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. SQN: A Stochastic Quasi-Newton Method

3. Proximal Method

4. Logistic Regression: An Example

5. Dictionary Learning

6. Conclusion

7. Appendix

INTRODUCTION

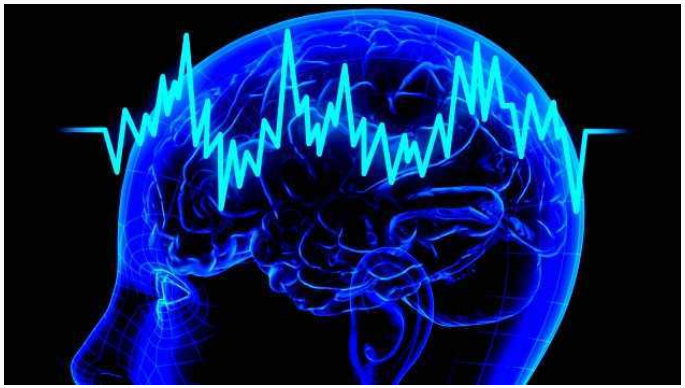
Introduction: What is machine learning (ML) ?

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

Training a Machine Learning model means finding optimal parameters ω:

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

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

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

Introduction: Challenges in Machine Learning

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

Ansatz: Stochastic Methods

INTRODUCTION: STOCHASTIC FRAMEWORK

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

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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.

Introduction: Stochastic Methods

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

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

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

"Mini Batch"

SQN: A STOCHASTIC QUASI-NEWTON METHOD

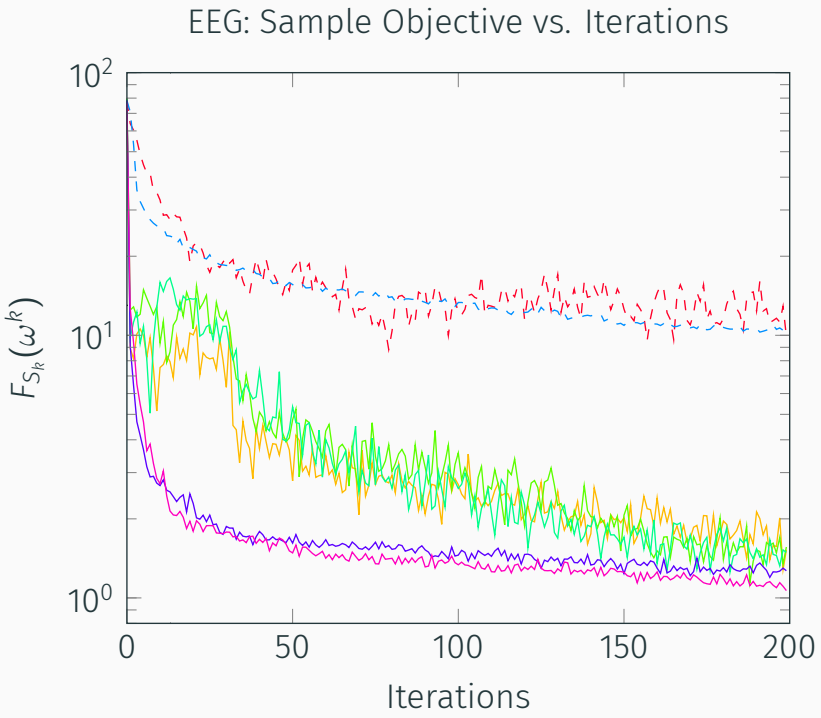
Stochastic quasi-Newton method (SQN)

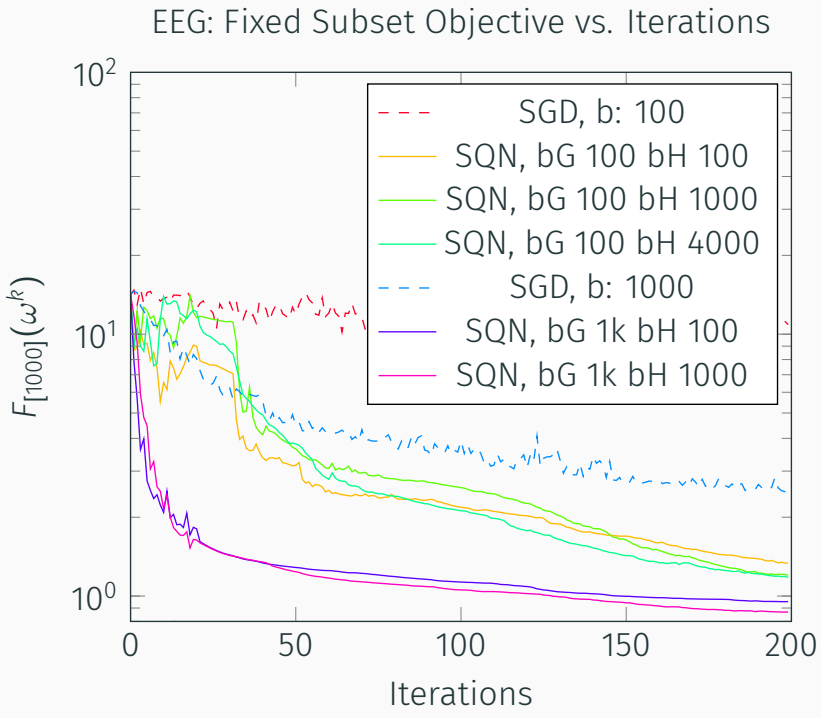
- Stochastically use second-order information
- Based on BFGS-method.
- Basic idea:

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

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

BEHAVIOR I

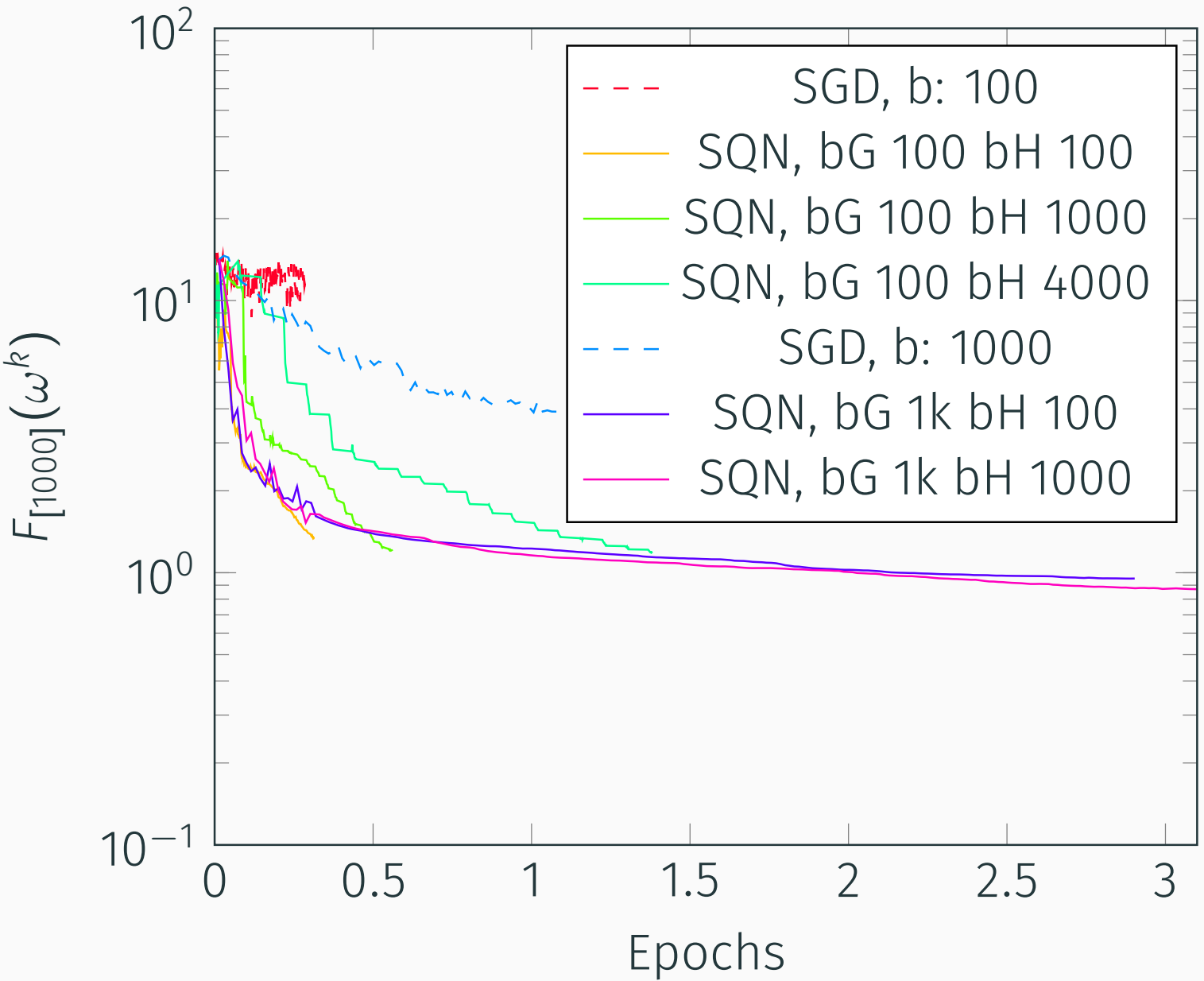




Performance on EEG Dataset, Problem size: 69550×600

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

EEG: Fixed Subset Objective vs. Accessed Data Points



RESULTS

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

PROXIMAL METHOD

Problem

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

Proximity Operator

$$\text{prox}_f(v) = \underset{x}{\text{argmin}} \left(f(x) + \frac{1}{2}\|x - v\|_2^2 \right)$$

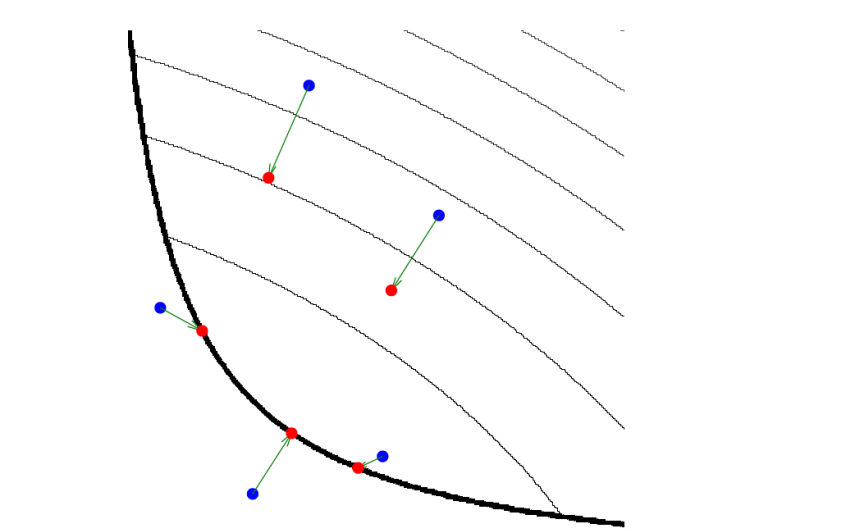


Figure 1: Evaluating a proximal operator at various points. *N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014*

Traditional Proximal Gradient Step:

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

Quasi-Newton Proximal Step:

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

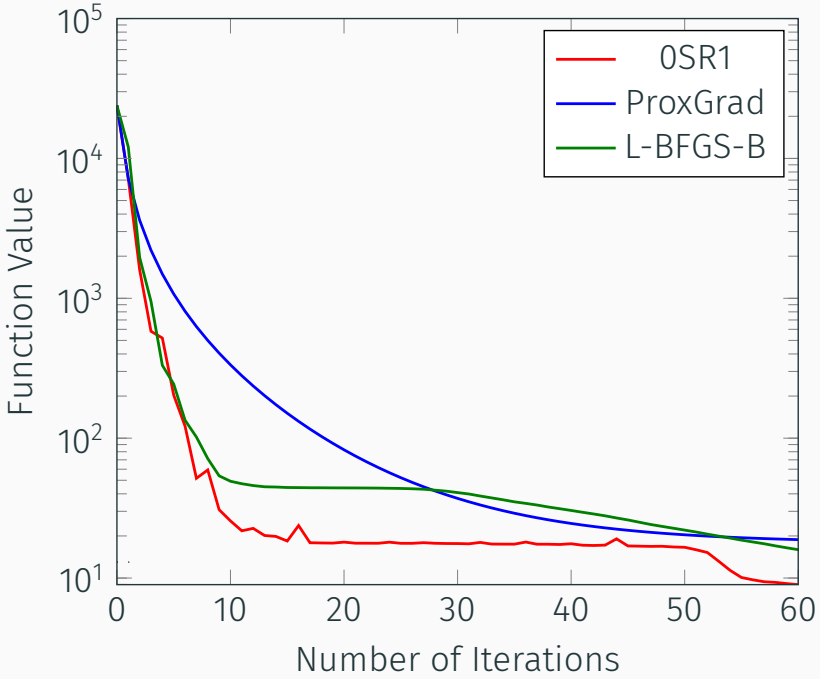
with $B_k = \underbrace{D_k}_{diag} + \underbrace{u_k}_{\in \mathbb{R}^n} u_k^T$.

PROXIMAL METHOD

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

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

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



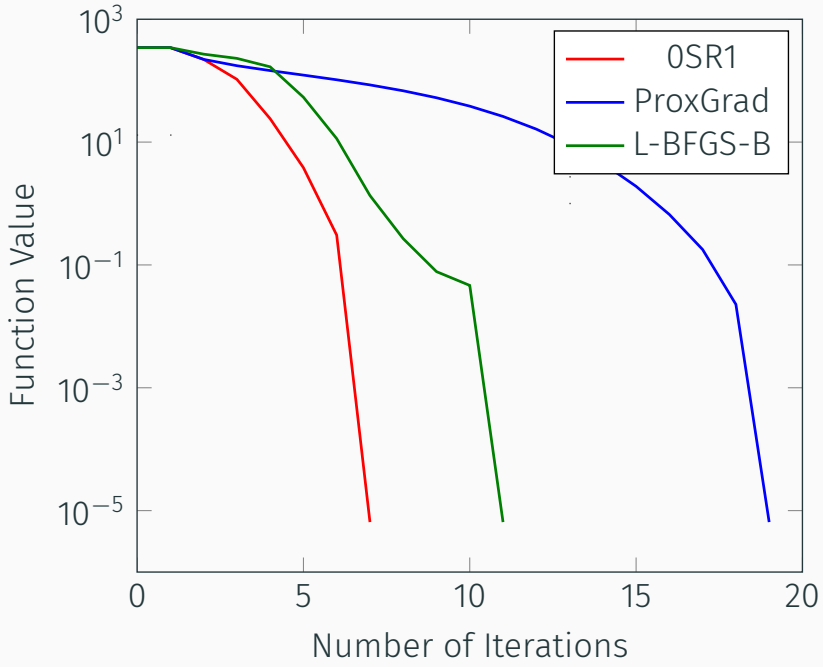
	0SR1	ProxGrad	L-BFGS-B
Iterations	1,822	135,328	1,989
Run-Time	68 s	1,144 s	56 s

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

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

A: Discretization of 3D Laplacian

$\lambda = 1$

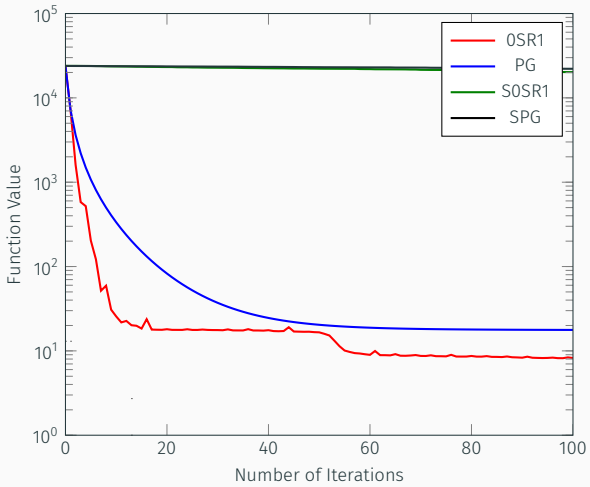


	0SR1	ProxGrad	L-BFGS-B
Iterations	7	18	10
Run-Time	0.037 s	0.004 s	0.022 s

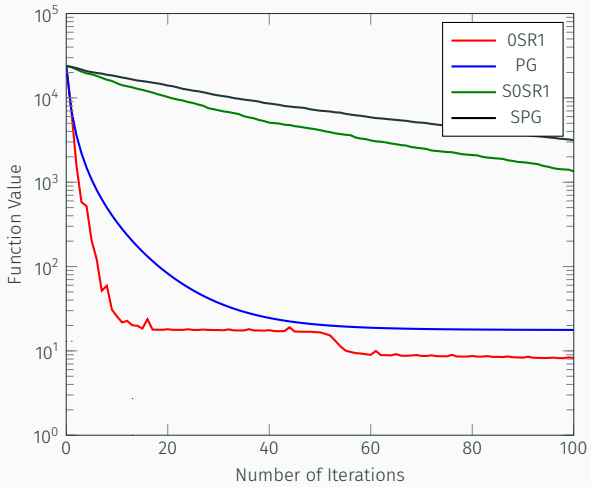
High-dimensional data: Extension to stochastic framework

Effect of batch size

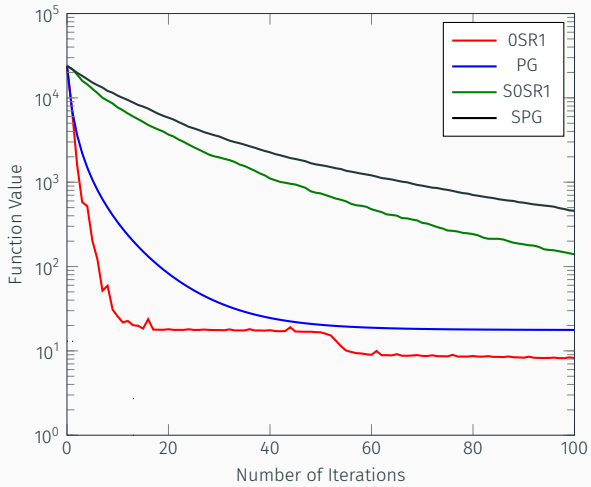
Batch size = 1



Batch size = 50



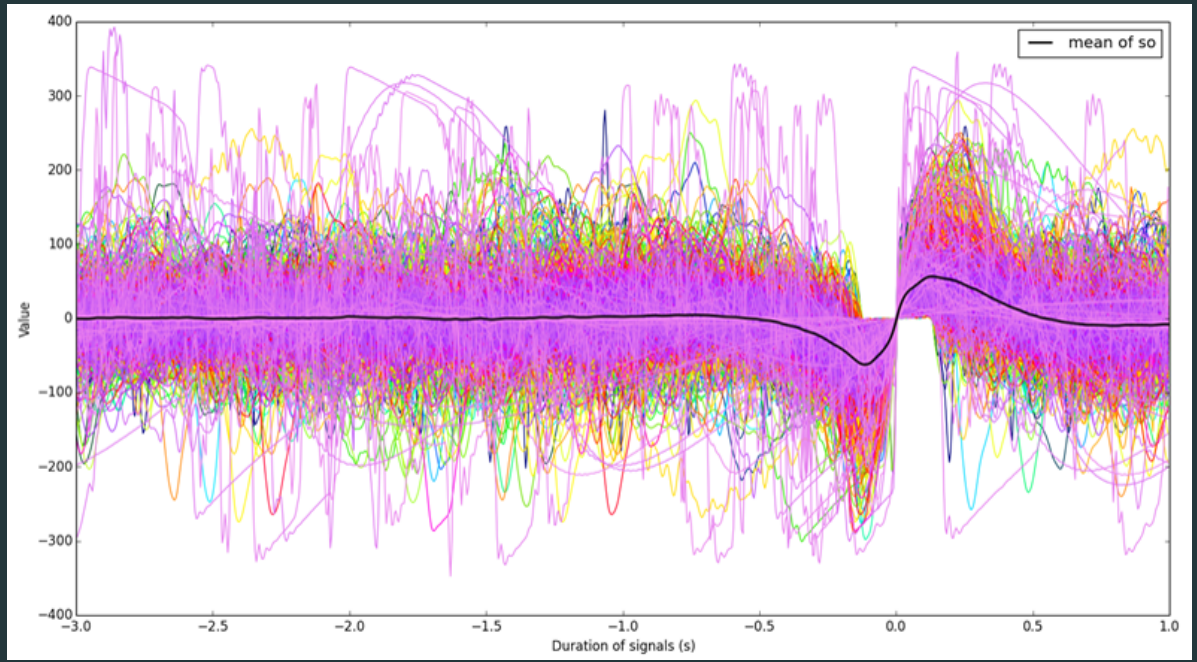
Batch size = 150



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

CONCLUSION

SUMMARY

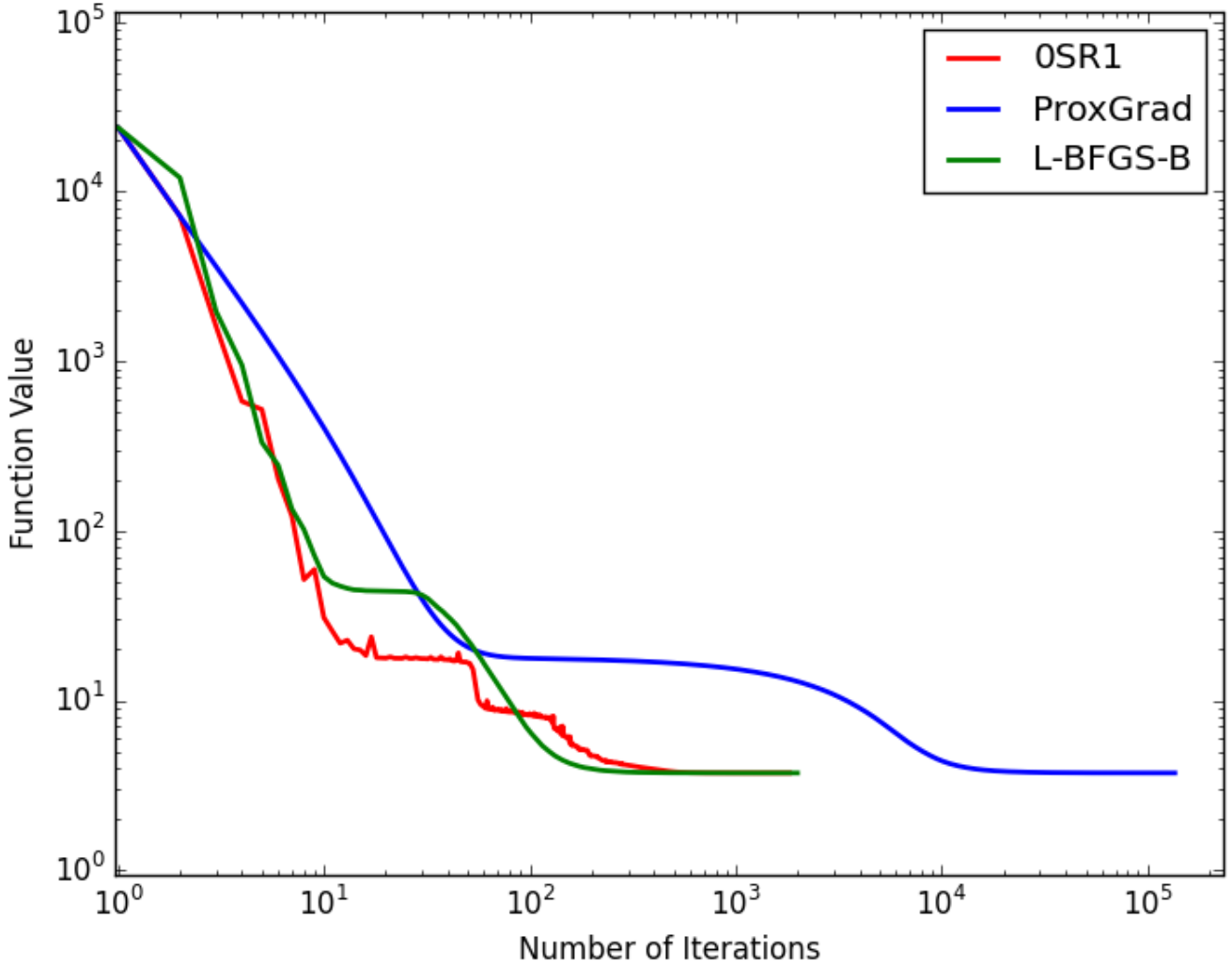
Questions?

MAIN REFERENCES I

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



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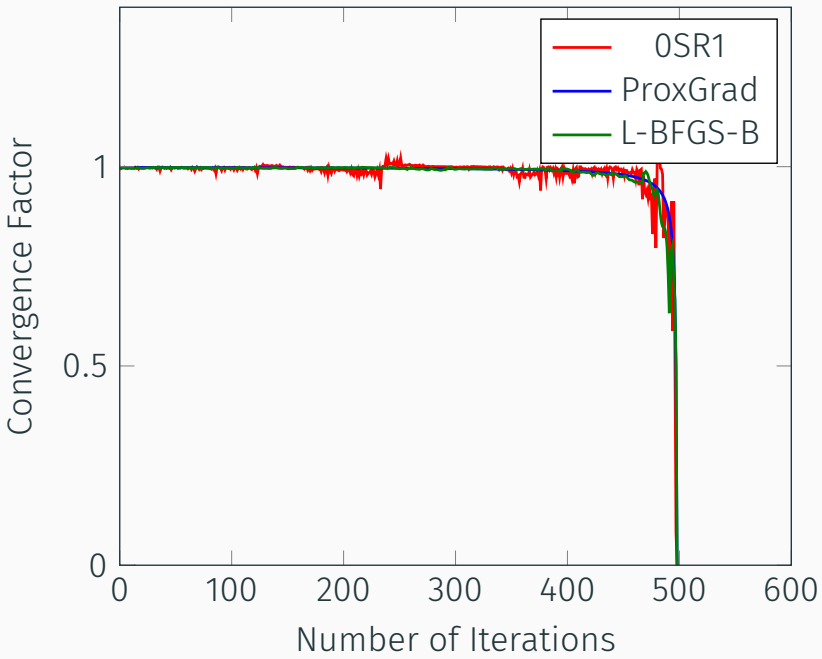

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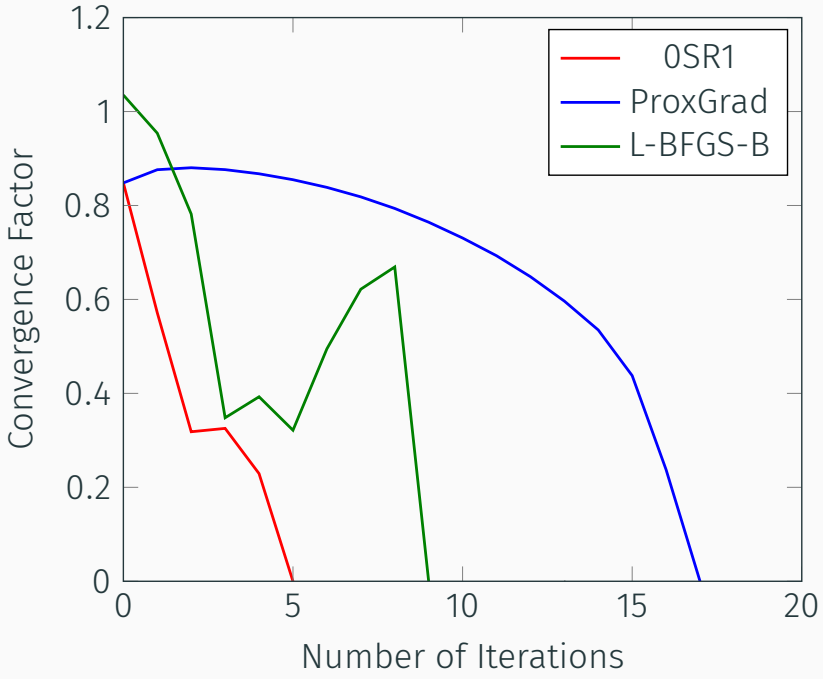
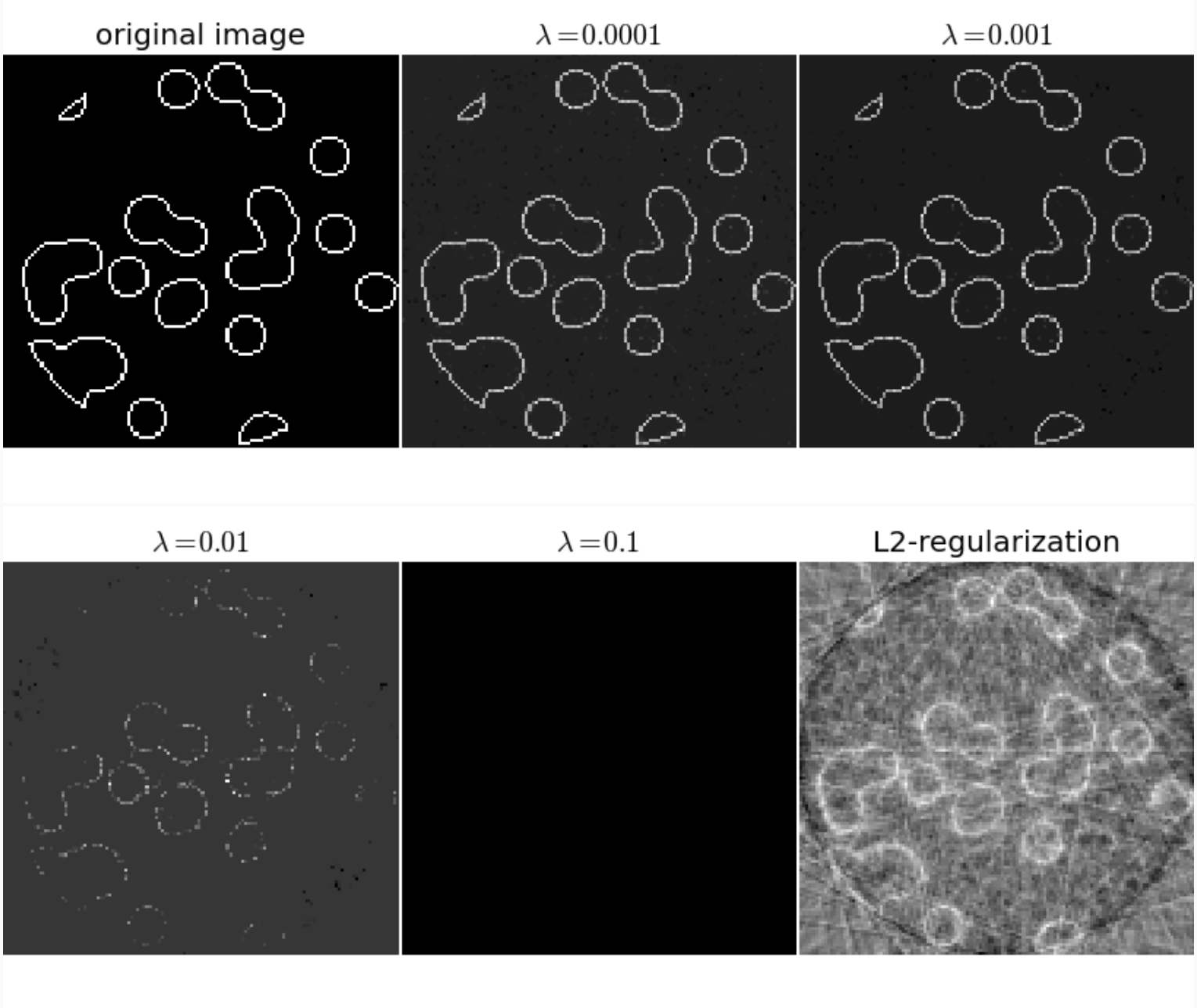
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