STOCHASTIC OPTIMIZATION IN MACHINE LEARNING

Case Studies in Nonlinear Optimization

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We're not running out of data anytime soon. It's maybe the only resource that grows exponentially.

Andreas Weigend

OUTLINE

1. Introduction
2. Stochastic Quasi-Newton Method (SQN)
3. Proximal Method
4. Classification
5. Dictionary Learning
6. Conclusion

INTRODUCTION

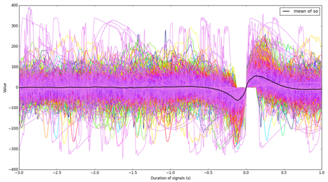
INTRODUCTION: WHAT IS MACHINE LEARNING (ML) ?

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

INTRODUCTION: ML AND OPTIMIZATION I

Training a Machine Learning model means finding optimal parameters ω:

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

- 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)

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

- 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.

Gradient Method

$$\min F(\omega)$$

Stochastic Gradient Descent

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

Gradient Method

$$\min F(\omega)$$

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

Stochastic Gradient Descent

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

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

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

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

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

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

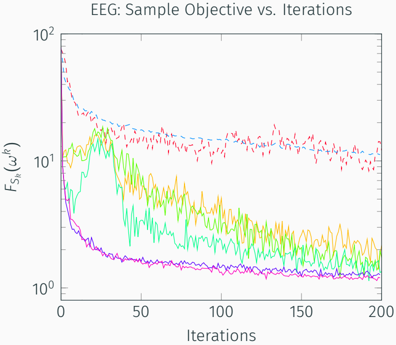
with

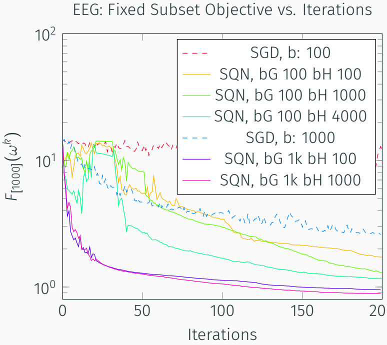
$$\nabla^2 \hat{F}(\omega^k) := \frac{1}{b_H} \sum_{i \in \mathcal{S}_{H,t}} \nabla^2 f(\omega^k, x_i, z_i)$$

where

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

SQN: PERFORMANCE I

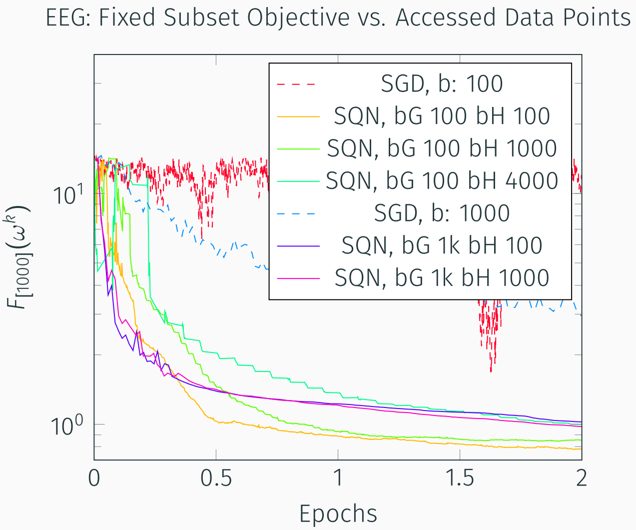




Performance on Logistic Regression, Problem size: 69550×600

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: $L = 10$, $M = 5$

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

PROXIMAL METHOD

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

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

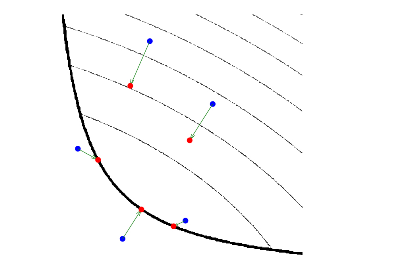


Figure 1: Evaluating a proximal operator at various points. *N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014*

Traditional Proximal Gradient Step:

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

Quasi-Newton Proximal Step:

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

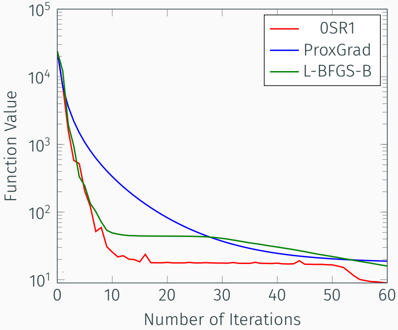
with $B_k = \underbrace{D_k}_{diag} + \underbrace{u_k}_{\in \mathbb{R}^n} u_k^T$.

A zero-memory approach is used

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

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

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



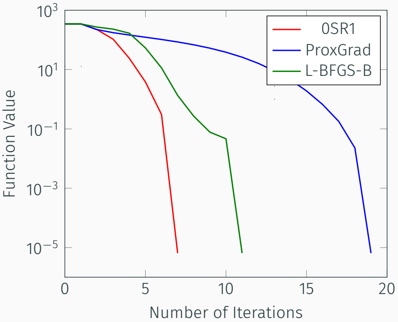
	0SR1	ProxGrad	L-BFGS-B
Iterations	1,822	135,328	1,989
Run-Time	68 s	1,144 s	56 s

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

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

A: Discretization of 3D Laplacian

$\lambda = 1$

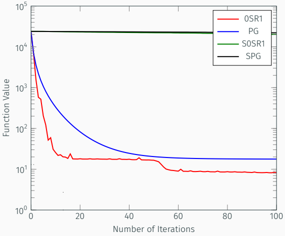


	0SR1	ProxGrad	L-BFGS-B
Iterations	7	18	10
Run-Time	0.037 s	0.004 s	0.022 s

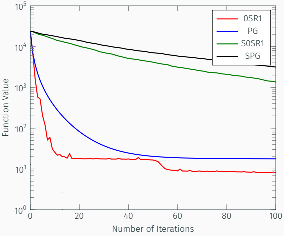
High-dimensional data: Extension to stochastic framework

Effect of batch size

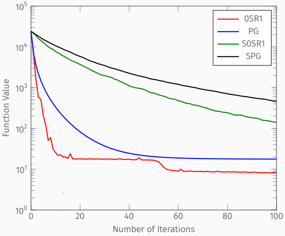
Batch size = 1



Batch size = 50



Batch size = 150



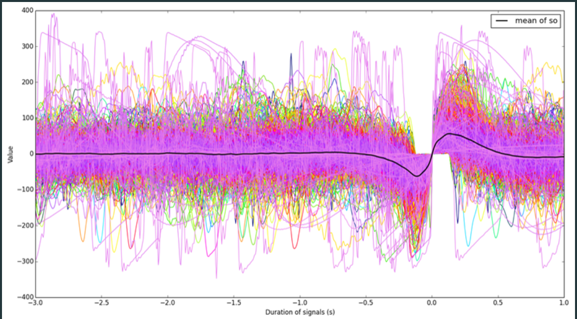
PROXIMAL METHOD: MAIN RESULTS

- 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

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

DICTIONARY LEARNING IN IMAGE RECONSTRUCTION I

Figure 2: Noisy image

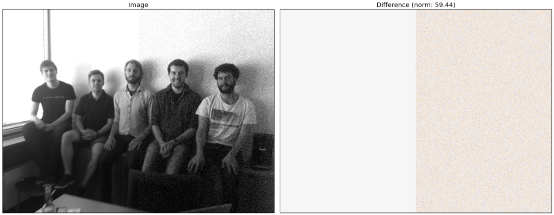
Figure 3: Reconstructed image

CONCLUSION

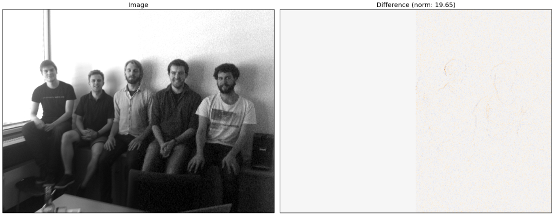
SUMMARY

- 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



first try (time: 619.9s)



Questions?

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