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. Conclusion

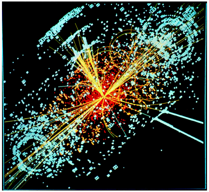
INTRODUCTION

Implementation of autonomously learning software for:

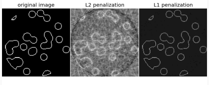
- Discovery of patterns and relationships in data
- Prediction of future events

Examples:

Higgs-Boson



Compressed Sensing



EEG

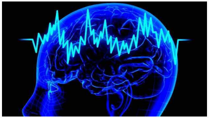


Image Reconstruction

Training a Machine Learning model means finding optimal parameters ω:

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

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- The dimension n of ω is model dependent, often #features$+1$

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

CHALLENGES IN MACHINE LEARNING

- Massive amounts of training data
- 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

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

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

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Stochastic Gradient Descent

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

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

with

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

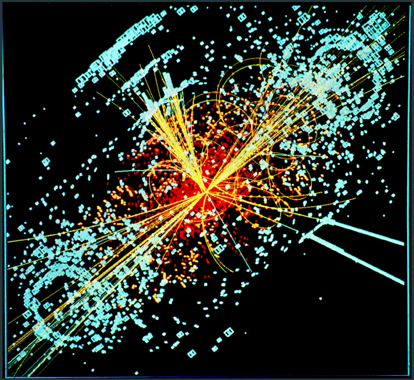
where $\mathcal{S}_k \subset [N], \quad b := |\mathcal{S}_k| \ll N$

"Mini Batch"

SQN: A STOCHASTIC QUASI-NEWTON METHOD

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

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

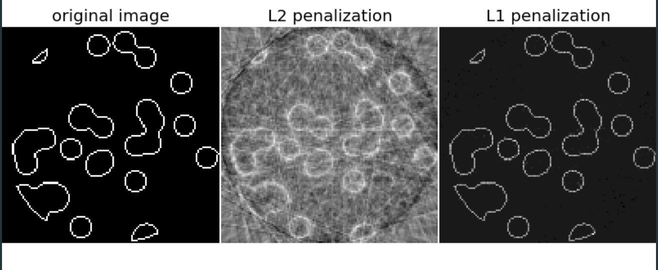
RESULTS

- 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

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

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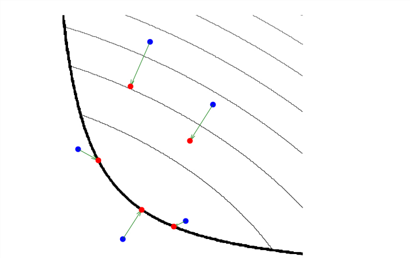
Proximity Operator $$\mathrm{prox}_f(v) = \operatorname*{argmin}_x \left(f(x) + \frac{1}{2}\|x - v\|_2^2\right)$$



Traditional Proximal Gradient Step:

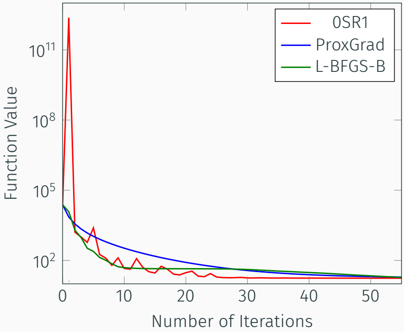
$$x_{k+1} = \mathrm{prox}_{\lambda_k h}(x_k - \lambda_k \nabla f(x_k))$$

Quasi-Newton Proximal Step:

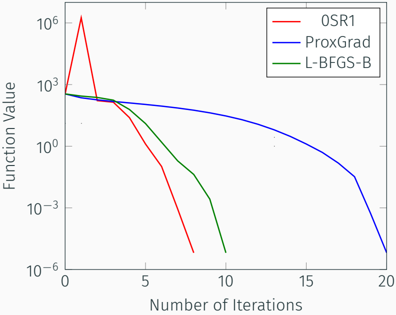
$$x_{k+1} = \mathrm{prox}_h^{B_k}(x_k - B_k^{-1} \nabla f(x_k)),$$

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

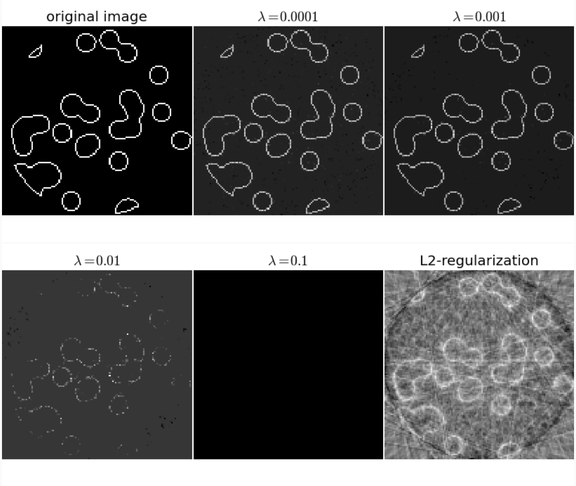
$F(x) = \|Ax - b\| + \lambda\|x\|_1$
$A \in \mathbb{R}^{1500\times3000},\ b \in \mathbb{R}^{1500}$
$A_{ij},\ b_i\ \sim \mathcal{N}(0,1),\ \lambda = 0.1$



$F(x) = \|Ax - b\| + \lambda\|x\|_1$
$A \in \mathbb{R}^{2197\times2197},\ b \in \mathbb{R}^{2197}$
A from 7-point finite difference stencil for 3D Laplacian on a Box
$\lambda = 1$



Effect of regularization parameter λ on solution:



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			
SGD	.71	55%	blablabla
SQN	0.01	96%	x sec, y AP

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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.