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

INTRODUCTION

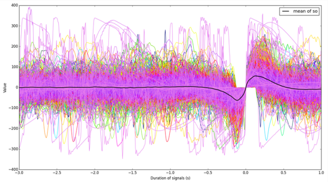
Implementation of autonomously learning software for:

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

Examples:

Image Denoising

Electroencephalography (EEG)



Section 4

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.

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.
- 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

$$\min F(\omega)$$

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

Stochastic Gradient Descent (SGD)

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

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

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

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

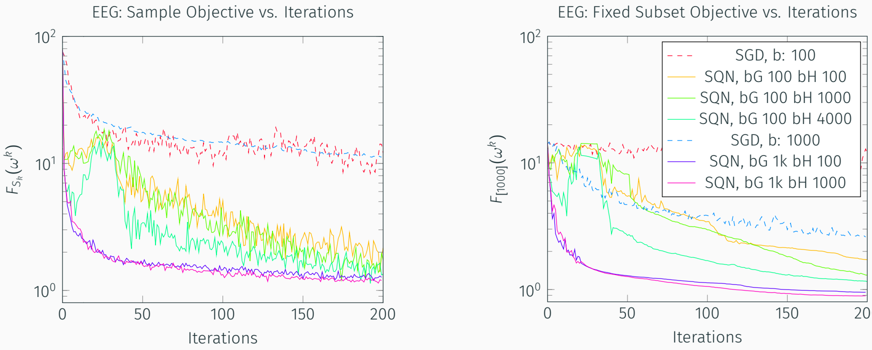
where

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

(t) subsequence of (k)

STOCHASTIC QUASI-NEWTON METHOD (SQN)

- 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

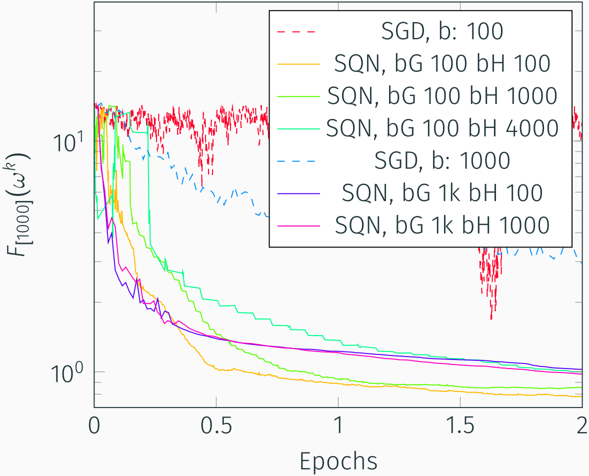


Performance on Logistic Regression, Problem size: 69550×600

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

SQN: PERFORMANCE II

EEG: Fixed Subset Objective vs. Accessed Data Points



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!
- Choice of termination criterion unclear.

PROXIMAL METHOD

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

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

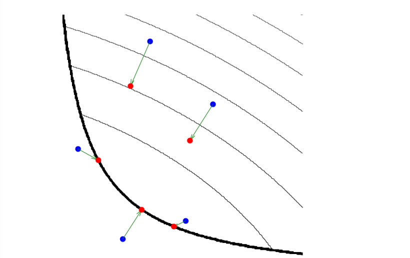


Figure 1: Evaluating a proximal operator at various points. *N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014*

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

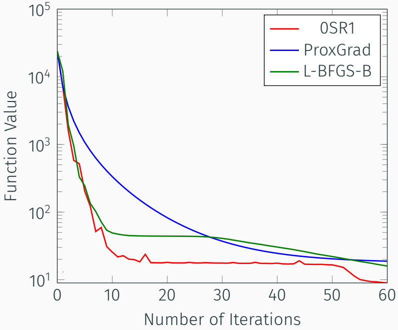
A zero-memory approach is used

PROXIMAL METHOD: PERFORMANCE I

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

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

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



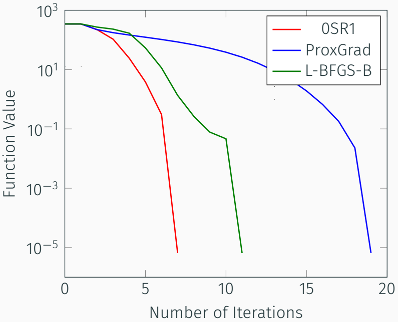
	0SR1	ProxGrad	L-BFGS-B
Iterations	1,822	135,328	1,989
Run-Time	68 s	1,144 s	56 s

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

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

A: Discretization of 3D Laplacian

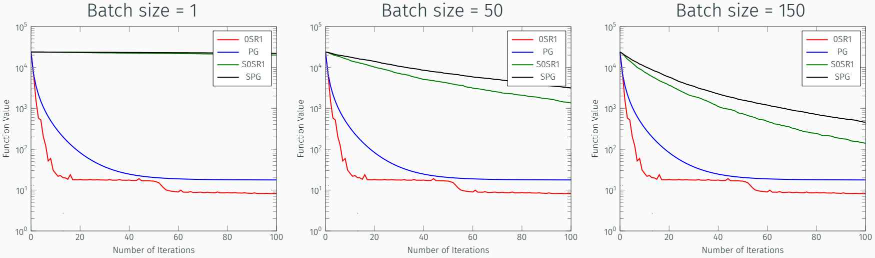
$\lambda = 1$



	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



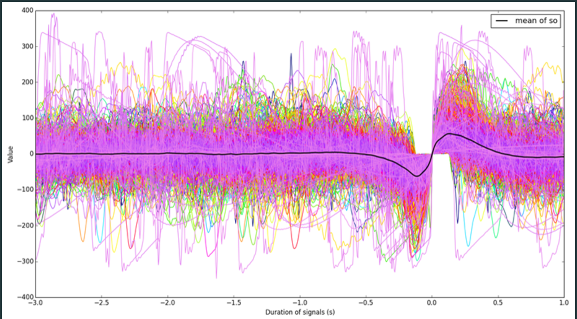
PROXIMAL METHOD: MAIN RESULTS

- 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

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

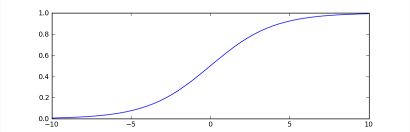


Figure 2: The sigmoid function.

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

	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

Figure 4: Reconstructed image

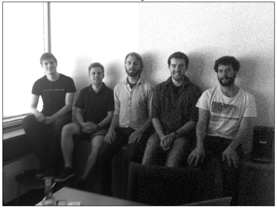
CONCLUSION

SUMMARY

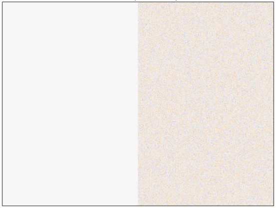
- Large amounts of data
- Need for stochastic algorithms
- Second order methods to improve speed
- For smooth and non-smooth problems
- Good performance of implementation on various problems

Distorted image

Image

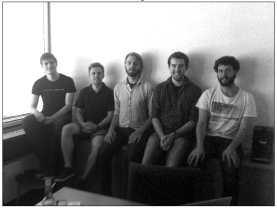


Difference (norm: 59.44)



first try (time: 619.9s)

Image



Difference (norm: 19.65)

Questions?

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

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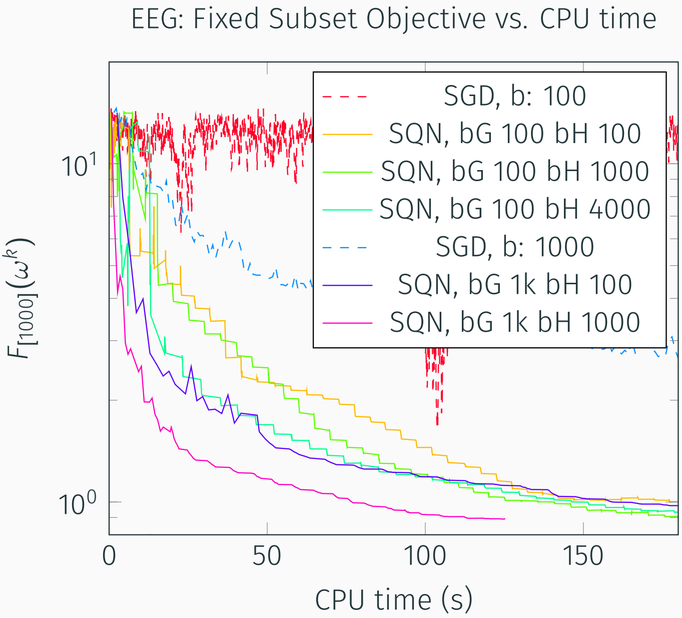
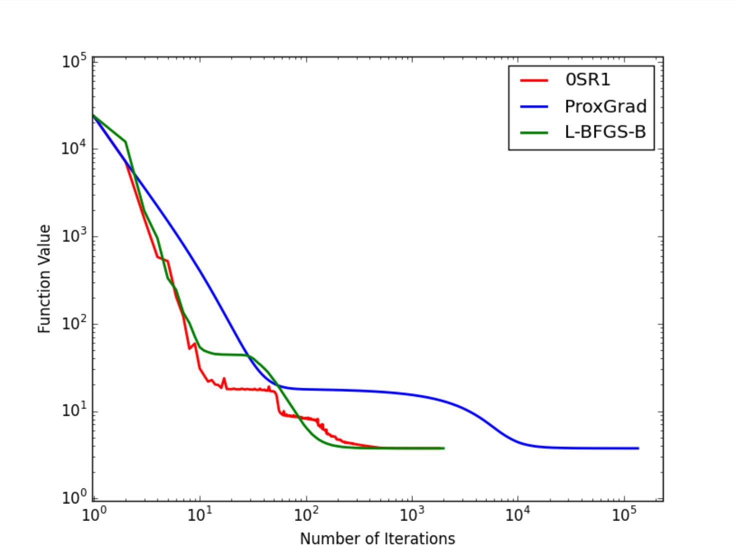
A stochastic quasi-newton method for large-scale optimization.
arXiv.org Preprint: arXiv:1401.7020, 2014.

J. Mairal, F. Bach, J. Ponce, and G. Sapiro.
Online learning for matrix factorization and sparse coding.
The Journal of Machine Learning Research, 11:19–60, 2010.

N. Parikh and S. Boyd.
Proximal algorithms.
Foundations and Trends in optimization, 1(3):123–231, 2013.

APPENDIX


EEG: Fixed Subset Objective vs. CPU time
SGD, b: 100
SQN, bG 100 bH 100
SQN, bG 100 bH 1000
SQN, bG 100 bH 4000
SGD, b: 1000
SQN, bG 1k bH 100
SQN, bG 1k bH 1000
10^1
10^0
$F_{[1000]}(\omega^k)$
0
50
100
150
CPU time (s)



0SR1
ProxGrad
L-BFGS-B
Function Value
Number of Iterations
10^0
10^1
10^2
10^3
10^4
10^5

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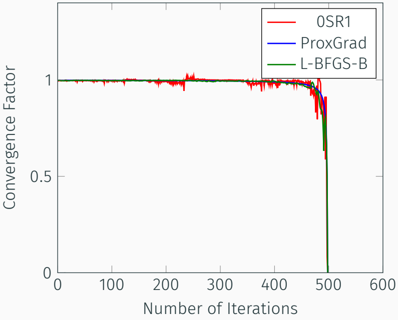

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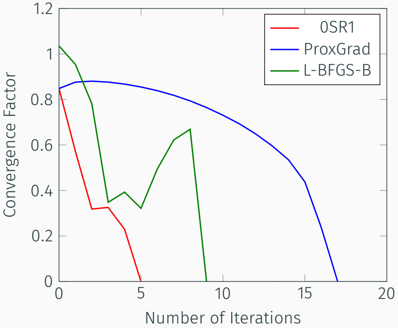
A: Discretization of 3D Laplacian
$\lambda = 1$



PROXIMAL METHOD

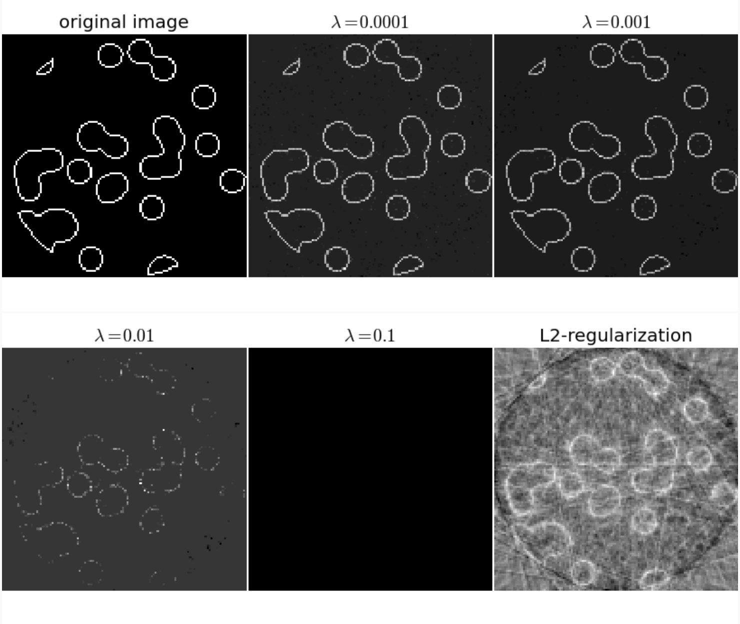


Figure 1: Dictionary learned