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

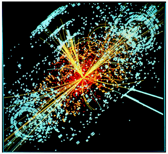
INTRODUCTION: WHAT IS MACHINE LEARNING?

Implementation of autonomously learning software for:

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

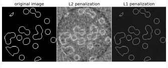
Examples:

Higgs-Boson



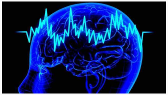
Section 2

Computed Tomography (CT)



Section 3

Electroence-phalography (EEG)



Section 4

Image Denoising

Section 5

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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$$F(\omega) := \mathbb{E}\left[f(\omega, \xi)\right] = \frac{1}{N} \sum_{i=1}^{N} f(\omega, x_i, z_i)$$

- 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.

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

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

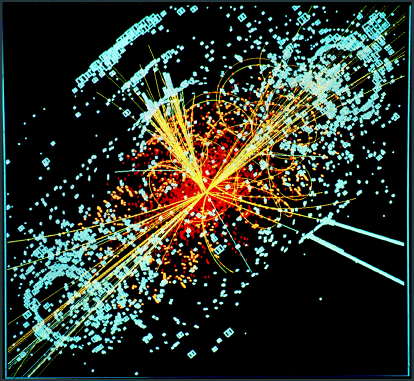
where $\mathcal{S}_k \subset [N], \quad b := |\mathcal{S}_k| \ll N$

"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.

- Stochastically use second-order information
- 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

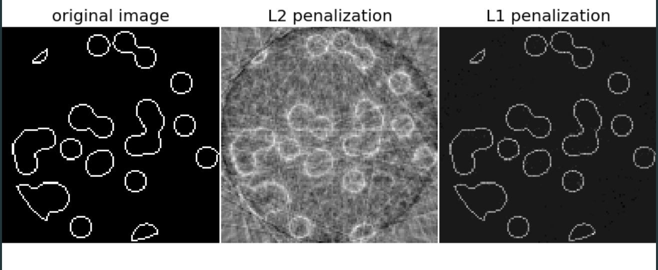
Pretty picures about the behaviour of SQN on HIGGS and comparison with traditional SGD

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

PROXIMAL METHOD

Computed Tomography (CT)

What did the original object look like?



Images of object from different angles

Reconstruct original object

Problem

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

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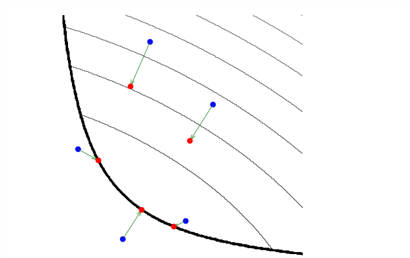
Proximity Operator $$\mathrm{prox}_f(v) = \operatorname*{argmin}_x \left(f(x) + \frac{1}{2}\|x - v\|_2^2\right)$$



Traditional Proximal Gradient Step:

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

Quasi-Newton Proximal Step:

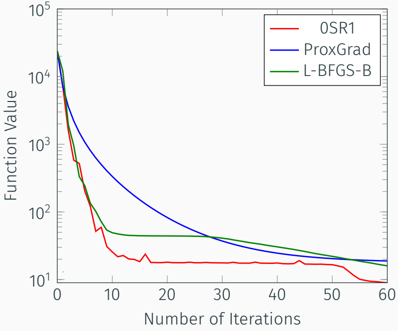
$$x_{k+1} = \operatorname{prox}_h^{B_k}(x_k - B_k^{-1} \nabla f(x_k)),$$

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

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

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

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

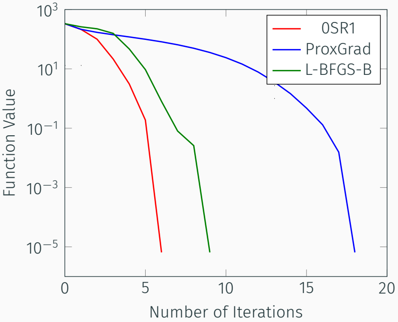


$F(x) = \|Ax - b\| + \lambda \|x\|_1$

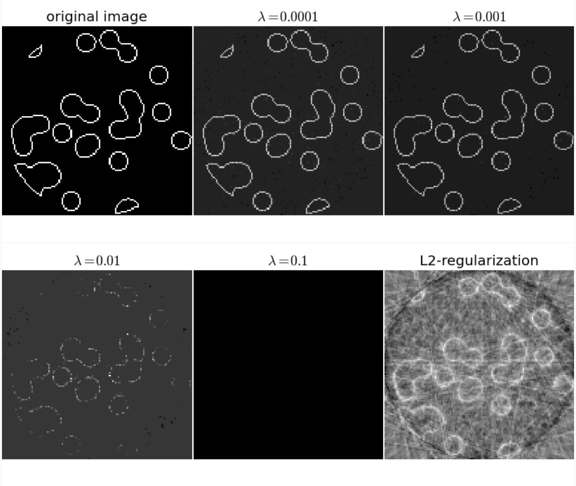
$A \in \mathbb{R}^{2197 \times 2197}, \; b \in \mathbb{R}^{2197}$

A from 7-point finite difference stencil for 3D Laplacian on a Box

$\lambda = 1$

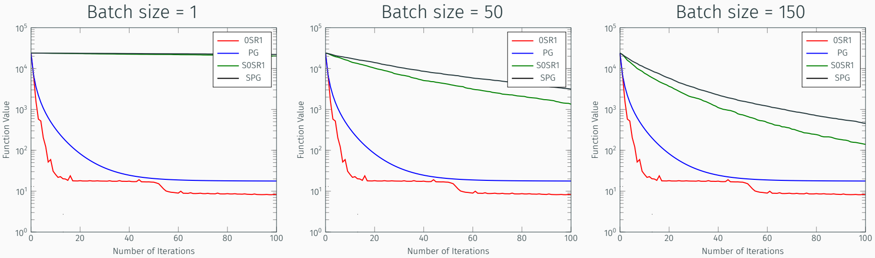


Effect of regularization parameter λ on solution:



High-dimensional data: Extension to stochastic framework

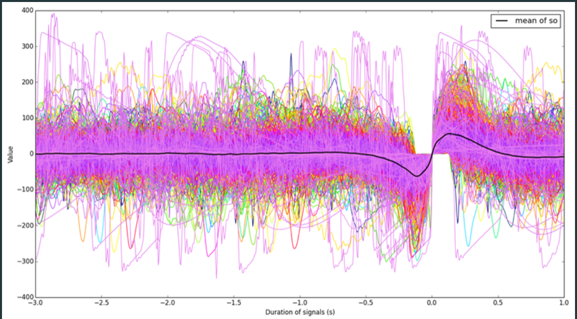
Effect of batch size



LOGISTIC REGRESSION: AN EXAMPLE

Electroencephalography (EEG)

How deep is your sleep?



Sleeping patient / 20 nights of EEG recordings

Predict next slow wave

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

CONCLUSION

Questions?

S. Becker and J. Fadili.
A quasi-newton proximal splitting method.
In *Advances in Neural Information Processing Systems*, pages 2618–2626, 2012.