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

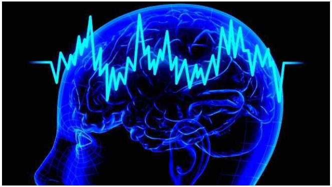
Introduction: What is Machine Learning (ML) ?

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

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 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$+1$

Introduction: 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

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

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

Introduction: Stochastic Methods

Gradient Method

$$\min F(\omega)$$

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

Stochastic Gradient Descent

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

Introduction: Stochastic Methods

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

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"

Stochastic Newton Method

Stochastic Gradient Descent

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

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"Mini Batch"

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

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

where

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

"Mini Batch"

Stochastic Quasi-Newton Method (SQN)

- Stochastically use second-order information
- Approximate $\nabla 2F(\hat{\omega}^k)$ 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

Behavior I

Performance on EEG Dataset, Problem size: 69550×600

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

Behavior II

Performance on EEG Dataset, Problem size: 69550×600

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

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

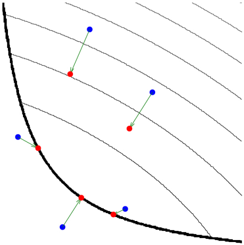


Figure : Evaluating a proximal operator at various points. *N Parikh, S Boyd, Proximal Methods, Foundations and Trends in Optimization 1, 2014*

Proximal Method

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

$F(x) = \|Ax - b\| + \lambda \|x\|_1$
$A \in \mathbb{R}^{1500 \times 3000}, \; b \in \mathbb{R}^{1500}$
$A_{ij}, \; b_i \; \tilde{} \, \mathcal{N}(0,1), \; \lambda = 0.1$

	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

Proximal Method: Stochastic Extension

High-dimensional data: Extension to stochastic framework

Effect of batch size

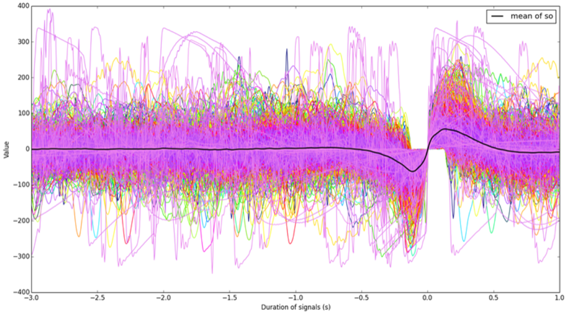
Batch size $= 1$

Batch size $= 50$

Batch size $= 150$

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

Can we recover the image?

Image is partially destroyed
Reconstruct image

Dictionary Learning

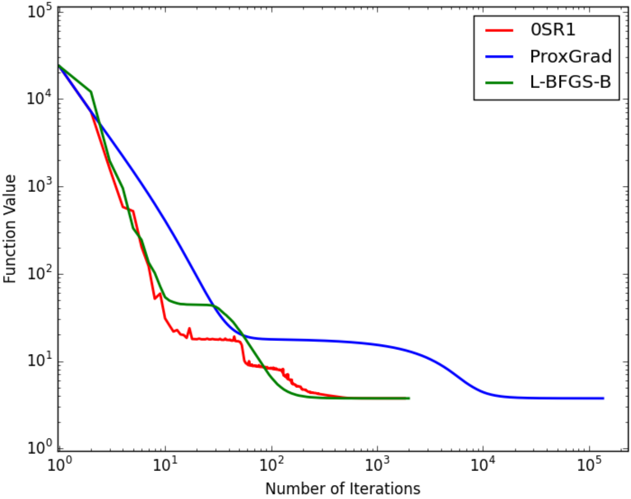
bla

Summary

Questions?

Main References I

Proximal Method



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

SQN: CPU Time

Proximal Method