METHOD

$$\min_{x} F(x) := \underbrace{f(x)}_{smooth} + \underbrace{h(x)}_{non-smooth}$$

Problem

$$\min_{x} F(x) := \underbrace{f(x)}_{smooth} + \underbrace{h(x)}_{non-smooth}$$

Proximity Operator

$$\operatorname{prox}_{f}(v) = \underset{x}{\operatorname{argmin}} (f(x) + \frac{1}{2} ||x - v||_{2}^{2})$$

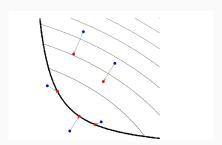


Figure 1: Evaluating a proximal operator at various points. N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014

Traditional Proximal Gradient Step:

$$x_{k+1} = \operatorname{prox}_{\lambda_k h}(x_k - \lambda_k \nabla f(x_k))$$

Quasi-Newton Proximal Step:

$$x_{k+1} = \text{prox}_{h}^{B_k}(x_k - B_k^{-1}\nabla f(x_k)),$$

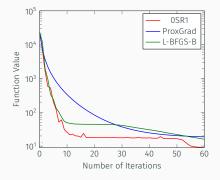
with
$$B_k = \underbrace{D_k}_{diag} + \underbrace{u_k}_{\in \mathbb{R}^n} u_k^T$$
.

PROXIMAL METHOD

$$F(x) = ||Ax - b|| + \lambda ||x||_1$$

$$A \in \mathbb{R}^{1500 \times 3000}, \ b \in \mathbb{R}^{1500}$$

$$A_{ij}, \ b_i \sim \mathcal{N}(0, 1), \ \lambda = 0.1$$



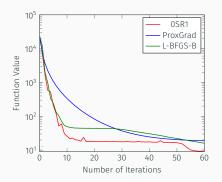
| | 0SR1 | ProxGrad | L-BFGS-B |
|------------|-------|----------|----------|
| Iterations | 1,822 | 135,328 | 1,989 |
| Run-Time | 68 s | 1,144 s | 56 s |

PROXIMAL METHOD

$$F(x) = ||Ax - b|| + \lambda ||x||_1$$

$$A \in \mathbb{R}^{1500 \times 3000}, \ b \in \mathbb{R}^{1500}$$

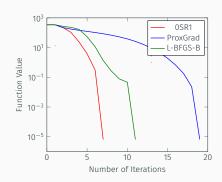
$$A_{ij}, \ b_i \sim \mathcal{N}(0, 1), \ \lambda = 0.1$$



| | 0SR1 | ProxGrad | L-BFGS-B |
|------------|-------|----------|----------|
| Iterations | 1,822 | 135,328 | 1,989 |
| Run-Time | 68 s | 1,144 s | 56 s |

$$F(x) = \|Ax - b\| + \lambda \|x\|_1$$

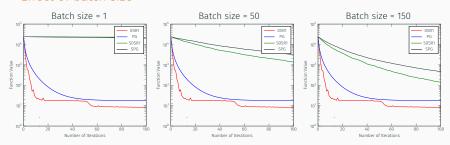
$$A \in \mathbb{R}^{2197 \times 2197}, \ b \in \mathbb{R}^{2197}$$
 A: Discretization of 3D Laplacian
$$\lambda = 1$$



| | 0SR1 | ProxGrad | L-BFGS-B |
|------------|---------|----------|----------|
| Iterations | 7 | 18 | 10 |
| Run-Time | 0.037 s | 0.004 s | 0.022 s |

High-dimensional data: Extension to stochastic framework

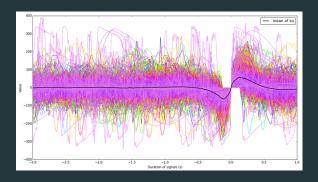
Effect of batch size



LOGISTIC REGRESSION: AN EXAMPLE

ELECTROENCEPHALOGRAPHY (EEG)

HOW DEEP IS YOUR SLEEP?



SLEEPING PATIENT / 20 NIGHTS OF EEG RECORDINGS

PREDICT NEXT SLOW WAVE

EEG: LOGISTIC REGRESSION

RESULTS

Nice table with SQN, SGD (no reg, L2), (Lasso,) Prox (L1) showing Obj. value in found optimum, CPU time, Iterations, F1 score of prediction model

| | $F(\omega^*)$ | Model Score | Cost |
|-------------------|---------------|-------------|-------------|
| No regularization | | | |
| SGD | 0.01 | 96% | x sec, y AP |
| SQN | 0.5 | 96% | x sec, y AP |
| Prox | 0.01 | 96% | x sec, y AP |
| L1 | | | |
| LASSO | .71 | 55 % | blablabla |
| Prox | 0.01 | 96% | x sec, y AP |
| L2 | | | |
| SGD | .71 | 55 % | blablabla |
| SQN | 0.01 | 96% | x sec, y AP |

DICTIONARY LEARNING

DICTIONARY LEARNING

CAN WE RECOVER THE IMAGE?



IMAGE IS PARTIALLY DESTROYED

RECONSTRUCT IMAGE

DICTIONARY LEARNING

bla







MAIN REFERENCES |



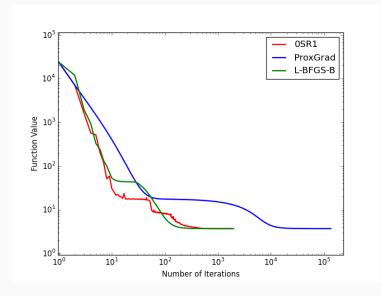
S. Becker and J. Fadili.

A quasi-newton proximal splitting method.

In Advances in Neural Information Processing Systems, pages 2618-2626, 2012.

APPENDIX

PROXIMAL METHOD

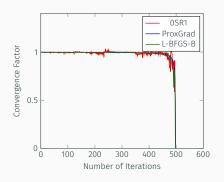


PROXIMAL METHOD

$$F(x) = ||Ax - b|| + \lambda ||x||_1$$

$$A \in \mathbb{R}^{1500 \times 3000}, \ b \in \mathbb{R}^{1500}$$

$$A_{ij}, \ b_i \sim \mathcal{N}(0, 1), \ \lambda = 0.1$$



$$\begin{split} F(x) &= \|Ax - b\| + \lambda \|x\|_1 \\ A &\in \mathbb{R}^{2197 \times 2197}, \ b \in \mathbb{R}^{2197} \\ A &: \text{ Discretization of 3D Laplacian} \\ \lambda &= 1 \end{split}$$

