

STOCHASTIC OPTIMIZATION IN MACHINE LEARNING

CASE STUDIES IN NONLINEAR OPTIMIZATION

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July 8, 2015

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*WE'RE NOT RUNNING OUT OF DATA ANYTIME
SOON. IT'S MAYBE THE ONLY RESOURCE THAT
GROWS EXPONENTIALLY.*

ANDREAS WEIGEND

1. Introduction
2. SQN: A Stochastic Quasi-Newton Method
3. Proximal Method
4. Logistic Regression: An Example
5. Conclusion

INTRODUCTION

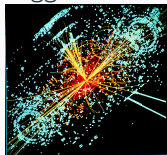
INTRODUCTION: WHAT IS MACHINE LEARNING?

Implementation of autonomously learning software for:

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

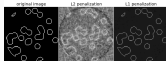
Examples:

Higgs-Boson



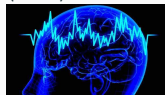
Section 2

Computed
Tomography
(CT)



Section 3

Electroence-
phalography
(EEG)



Section 4

Image
Denoising



Section 5

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- z : Training labels (only in classification models; vector of size N)
- The dimension n of ω is model dependent, often $\text{\#features}+1$

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- x_i : new data point with *unknown* label z_i
- h : hypothesis function of the ML model

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- Construction of very large models
- Handling high memory/computational demands

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Ansatz: Stochastic Methods

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- 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

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

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

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with

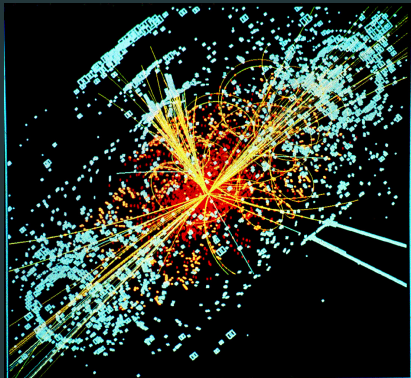
$$\nabla \hat{F}(\omega^{(k)}) := \frac{1}{b} \sum_{i \in \mathcal{S}_k} f(\omega, x_i, z_i)$$

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

SQN: A STOCHASTIC QUASI-NEWTON METHOD

CLASSIFICATION

DID WE JUST DETECT A HIGGS-BOSON?



- Data from Monte-Carlo simulations
- $X \in \mathbb{R}^{11.000.000 \times 29}$
Lots of samples, relatively small, dense feature set.
- Here, we use *Logistic Regression* for classification.

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- Based on BFGS-method.

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

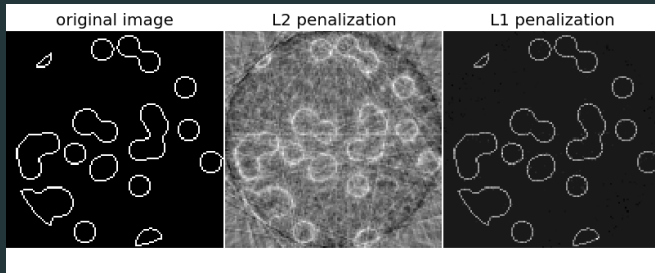
Pretty pictures about the behaviour of SQN on HIGGS and comparison with traditional SGD

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

PROXIMAL METHOD

IMAGE RECONSTRUCTION

WHAT DID THE ORIGINAL IMAGE LOOK LIKE?



Problem

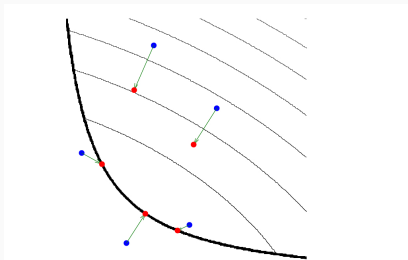
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Proximity Operator

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



Traditional Proximal Gradient Step:

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

Quasi-Newton Proximal Step:

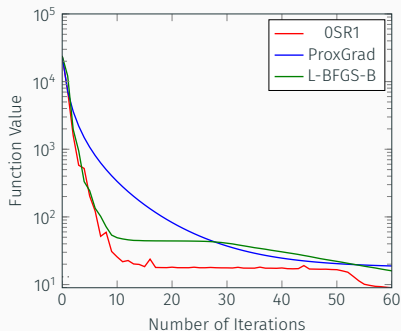
$$x_{k+1} = \text{prox}_h^{B_k}(x_k - B_k^{-1} \nabla f(x_k)),$$

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

PROXIMAL METHOD

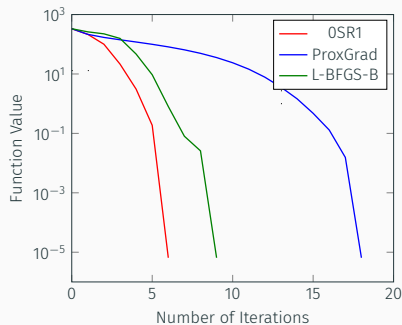
$$F(x) = \|Ax - b\| + \lambda \|x\|_1$$

$A \in \mathbb{R}^{1500 \times 3000}$, $b \in \mathbb{R}^{1500}$
 A_{ij} , $b_i \sim \mathcal{N}(0, 1)$, $\lambda = 0.1$

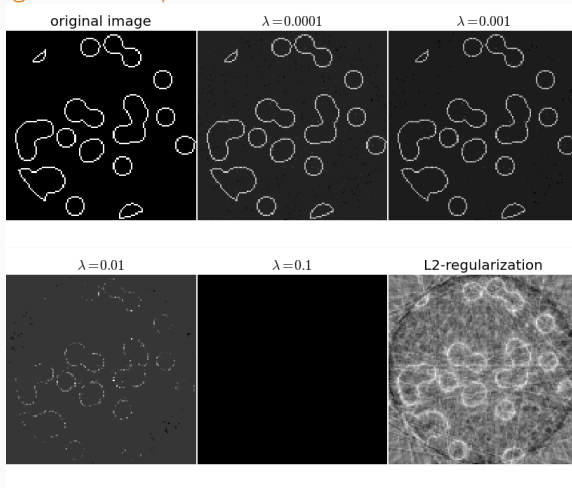


$$F(x) = \|Ax - b\| + \lambda \|x\|_1$$

$A \in \mathbb{R}^{2197 \times 2197}$, $b \in \mathbb{R}^{2197}$
A from 7-point finite difference stencil for 3D Laplacian on a Box
 $\lambda = 1$

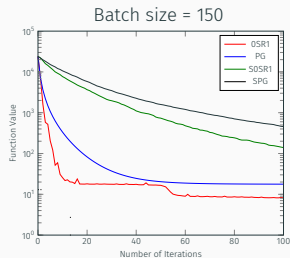
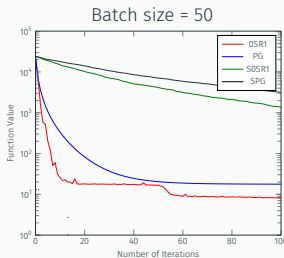
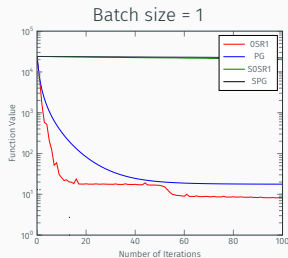


Effect of regularization parameter λ on solution:



High-dimensional data: Extension to stochastic framework

Effect of batch size



LOGISTIC REGRESSION: AN EXAMPLE

Explain what we want to do, and explain the dataset, and why using both SQN and Prox makes sense

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 | | | |
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CONCLUSION



QUESTIONS?



S. Becker and J. Fadili.

A quasi-newton proximal splitting method.

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