STOCHASTIC OPTIMIZATION IN MACHINE LEARNING

Case Studies in Nonlinear Optimization

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

July 11, 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

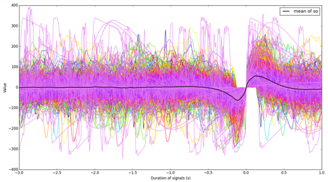
INTRODUCTION

Implementation of autonomously learning software for:

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

Examples:

Electroencephalography (EEG)



Section 4

Image Denoising

Section 5

Training a Machine Learning model means finding optimal parameters ω:

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

- F: Loss function
- X: The training data
- z: Training labels

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

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

Stochastic Methods

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

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

INTRODUCTION: STOCHASTIC FRAMEWORK

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

- 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.

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

- 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.
- Example loss function: $f(\omega, x_i, z_i) = |z_i - \omega^T x_i|$ (Linear Regression)

Gradient Method

$$\min F(\omega)$$

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

Stochastic Gradient Descent (SGD)

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

Gradient Method

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

Stochastic Gradient Descent (SGD)

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

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

with

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

where $\mathcal{S}_k \subset [N], \quad b := |\mathcal{S}_k| \ll N$

”Mini Batch”

STOCHASTIC QUASI-NEWTON METHOD (SQN)

Stochastic Gradient Descent

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

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

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

Stochastic Newton Method

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

Stochastic Gradient Descent

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

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

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

Stochastic Newton Method

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

$$\omega^{k+1} := \omega^k - \alpha_k \nabla^2 \hat{F}(\omega^k)^{-1} \nabla \hat{F}(\omega^k)$$

with

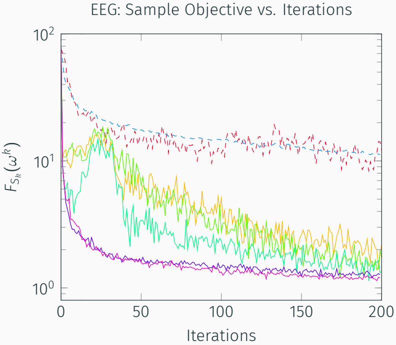
$$\nabla^2 \hat{F}(\omega^k) := \frac{1}{b_H} \sum_{i \in \mathcal{S}_{H,t}} \nabla^2 f(\omega^t, x_i, z_i)$$

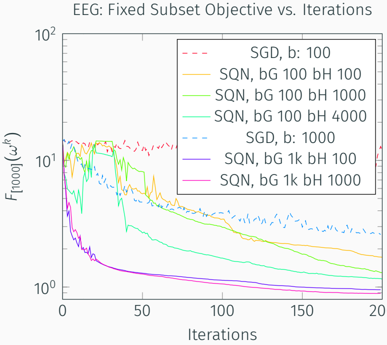
where

$$\mathcal{S}_{H,t} \subset [N], \quad b_H := |\mathcal{S}_{H,t}| \ll N,$$

(t) subsequence of (k)

- Stochastically use second-order information
- Approximate $\nabla^2 \hat{F}(\omega^k)$ by BFGS matrix H_t
- t running on slower time-scale than k.
- H_t update in $\mathcal{O}(n)$ time and constant memory, using several tricks

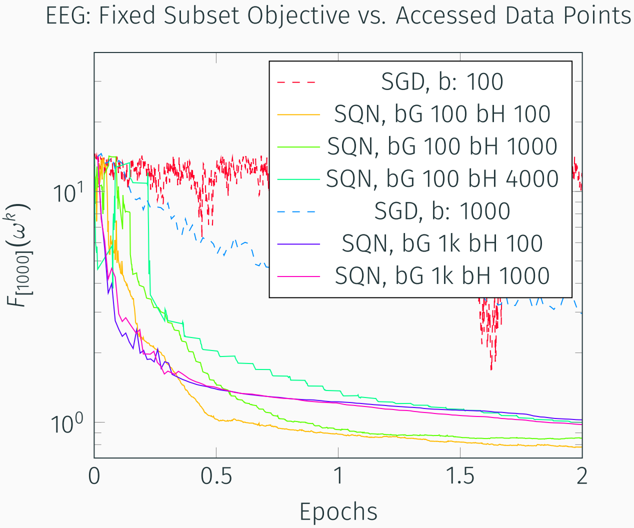




Performance on Logistic Regression, Problem size: 69550×600

Armijo-stepsizes, Further SQN-parameters: $L = 10$, $M = 5$

SQN: PERFORMANCE II



Performance on Logistic Regression, Problem size: 69550×600

Armijo-stepsizes, Further SQN-parameters: $L = 10$, $M = 5$

SQN: MAIN RESULTS

- Can be faster than SGD on appropriate Datasets
- Requires tedious, manual tuning of hyperparameters to be efficient!
- Choice of termination criterion unclear.

PROXIMAL METHOD

Problem

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

Proximity Operator

$$\mathrm{prox}_h(v) = \operatorname*{argmin}_x \left(h(x) + \frac{1}{2}\|x - v\|_2^2 \right)$$

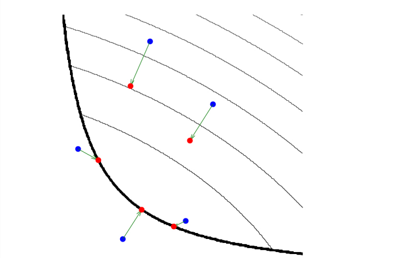


Figure 1: Evaluating a proximal operator at various points. *N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014*

PROXIMAL METHOD: ZERO-MEMORY RANK-ONE UPDATE

Traditional Proximal Gradient Step:

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

Quasi-Newton Proximal Step:

$$x_{k+1} = \mathrm{prox}_h^{B_k}(x_k - B_k^{-1}\nabla f(x_k)),$$

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

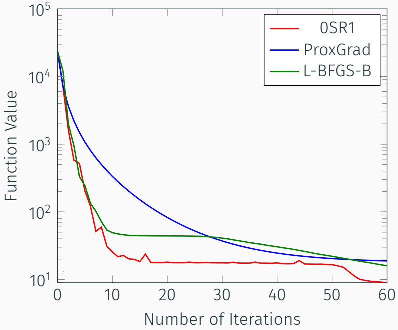
A zero-memory approach is used

PROXIMAL METHOD: PERFORMANCE I

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

$A \in \mathbb{R}^{1500\times3000}, \; b \in \mathbb{R}^{1500}$

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



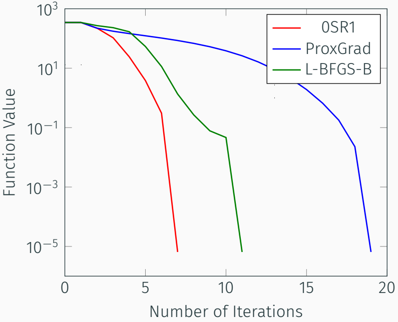
	0SR1	ProxGrad	L-BFGS-B
Iterations	1,822	135,328	1,989
Run-Time	68 s	1,144 s	56 s

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

$A \in \mathbb{R}^{2197\times2197}, \; b \in \mathbb{R}^{2197}$

A: Discretization of 3D Laplacian

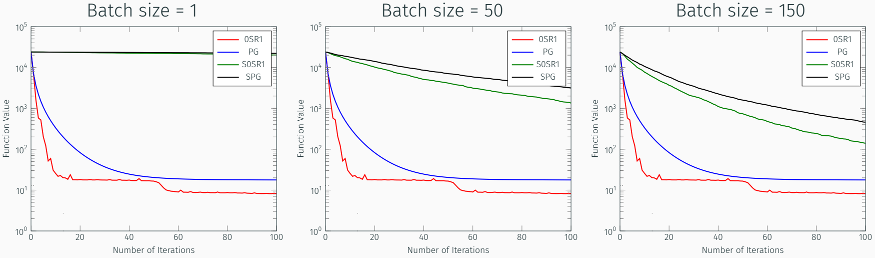
$\lambda = 1$



	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



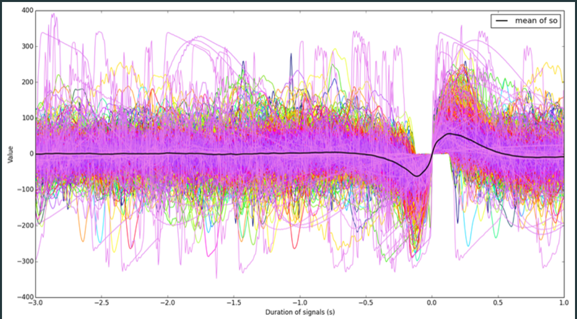
PROXIMAL METHOD: MAIN RESULTS

- Superior results to standard proximal gradient
- Competitive with other standard methods
- Extension to stochastic framework possible
- Applicable to large-scale problems

CLASSIFICATION

Electroencephalography (EEG)

How deep is your sleep?



Sleeping patient / 20 nights of EEG recordings

Predict next slow wave

$$f(\omega, x_i, y_i) = -y_i \log(h(\omega, x_i)) - (1 - y_i) \log(1 - h(\omega, x_i))$$

with

$$h(\omega, x_i) := sigmoid(\omega^T x_i) := \frac{1}{1 + e^{-\omega^T x_i}}$$

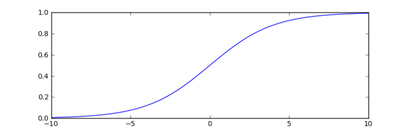


Figure 2: The sigmoid function.

Batch-size	1000, 1000	500, 500
Mean Score	0.8	0.8
Std	0.007	0.006
Running Time	65 s	31 s
M	5	5
L	10	10

CLASSIFICATION: RESULTS FOR 0SR1

	λ=0.1	λ=0.01	λ=0.1	λ=0.01
Batch-size	100	100	1000	1000
Mean Score	0.8	0.67	0.8	0.8
Std	0.01	0.14	0.01	0.016
Running Time	63 s	45 s	68 s	69 s

DICTIONARY LEARNING

Image Denoising

Can we recover the image?

Image is partially destroyed

Reconstruct image

Well-known machine learning model:

$$\min_{D,\alpha} \frac{1}{N} \sum_{i=1}^{N} \| \underbrace{x_i - D\alpha_i}_{\text{a) SQN}} \|_2^2 + \underbrace{\lambda \|\alpha_i\|_1}_{\text{b) Prox}}$$

2-phase optimization problem

1. Update "dictionary"
2. Induce sparsity

$\Rightarrow$ Example: Reconstruction of partially distorted images

Figure 3: Noisy image

DICTIONARY LEARNING IN IMAGE RECONSTRUCTION II

Figure 4: Reconstructed image

CONCLUSION

SUMMARY

- Large amounts of data
- Need for stochastic algorithms
- Second order methods to improve speed
- For smooth and non-smooth problems
- Good performance of implementation on various problems


Distorted image
Image
Difference (norm: 59.44)


first try (time: 619.9s)
Image
Difference (norm: 19.65)

Questions?

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