# Statistical machine learning and convex optimization

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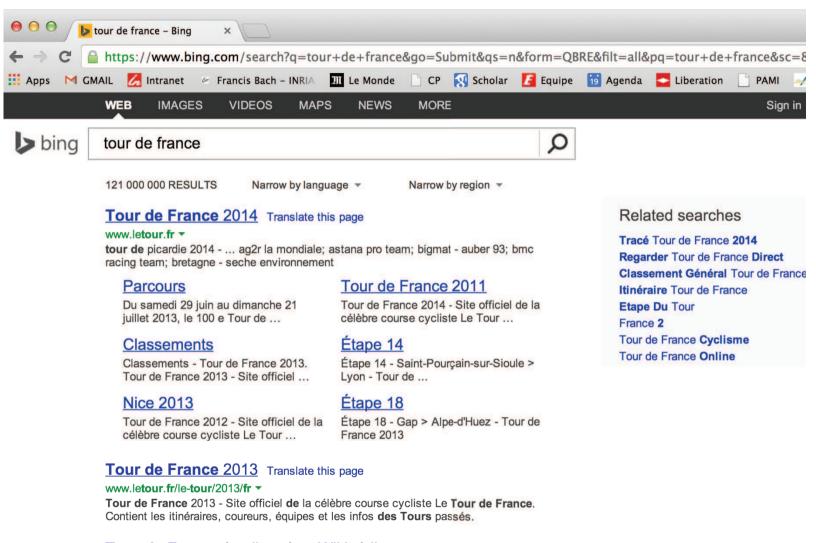
Machine learning summer school - Cadiz 2016

Slides available: www.di.ens.fr/~fbach/mlss\_2016\_cadiz\_slides.pdf

## "Big data" revolution? A new scientific context

- Data everywhere: size does not (always) matter
- Science and industry
- Size and variety
- Learning from examples
  - n observations in dimension d

## **Search engines - Advertising**

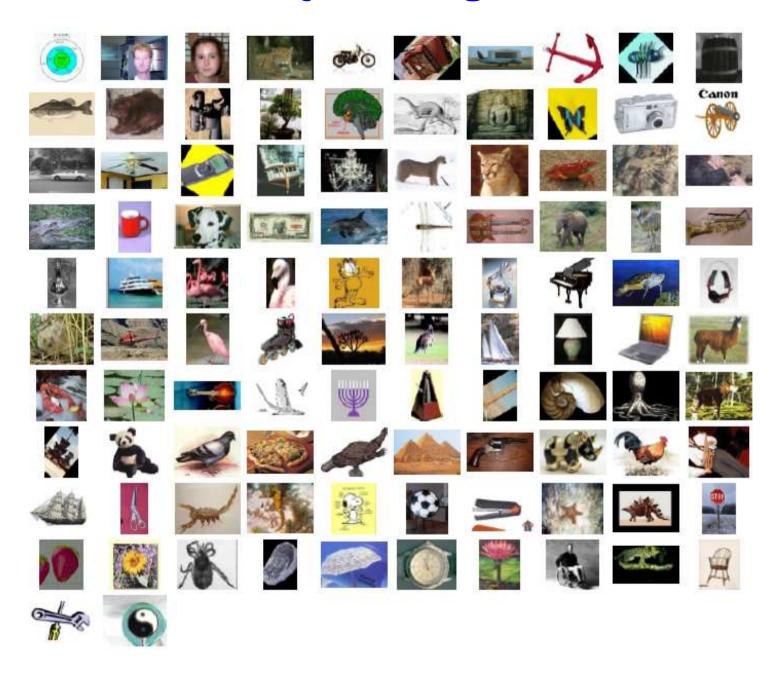


Tour de France (cyclisme) — Wikipédia Translate this page

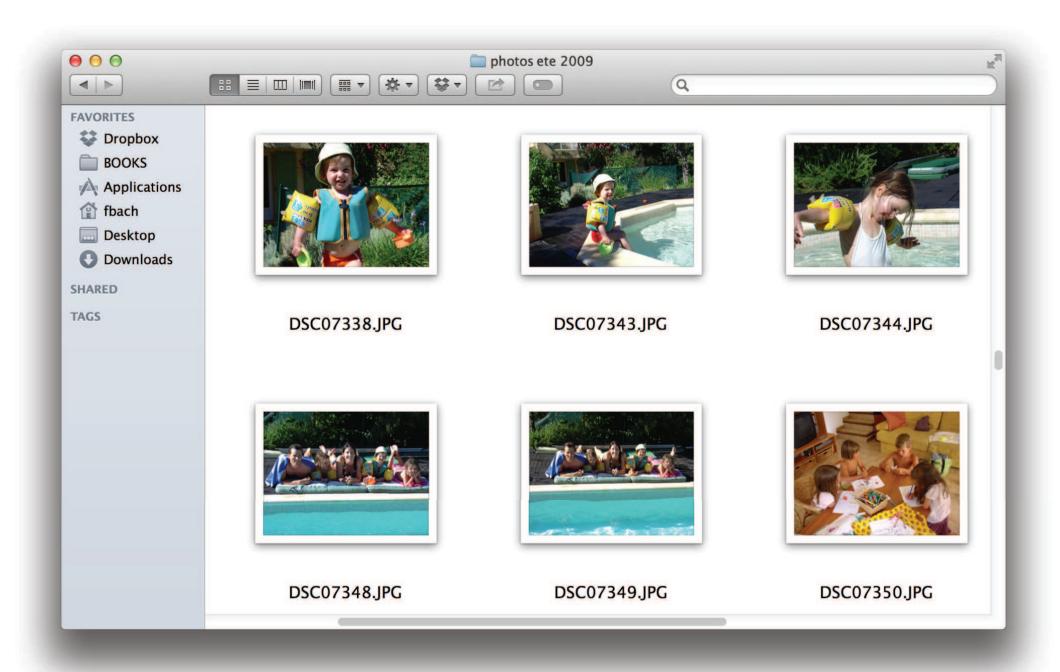
fr.wikipedia.org/wiki/Tour\_de\_France (cyclisme) -

Le **Tour de France** est une compétition cycliste par étapes créée en 1903 par Henri Desgrange et Géo Lefèvre, chef **de** la rubrique cyclisme du journal L'Auto. Histoire · Médiatisation du ... · Équipes et participation

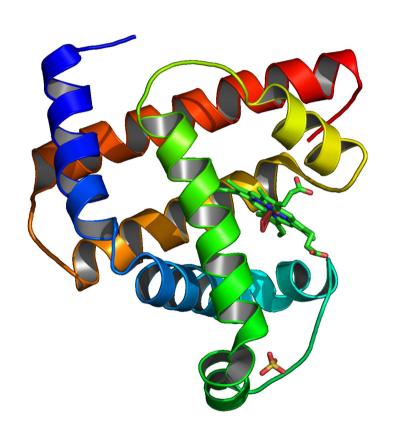
## Visual object recognition



## **Personal photos**



#### **Bioinformatics**



- Protein: Crucial elements of cell life
- Massive data: 2 millions for humans
- Complex data

# Context Machine learning for "big data"

- Large-scale machine learning: large d, large n
  - -d: dimension of each observation (input)
  - -n: number of observations
- Examples: computer vision, bioinformatics, advertising

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- Examples: computer vision, bioinformatics, advertising
- Ideal running-time complexity: O(dn)

# Context Machine learning for "big data"

- Large-scale machine learning: large d, large n
  - -d: dimension of each observation (input)
  - -n: number of observations
- Examples: computer vision, bioinformatics, advertising
- Ideal running-time complexity: O(dn)
- Going back to simple methods
  - Stochastic gradient methods (Robbins and Monro, 1951)
  - Mixing statistics and optimization

#### **Outline** - I

#### 1. Introduction

- Large-scale machine learning and optimization
- Classes of functions (convex, smooth, etc.)
- Traditional statistical analysis through Rademacher complexity

#### 2. Classical methods for convex optimization

- Smooth optimization (gradient descent, Newton method)
- Non-smooth optimization (subgradient descent)

#### 3. Classical stochastic approximation (not covered)

• Robbins-Monro algorithm (1951)

#### **Outline** - II

#### 4. Non-smooth stochastic approximation

- Stochastic (sub)gradient and averaging
- Non-asymptotic results and lower bounds

#### 5. Smooth stochastic approximation algorithms

- Non-asymptotic analysis for smooth functions
- Least-squares regression without decaying step-sizes

#### 6. Finite data sets

Gradient methods with exponential convergence rates

- Data: n observations  $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ ,  $i = 1, \ldots, n$ , i.i.d.
- Prediction as a linear function  $\theta^{\top}\Phi(x)$  of features  $\Phi(x) \in \mathbb{R}^d$
- (regularized) empirical risk minimization: find  $\hat{\theta}$  solution of

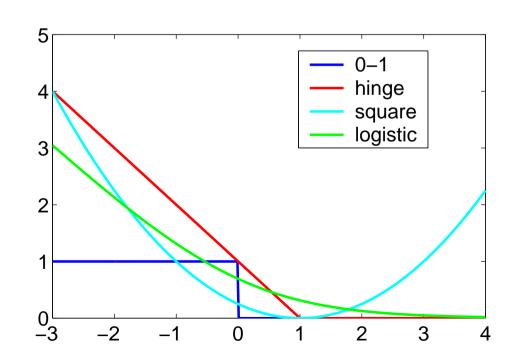
$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i)) \quad + \quad \mu \Omega(\theta)$$

#### **Usual losses**

- Regression:  $y \in \mathbb{R}$ , prediction  $\hat{y} = \theta^{\top} \Phi(x)$ 
  - quadratic loss  $\frac{1}{2}(y-\hat{y})^2 = \frac{1}{2}(y-\theta^\top\Phi(x))^2$

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- Classification :  $y \in \{-1, 1\}$ , prediction  $\hat{y} = \text{sign}(\theta^{\top} \Phi(x))$ 
  - loss of the form  $\ell(y \theta^{\top} \Phi(x))$
  - "True" 0-1 loss:  $\ell(y\,\theta^{\top}\Phi(x))=1_{y\,\theta^{\top}\Phi(x)<0}$
  - Usual convex losses:



#### Main motivating examples

• Support vector machine (hinge loss): non-smooth

$$\ell(Y, \theta^{\top} \Phi(X)) = \max\{1 - Y \theta^{\top} \Phi(X), 0\}$$

• Logistic regression: smooth

$$\ell(Y, \theta^{\top} \Phi(X)) = \log(1 + \exp(-Y\theta^{\top} \Phi(X)))$$

Least-squares regression

$$\ell(Y, \theta^{\top} \Phi(X)) = \frac{1}{2} (Y - \theta^{\top} \Phi(X))^2$$

- Structured output regression
  - See Tsochantaridis et al. (2005); Lacoste-Julien et al. (2013)

#### **Usual regularizers**

- Main goal: avoid overfitting
- (squared) Euclidean norm:  $\|\theta\|_2^2 = \sum_{j=1}^d |\theta_j|^2$ 
  - Numerically well-behaved
  - Representer theorem and kernel methods :  $\theta = \sum_{i=1}^{n} \alpha_i \Phi(x_i)$
  - See, e.g., Schölkopf and Smola (2001); Shawe-Taylor and Cristianini (2004)

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#### Sparsity-inducing norms

- Main example:  $\ell_1$ -norm  $\|\theta\|_1 = \sum_{j=1}^d |\theta_j|$
- Perform model selection as well as regularization
- Non-smooth optimization and structured sparsity
- See, e.g., Bach, Jenatton, Mairal, and Obozinski (2012b,a)

- Data: n observations  $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ ,  $i = 1, \ldots, n$ , i.i.d.
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- (regularized) empirical risk minimization: find  $\hat{\theta}$  solution of

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i)) \quad + \quad \mu \Omega(\theta)$$

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- Empirical risk:  $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^{\top} \Phi(x_i))$  training cost
- Expected risk:  $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \theta^{\top} \Phi(x))$  testing cost
- Two fundamental questions: (1) computing  $\hat{\theta}$  and (2) analyzing  $\hat{\theta}$

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$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i)) \text{ such that } \Omega(\theta) \leqslant D$$

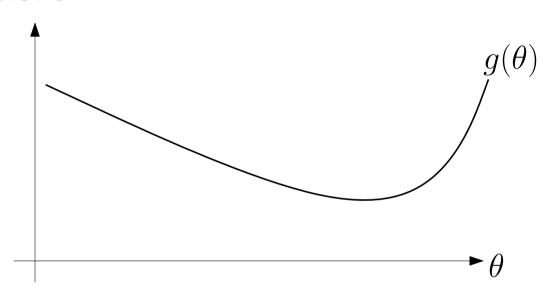
convex data fitting term + constraint

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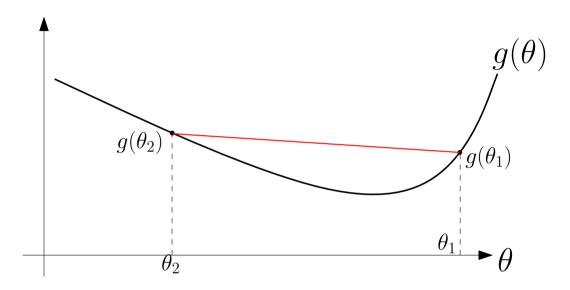
#### **General assumptions**

- Data: n observations  $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$ ,  $i = 1, \ldots, n$ , i.i.d.
- Bounded features  $\Phi(x) \in \mathbb{R}^d$ :  $\|\Phi(x)\|_2 \leqslant R$
- Empirical risk:  $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^{\top} \Phi(x_i))$  training cost
- Expected risk:  $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \theta^{\top} \Phi(x))$  testing cost
- Loss for a single observation:  $f_i(\theta) = \ell(y_i, \theta^\top \Phi(x_i))$  $\Rightarrow \forall i, \ f(\theta) = \mathbb{E}f_i(\theta)$
- Properties of  $f_i, f, \hat{f}$ 
  - Convex on  $\mathbb{R}^d$
  - Additional regularity assumptions: Lipschitz-continuity, smoothness and strong convexity

#### • Global definitions



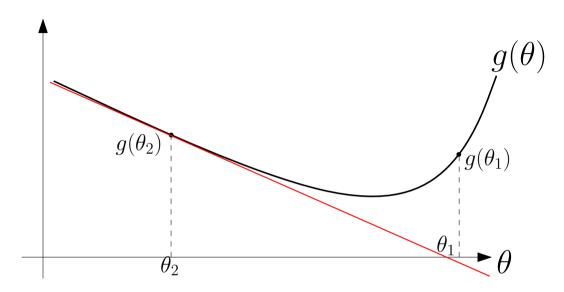
• Global definitions (full domain)



Not assuming differentiability:

$$\forall \theta_1, \theta_2, \alpha \in [0, 1], \quad g(\alpha \theta_1 + (1 - \alpha)\theta_2) \leq \alpha g(\theta_1) + (1 - \alpha)g(\theta_2)$$

Global definitions (full domain)

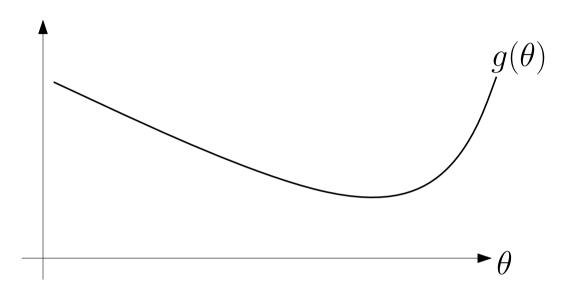


– Assuming differentiability:

$$\forall \theta_1, \theta_2, \quad g(\theta_1) \geqslant g(\theta_2) + g'(\theta_2)^\top (\theta_1 - \theta_2)$$

• Extensions to all functions with subgradients / subdifferential

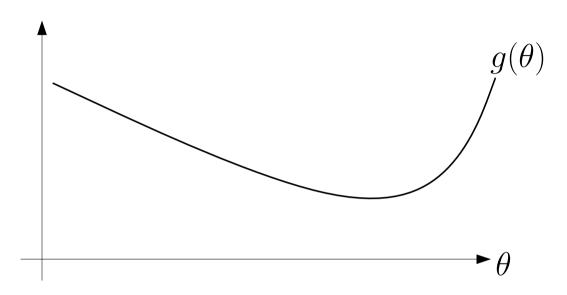
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#### • Local definitions

- Twice differentiable functions
- $\forall \theta, g''(\theta) \geq 0$  (positive semi-definite Hessians)

Global definitions (full domain)



#### Local definitions

- Twice differentiable functions
- $\forall \theta, g''(\theta) \geq 0$  (positive semi-definite Hessians)
- Why convexity?

### Why convexity?

- Local minimum = global minimum
  - Optimality condition (non-smooth):  $0 \in \partial g(\theta)$
  - Optimality condition (smooth):  $g'(\theta) = 0$
- Convex duality
  - See Boyd and Vandenberghe (2003)
- Recognizing convex problems
  - See Boyd and Vandenberghe (2003)

#### **Lipschitz continuity**

• Bounded gradients of g ( $\Leftrightarrow$  Lipschitz-continuity): the function g if convex, differentiable and has (sub)gradients uniformly bounded by B on the ball of center 0 and radius D:

$$\forall \theta \in \mathbb{R}^d, \|\theta\|_2 \leqslant D \Rightarrow \|g'(\theta)\|_2 \leqslant B$$

$$\Leftrightarrow$$

$$\forall \theta, \theta' \in \mathbb{R}^d, \|\theta\|_2, \|\theta'\|_2 \leqslant D \Rightarrow |g(\theta) - g(\theta')| \leqslant B\|\theta - \theta'\|_2$$

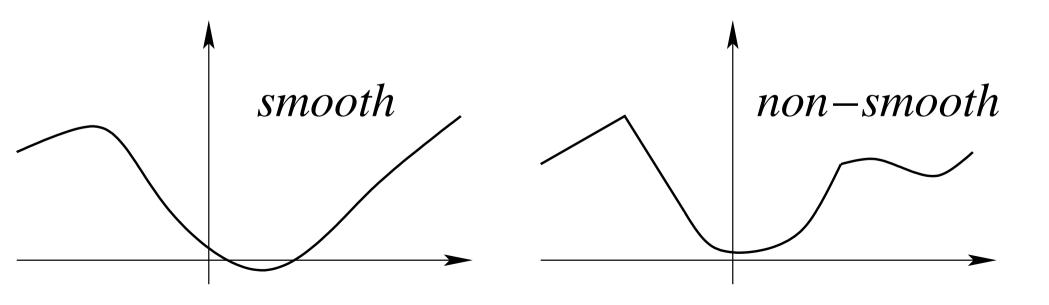
#### Machine learning

- with  $g(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^{\top} \Phi(x_i))$
- G-Lipschitz loss and R-bounded data: B=GR

ullet A function  $g:\mathbb{R}^d o \mathbb{R}$  is L-smooth if and only if it is differentiable and its gradient is L-Lipschitz-continuous

$$\forall \theta_1, \theta_2 \in \mathbb{R}^d, \|g'(\theta_1) - g'(\theta_2)\|_2 \le L \|\theta_1 - \theta_2\|_2$$

• If g is twice differentiable:  $\forall \theta \in \mathbb{R}^d, \ g''(\theta) \preccurlyeq L \cdot Id$ 



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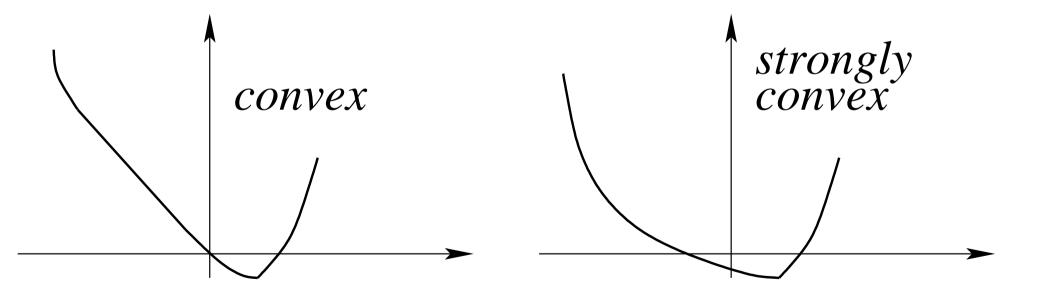
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- Machine learning
  - with  $g(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^{\top} \Phi(x_i))$
  - Hessian  $\approx$  covariance matrix  $\frac{1}{n} \sum_{i=1}^{n} \Phi(x_i) \Phi(x_i)^{\top}$
  - $L_{
    m loss}$ -smooth loss and R-bounded data:  $L=L_{
    m loss}R^2$

ullet A function  $g:\mathbb{R}^d o \mathbb{R}$  is  $\mu$ -strongly convex if and only if

$$\forall \theta_1, \theta_2 \in \mathbb{R}^d, \ g(\theta_1) \geqslant g(\theta_2) + g'(\theta_2)^\top (\theta_1 - \theta_2) + \frac{\mu}{2} \|\theta_1 - \theta_2\|_2^2$$

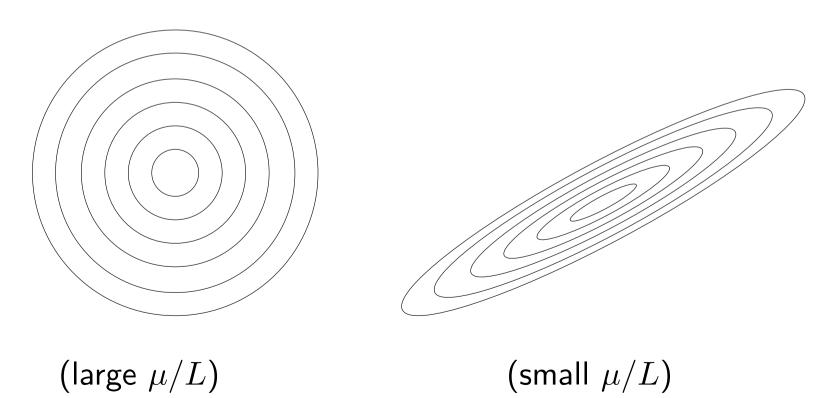
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- Hessian  $\approx$  covariance matrix  $\frac{1}{n} \sum_{i=1}^{n} \Phi(x_i) \Phi(x_i)^{\top}$
- Data with invertible covariance matrix (low correlation/dimension)

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- Data with invertible covariance matrix (low correlation/dimension)
- ullet Adding regularization by  $rac{\mu}{2} \| heta \|^2$ 
  - creates additional bias unless  $\mu$  is small

## Summary of smoothness/convexity assumptions

• Bounded gradients of g (Lipschitz-continuity): the function g if convex, differentiable and has (sub)gradients uniformly bounded by B on the ball of center 0 and radius D:

$$\forall \theta \in \mathbb{R}^d, \|\theta\|_2 \leqslant D \Rightarrow \|g'(\theta)\|_2 \leqslant B$$

• Smoothness of g: the function g is convex, differentiable with L-Lipschitz-continuous gradient g' (e.g., bounded Hessians):

$$\forall \theta_1, \theta_2 \in \mathbb{R}^d, \|g'(\theta_1) - g'(\theta_2)\|_2 \le L\|\theta_1 - \theta_2\|_2$$

• Strong convexity of g: The function g is strongly convex with respect to the norm  $\|\cdot\|$ , with convexity constant  $\mu > 0$ :

$$\forall \theta_1, \theta_2 \in \mathbb{R}^d, \ g(\theta_1) \geqslant g(\theta_2) + g'(\theta_2)^\top (\theta_1 - \theta_2) + \frac{\mu}{2} \|\theta_1 - \theta_2\|_2^2$$

## **Analysis of empirical risk minimization**

• Approximation and estimation errors:  $\Theta = \{\theta \in \mathbb{R}^d, \Omega(\theta) \leq D\}$ 

$$f(\hat{\theta}) - \min_{\theta \in \mathbb{R}^d} f(\theta) = \left[ f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) \right] + \left[ \min_{\theta \in \Theta} f(\theta) - \min_{\theta \in \mathbb{R}^d} f(\theta) \right]$$

Estimation error Approximation error

– NB: may replace  $\min_{\theta \in \mathbb{R}^d} f(\theta)$  by best (non-linear) predictions

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Estimation error Approximation error

1. Uniform deviation bounds, with  $|\hat{\theta} \in \arg\min_{\theta \in \Theta} \hat{f}(\theta)$ 

$$\hat{\theta} \in \arg\min_{\theta \in \Theta} \hat{f}(\theta)$$

$$f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) \leqslant 2 \cdot \sup_{\theta \in \Theta} |f(\theta) - \hat{f}(\theta)|$$

- Typically slow rate  $O(1/\sqrt{n})$
- **2**. More refined concentration results with faster rates O(1/n)

## Slow rate for supervised learning

- Assumptions (f is the expected risk,  $\hat{f}$  the empirical risk)
  - $-\Omega(\theta) = \|\theta\|_2$  (Euclidean norm)
  - "Linear" predictors:  $\theta(x) = \theta^{\top} \Phi(x)$ , with  $\|\Phi(x)\|_2 \leqslant R$  a.s.
  - G-Lipschitz loss: f and  $\hat{f}$  are GR-Lipschitz on  $\Theta = \{\|\theta\|_2 \leqslant D\}$
  - No assumptions regarding convexity

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  - G-Lipschitz loss: f and  $\hat{f}$  are GR-Lipschitz on  $\Theta = \{\|\theta\|_2 \leqslant D\}$
  - No assumptions regarding convexity
- ullet With probability greater than  $1-\delta$

$$\sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| \leqslant \frac{\ell_0 + GRD}{\sqrt{n}} \left[ 2 + \sqrt{2 \log \frac{2}{\delta}} \right]$$

- $\bullet \ \, \text{Expectated estimation error:} \, \, \mathbb{E} \big[ \sup_{\theta \in \Theta} |\hat{f}(\theta) f(\theta)| \big] \leqslant \frac{4\ell_0 + 4GRD}{\sqrt{n}}$
- Using Rademacher averages (see, e.g., Boucheron et al., 2005)
- Lipschitz functions ⇒ slow rate

#### **Motivation from mean estimation**

• Estimator  $\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} z_i = \arg\min_{\theta \in \mathbb{R}} \frac{1}{2n} \sum_{i=1}^{n} (\theta - z_i)^2 = \hat{f}(\theta)$ 

• From before:

$$- f(\theta) = \frac{1}{2} \mathbb{E}(\theta - z)^2 = \frac{1}{2} (\theta - \mathbb{E}z)^2 + \frac{1}{2} \operatorname{var}(z) = \hat{f}(\theta) + O(1/\sqrt{n})$$
$$- f(\hat{\theta}) = \frac{1}{2} (\hat{\theta} - \mathbb{E}z)^2 + \frac{1}{2} \operatorname{var}(z) = f(\mathbb{E}z) + O(1/\sqrt{n})$$

#### Motivation from mean estimation

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- From before:

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$$- f(\hat{\theta}) = \frac{1}{2} (\hat{\theta} - \mathbb{E}z)^2 + \frac{1}{2} \operatorname{var}(z) = f(\mathbb{E}z) + O(1/\sqrt{n})$$

More refined/direct bound:

$$f(\hat{\theta}) - f(\mathbb{E}z) = \frac{1}{2}(\hat{\theta} - \mathbb{E}z)^{2}$$

$$\mathbb{E}[f(\hat{\theta}) - f(\mathbb{E}z)] = \frac{1}{2}\mathbb{E}\left(\frac{1}{n}\sum_{i=1}^{n}z_{i} - \mathbb{E}z\right)^{2} = \frac{1}{2n}\operatorname{var}(z)$$

• Bound only at  $\hat{\theta}$  + strong convexity (instead of uniform bound)

## Fast rate for supervised learning

- **Assumptions** (f is the expected risk,  $\hat{f}$  the empirical risk)
  - Same as before (bounded features, Lipschitz loss)
  - Regularized risks:  $f^{\mu}(\theta) = f(\theta) + \frac{\mu}{2} \|\theta\|_2^2$  and  $\hat{f}^{\mu}(\theta) = \hat{f}(\theta) + \frac{\mu}{2} \|\theta\|_2^2$
  - Convexity
- ullet For any a>0, with probability greater than  $1-\delta$ , for all  $\theta\in\mathbb{R}^d$ ,

$$f^{\mu}(\hat{\theta}) - \min_{\eta \in \mathbb{R}^d} f^{\mu}(\eta) \leqslant \frac{8(1 + \frac{1}{a})G^2R^2(32 + \log\frac{1}{\delta})}{\mu n}$$

- Results from Sridharan, Srebro, and Shalev-Shwartz (2008)
  - see also Boucheron and Massart (2011) and references therein
- Strongly convex functions ⇒ fast rate
  - Warning:  $\mu$  should decrease with n to reduce approximation error

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#### 2. Classical methods for convex optimization

- Smooth optimization (gradient descent, Newton method)
- Non-smooth optimization (subgradient descent)

#### 3. Classical stochastic approximation (not covered)

• Robbins-Monro algorithm (1951)

#### **Outline** - II

#### 4. Non-smooth stochastic approximation

- Stochastic (sub)gradient and averaging
- Non-asymptotic results and lower bounds

#### 5. Smooth stochastic approximation algorithms

- Non-asymptotic analysis for smooth functions
- Least-squares regression without decaying step-sizes

#### 6. Finite data sets

Gradient methods with exponential convergence rates

## Complexity results in convex optimization

- **Assumption**: g convex on  $\mathbb{R}^d$
- Classical generic algorithms
  - Gradient descent and accelerated gradient descent
  - Newton method
  - Subgradient method and ellipsoid algorithm
- ullet Key additional properties of g
  - Lipschitz continuity, smoothness or strong convexity
- Key insight from Bottou and Bousquet (2008)
  - In machine learning, no need to optimize below estimation error
- **Key references**: Nesterov (2004), Bubeck (2015)

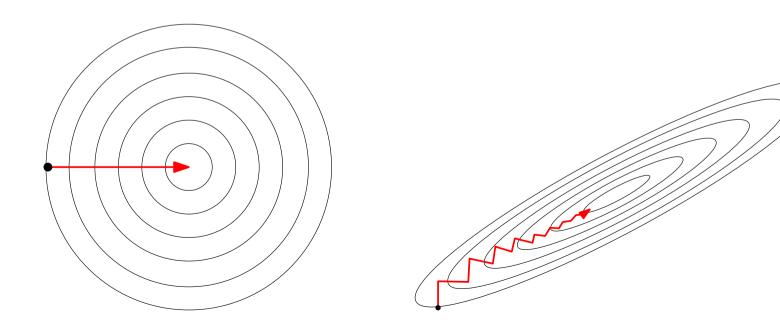
# (smooth) gradient descent

#### Assumptions

- g convex with L-Lipschitz-continuous gradient (e.g., L-smooth)

#### • Algorithm:

$$\theta_t = \theta_{t-1} - \frac{1}{L}g'(\theta_{t-1})$$



# (smooth) gradient descent - strong convexity

#### Assumptions

- g convex with L-Lipschitz-continuous gradient (e.g., L-smooth)
- $g \mu$ -strongly convex
- Algorithm:

$$\theta_t = \theta_{t-1} - \frac{1}{L}g'(\theta_{t-1})$$

• Bound:

$$g(\theta_t) - g(\theta_*) \leq (1 - \mu/L)^t \left[ g(\theta_0) - g(\theta_*) \right]$$

- Three-line proof
- Line search, steepest descent or constant step-size

# (smooth) gradient descent - slow rate

#### Assumptions

- g convex with L-Lipschitz-continuous gradient (e.g., L-smooth)
- Minimum attained at  $\theta_*$
- Algorithm:

$$\theta_t = \theta_{t-1} - \frac{1}{L}g'(\theta_{t-1})$$

Bound:

$$g(\theta_t) - g(\theta_*) \leqslant \frac{2L\|\theta_0 - \theta_*\|^2}{t+4}$$

- Four-line proof
- Adaptivity of gradient descent to problem difficulty
- Not best possible convergence rates after O(d) iterations

## Gradient descent - Proof for quadratic functions

- Quadratic convex function:  $g(\theta) = \frac{1}{2}\theta^{\top}H\theta c^{\top}\theta$ 
  - $\mu$  and L are smallest largest eigenvalues of H
  - Global optimum  $\theta_* = H^{-1}c$  (or  $H^{\dagger}c$ )
- Gradient descent:

$$\theta_{t} = \theta_{t-1} - \frac{1}{L}(H\theta - c) = \theta_{t-1} - \frac{1}{L}(H\theta - H\theta_{*})$$

$$\theta_{t} - \theta_{*} = (I - \frac{1}{L}H)(\theta_{t-1} - \theta_{*}) = (I - \frac{1}{L}H)^{t}(\theta_{0} - \theta_{*})$$

- Strong convexity  $\mu > 0$ : eigenvalues of  $(I \frac{1}{L}H)^t$  in  $[0, (1 \frac{\mu}{L})^t]$ 
  - Convergence of iterates:  $\|\theta_t \theta_*\|^2 \leq (1 \mu/L)^{2t} \|\theta_0 \theta_*\|^2$
  - Function values:  $g(\theta_t) g(\theta_*) \leq (1 \mu/L)^{2t} [g(\theta_0) g(\theta_*)]$

## **Gradient descent - Proof for quadratic functions**

- Quadratic convex function:  $g(\theta) = \frac{1}{2}\theta^{\top}H\theta c^{\top}\theta$ 
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$$\theta_{t} - \theta_{*} = (I - \frac{1}{L}H)(\theta_{t-1} - \theta_{*}) = (I - \frac{1}{L}H)^{t}(\theta_{0} - \theta_{*})$$

- Convexity  $\mu=0$ : eigenvalues of  $(I-\frac{1}{L}H)^t$  in [0,1]
  - No convergence of iterates:  $\|\theta_t \theta_*\|^2 \leq \|\theta_0 \theta_*\|^2$
  - Function values:  $g(\theta_t) g(\theta_*) \leqslant \max_{v \in [0,L]} v (1 v/L)^{2t} \|\theta_0 \theta_*\|^2$   $g(\theta_t) g(\theta_*) \leqslant \frac{L}{t} \|\theta_0 \theta_*\|^2$

# Accelerated gradient methods (Nesterov, 1983)

#### Assumptions

– g convex with L-Lipschitz-cont. gradient , min. attained at  $\theta_*$ 

• Algorithm:

$$\theta_t = \eta_{t-1} - \frac{1}{L}g'(\eta_{t-1})$$

$$\eta_t = \theta_t + \frac{t-1}{t+2}(\theta_t - \theta_{t-1})$$

• Bound:

$$g(\theta_t) - g(\theta_*) \leqslant \frac{2L\|\theta_0 - \theta_*\|^2}{(t+1)^2}$$

- Ten-line proof (see, e.g., Schmidt, Le Roux, and Bach, 2011)
- Not improvable
- Extension to strongly-convex functions

## Accelerated gradient methods - strong convexity

#### Assumptions

- g convex with L-Lipschitz-cont. gradient, min. attained at  $\theta_*$
- $-g \mu$ -strongly convex

#### • Algorithm:

$$\theta_t = \eta_{t-1} - \frac{1}{L}g'(\eta_{t-1})$$

$$\eta_t = \theta_t + \frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}}(\theta_t - \theta_{t-1})$$

- Bound:  $g(\theta_t) f(\theta_*) \leq L \|\theta_0 \theta_*\|^2 (1 \sqrt{\mu/L})^t$ 
  - Ten-line proof (see, e.g., Schmidt, Le Roux, and Bach, 2011)
  - Not improvable
  - Relationship with conjugate gradient for quadratic functions

# Optimization for sparsity-inducing norms (see Bach, Jenatton, Mairal, and Obozinski, 2012b)

Gradient descent as a proximal method (differentiable functions)

$$-\theta_{t+1} = \arg\min_{\theta \in \mathbb{R}^d} f(\theta_t) + (\theta - \theta_t)^{\top} \nabla f(\theta_t) + \frac{L}{2} \|\theta - \theta_t\|_2^2$$
$$-\theta_{t+1} = \theta_t - \frac{1}{L} \nabla f(\theta_t)$$

# **Optimization for sparsity-inducing norms** (see Bach, Jenatton, Mairal, and Obozinski, 2012b)

Gradient descent as a proximal method (differentiable functions)

$$-\theta_{t+1} = \arg\min_{\theta \in \mathbb{R}^d} f(\theta_t) + (\theta - \theta_t)^{\top} \nabla f(\theta_t) + \frac{L}{2} \|\theta - \theta_t\|_2^2$$
$$-\theta_{t+1} = \theta_t - \frac{1}{L} \nabla f(\theta_t)$$

$$ullet$$
 Problems of the form:  $\min_{\theta \in \mathbb{R}^d} f(\theta) + \mu \Omega(\theta)$ 

$$-\theta_{t+1} = \arg\min_{\theta \in \mathbb{R}^d} f(\theta_t) + (\theta - \theta_t)^{\top} \nabla f(\theta_t) + \mu \Omega(\theta) + \frac{L}{2} \|\theta - \theta_t\|_2^2$$

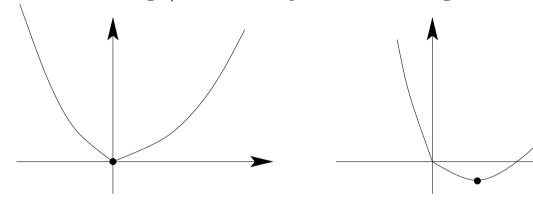
- $-\Omega(\theta) = \|\theta\|_1 \Rightarrow$  Thresholded gradient descent
- Similar convergence rates than smooth optimization
  - Acceleration methods (Nesterov, 2007; Beck and Teboulle, 2009)

# **S**oft-thresholding for the $\ell_1$ -norm

• Example 1: quadratic problem in 1D, i.e.  $\left| \min_{x \in \mathbb{R}} \frac{1}{2} x^2 - xy + \lambda |x| \right|$ 

$$\min_{x \in \mathbb{R}} \frac{1}{2}x^2 - xy + \lambda |x|$$

- Piecewise quadratic function with a kink at zero
  - Derivative at 0+:  $g_+=\lambda-y$  and 0-:  $g_-=-\lambda-y$



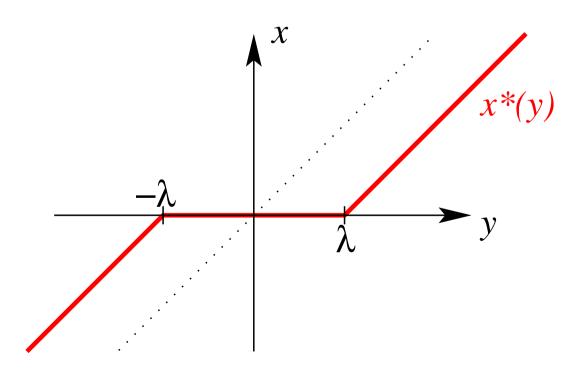
- -x=0 is the solution iff  $g_{+}\geqslant 0$  and  $g_{-}\leqslant 0$  (i.e.,  $|y|\leqslant \lambda$ )
- $-x \geqslant 0$  is the solution iff  $g_+ \leqslant 0$  (i.e.,  $y \geqslant \lambda$ )  $\Rightarrow x^* = y \lambda$
- $-x \leq 0$  is the solution iff  $g_{-} \leq 0$  (i.e.,  $y \leq -\lambda$ )  $\Rightarrow x^* = y + \lambda$
- Solution  $|x^* = \operatorname{sign}(y)(|y| \lambda)_+| = \operatorname{soft\ thresholding}$

# **Soft-thresholding for the** $\ell_1$ **-norm**

• Example 1: quadratic problem in 1D, i.e.  $\left| \min_{x \in \mathbb{R}} \frac{1}{2} x^2 - xy + \lambda |x| \right|$ 

$$\min_{x \in \mathbb{R}} \frac{1}{2} x^2 - xy + \lambda |x|$$

- Piecewise quadratic function with a kink at zero
- Solution  $x^* = sign(y)(|y| \lambda)_+ = soft thresholding$



#### **Newton method**

• Given  $\theta_{t-1}$ , minimize second-order Taylor expansion

$$\tilde{g}(\theta) = g(\theta_{t-1}) + g'(\theta_{t-1})^{\top} (\theta - \theta_{t-1}) + \frac{1}{2} (\theta - \theta_{t-1})^{\top} g''(\theta_{t-1})^{\top} (\theta - \theta_{t-1})$$

- Expensive Iteration:  $\theta_t = \theta_{t-1} g''(\theta_{t-1})^{-1}g'(\theta_{t-1})$ 
  - Running-time complexity:  $O(d^3)$  in general
- Quadratic convergence: If  $\|\theta_{t-1} \theta_*\|$  small enough, for some constant C, we have

$$(C\|\theta_t - \theta_*\|) = (C\|\theta_{t-1} - \theta_*\|)^2$$

- See Boyd and Vandenberghe (2003)

## **Summary: minimizing smooth convex functions**

- **Assumption**: *g* convex
- Gradient descent:  $\theta_t = \theta_{t-1} \gamma_t g'(\theta_{t-1})$ 
  - -O(1/t) convergence rate for smooth convex functions
  - $O(e^{-t\mu/L})$  convergence rate for strongly smooth convex functions
  - Optimal rates  $O(1/t^2)$  and  $O(e^{-t\sqrt{\mu/L}})$
- Newton method:  $\theta_t = \theta_{t-1} f''(\theta_{t-1})^{-1} f'(\theta_{t-1})$ 
  - $-O(e^{-\rho 2^t})$  convergence rate

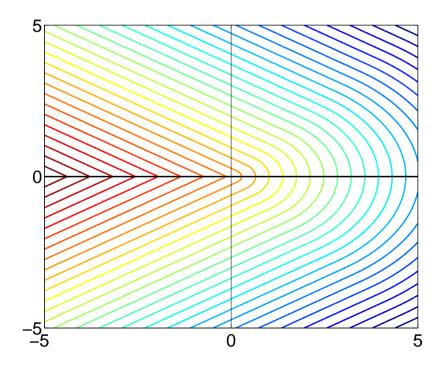
## **Summary: minimizing smooth convex functions**

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  - Optimal rates  $O(1/t^2)$  and  $O(e^{-t\sqrt{\mu/L}})$
- Newton method:  $\theta_t = \theta_{t-1} f''(\theta_{t-1})^{-1} f'(\theta_{t-1})$ 
  - $-O(e^{-\rho 2^t})$  convergence rate
- From smooth to non-smooth
  - Subgradient method and ellipsoid (not covered)

# Counter-example (Bertsekas, 1999) Steepest descent for nonsmooth objectives

• 
$$g(\theta_1, \theta_2) = \begin{cases} -5(9\theta_1^2 + 16\theta_2^2)^{1/2} & \text{if } \theta_1 > |\theta_2| \\ -(9\theta_1 + 16|\theta_2|)^{1/2} & \text{if } \theta_1 \leqslant |\theta_2| \end{cases}$$

• Steepest descent starting from any  $\theta$  such that  $\theta_1 > |\theta_2| > (9/16)^2 |\theta_1|$ 



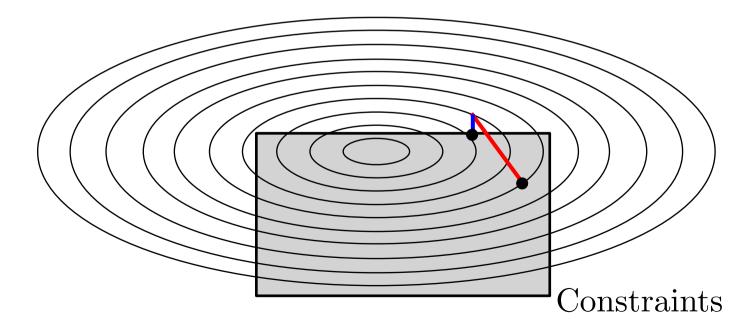
# Subgradient method/"descent" (Shor et al., 1985)

#### Assumptions

- g convex and B-Lipschitz-continuous on  $\{\|\theta\|_2 \leqslant D\}$ 

• Algorithm: 
$$\theta_t = \Pi_D \left( \theta_{t-1} - \frac{2D}{B\sqrt{t}} g'(\theta_{t-1}) \right)$$

-  $\Pi_D$ : orthogonal projection onto  $\{\|\theta\|_2 \leqslant D\}$ 



# Subgradient method/"descent" (Shor et al., 1985)

#### Assumptions

- g convex and B-Lipschitz-continuous on  $\{\|\theta\|_2 \leqslant D\}$
- Algorithm:  $\theta_t = \Pi_D \left( \theta_{t-1} \frac{2D}{B\sqrt{t}} g'(\theta_{t-1}) \right)$ 
  - $\Pi_D$ : orthogonal projection onto  $\{\|\theta\|_2 \leq D\}$
- Bound:

$$g\left(\frac{1}{t}\sum_{k=0}^{t-1}\theta_k\right) - g(\theta_*) \leqslant \frac{2DB}{\sqrt{t}}$$

- Three-line proof
- Best possible convergence rate after O(d) iterations (Bubeck, 2015)

# Subgradient method/"descent" - proof - I

- Iteration:  $\theta_t = \Pi_D(\theta_{t-1} \gamma_t g'(\theta_{t-1}))$  with  $\gamma_t = \frac{2D}{B\sqrt{t}}$
- Assumption:  $||g'(\theta)||_2 \leqslant B$  and  $||\theta||_2 \leqslant D$

$$\|\theta_t - \theta_*\|_2^2 \leqslant \|\theta_{t-1} - \theta_* - \gamma_t g'(\theta_{t-1})\|_2^2 \text{ by contractivity of projections}$$

$$\leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2 \gamma_t^2 - 2\gamma_t (\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \text{ because } \|g'(\theta_{t-1})\|_2 \leqslant B$$

$$\leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2 \gamma_t^2 - 2\gamma_t \left[g(\theta_{t-1}) - g(\theta_*)\right] \text{ (property of subgradients)}$$

leading to

$$g(\theta_{t-1}) - g(\theta_*) \leqslant \frac{B^2 \gamma_t}{2} + \frac{1}{2\gamma_t} [\|\theta_{t-1} - \theta_*\|_2^2 - \|\theta_t - \theta_*\|_2^2]$$

# Subgradient method/"descent" - proof - II

- Starting from  $g(\theta_{t-1}) g(\theta_*) \leqslant \frac{B^2 \gamma_t}{2} + \frac{1}{2\gamma_t} \left[ \|\theta_{t-1} \theta_*\|_2^2 \|\theta_t \theta_*\|_2^2 \right]$
- Constant step-size  $\gamma_t = \gamma$

$$\sum_{u=1}^{t} \left[ g(\theta_{u-1}) - g(\theta_{*}) \right] \leqslant \sum_{u=1}^{t} \frac{B^{2}\gamma}{2} + \sum_{u=1}^{t} \frac{1}{2\gamma} \left[ \|\theta_{u-1} - \theta_{*}\|_{2}^{2} - \|\theta_{u} - \theta_{*}\|_{2}^{2} \right]$$

$$\leqslant t \frac{B^{2}\gamma}{2} + \frac{1}{2\gamma} \|\theta_{0} - \theta_{*}\|_{2}^{2} \leqslant t \frac{B^{2}\gamma}{2} + \frac{2}{\gamma} D^{2}$$

- Optimized step-size  $\gamma_t = \frac{2D}{B\sqrt{t}}$  depends on "horizon"
  - Leads to bound of  $2DB\sqrt{t}$
- Using convexity:  $g\left(\frac{1}{t}\sum_{k=0}^{t-1}\theta_k\right) g(\theta_*) \leqslant \frac{2DB}{\sqrt{t}}$

# Subgradient method/"descent" - proof - III

• Starting from 
$$g(\theta_{t-1}) - g(\theta_*) \leqslant \frac{B^2 \gamma_t}{2} + \frac{1}{2\gamma_t} \left[ \|\theta_{t-1} - \theta_*\|_2^2 - \|\theta_t - \theta_*\|_2^2 \right]$$

Decreasing step-size

$$\begin{split} \sum_{u=1}^{t} \left[ g(\theta_{u-1}) - g(\theta_*) \right] &\leqslant \sum_{u=1}^{t} \frac{B^2 \gamma_u}{2} + \sum_{u=1}^{t} \frac{1}{2\gamma_u} \left[ \|\theta_{u-1} - \theta_*\|_2^2 - \|\theta_u - \theta_*\|_2^2 \right] \\ &= \sum_{u=1}^{t} \frac{B^2 \gamma_u}{2} + \sum_{u=1}^{t-1} \|\theta_u - \theta_*\|_2^2 \left( \frac{1}{2\gamma_{u+1}} - \frac{1}{2\gamma_u} \right) + \frac{\|\theta_0 - \theta_*\|_2^2}{2\gamma_1} - \frac{\|\theta_t - \theta_*\|_2^2}{2\gamma_t} \\ &\leqslant \sum_{u=1}^{t} \frac{B^2 \gamma_u}{2} + \sum_{u=1}^{t-1} 4D^2 \left( \frac{1}{2\gamma_{u+1}} - \frac{1}{2\gamma_u} \right) + \frac{4D^2}{2\gamma_1} \\ &= \sum_{u=1}^{t} \frac{B^2 \gamma_u}{2} + \frac{4D^2}{2\gamma_t} \leqslant 2DB\sqrt{t} \text{ with } \gamma_t = \frac{2D}{B\sqrt{t}} \end{split}$$

• Using convexity:  $g\left(\frac{1}{t}\sum_{k=0}^{t-1}\theta_k\right) - g(\theta_*) \leqslant \frac{2DB}{\sqrt{t}}$ 

# Subgradient descent for machine learning

- Assumptions (f is the expected risk,  $\hat{f}$  the empirical risk)
  - "Linear" predictors:  $\theta(x) = \theta^{\top} \Phi(x)$ , with  $\|\Phi(x)\|_2 \leqslant R$  a.s.
  - $-\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \Phi(x_i)^{\top} \theta)$
  - G-Lipschitz loss: f and  $\hat{f}$  are GR-Lipschitz on  $\Theta = \{\|\theta\|_2 \leqslant D\}$
- ullet Statistics: with probability greater than  $1-\delta$

$$\sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| \leqslant \frac{GRD}{\sqrt{n}} \left[ 2 + \sqrt{2 \log \frac{2}{\delta}} \right]$$

• Optimization: after t iterations of subgradient method

$$\hat{f}(\hat{\theta}) - \min_{\eta \in \Theta} \hat{f}(\eta) \leqslant \frac{GRD}{\sqrt{t}}$$

• t=n iterations, with total running-time complexity of  $O(n^2d)$ 

## Subgradient descent - strong convexity

#### Assumptions

- g convex and B-Lipschitz-continuous on  $\{\|\theta\|_2 \leq D\}$
- $-g \mu$ -strongly convex

• Algorithm: 
$$\theta_t = \Pi_D \left( \theta_{t-1} - \frac{2}{\mu(t+1)} g'(\theta_{t-1}) \right)$$

• Bound:

$$g\left(\frac{2}{t(t+1)}\sum_{k=1}^{t} k\theta_{k-1}\right) - g(\theta_*) \leqslant \frac{2B^2}{\mu(t+1)}$$

- Three-line proof
- Best possible convergence rate after O(d) iterations (Bubeck, 2015)

# Subgradient method - strong convexity - proof - I

- Iteration:  $\theta_t = \Pi_D(\theta_{t-1} \gamma_t g'(\theta_{t-1}))$  with  $\gamma_t = \frac{2}{\mu(t+1)}$
- Assumption:  $||g'(\theta)||_2 \leqslant B$  and  $||\theta||_2 \leqslant D$  and  $\mu$ -strong convexity of f

$$\begin{split} \|\theta_{t} - \theta_{*}\|_{2}^{2} & \leqslant \quad \|\theta_{t-1} - \theta_{*} - \gamma_{t} g'(\theta_{t-1})\|_{2}^{2} \text{ by contractivity of projections} \\ & \leqslant \quad \|\theta_{t-1} - \theta_{*}\|_{2}^{2} + B^{2} \gamma_{t}^{2} - 2\gamma_{t} (\theta_{t-1} - \theta_{*})^{\top} g'(\theta_{t-1}) \text{ because } \|g'(\theta_{t-1})\|_{2} \leqslant B \\ & \leqslant \quad \|\theta_{t-1} - \theta_{*}\|_{2}^{2} + B^{2} \gamma_{t}^{2} - 2\gamma_{t} \big[ g(\theta_{t-1}) - g(\theta_{*}) + \frac{\mu}{2} \|\theta_{t-1} - \theta_{*}\|_{2}^{2} \big] \end{split}$$

(property of subgradients and strong convexity)

leading to

$$g(\theta_{t-1}) - g(\theta_*) \leq \frac{B^2 \gamma_t}{2} + \frac{1}{2} \left[ \frac{1}{\gamma_t} - \mu \right] \|\theta_{t-1} - \theta_*\|_2^2 - \frac{1}{2\gamma_t} \|\theta_t - \theta_*\|_2^2$$

$$\leq \frac{B^2}{\mu(t+1)} + \frac{\mu}{2} \left[ \frac{t-1}{2} \right] \|\theta_{t-1} - \theta_*\|_2^2 - \frac{\mu(t+1)}{4} \|\theta_t - \theta_*\|_2^2$$

# Subgradient method - strong convexity - proof - II

$$\quad \text{From} \quad g(\theta_{t-1}) - g(\theta_*) \leqslant \frac{B^2}{\mu(t+1)} + \frac{\mu}{2} \big[ \frac{t-1}{2} \big] \|\theta_{t-1} - \theta_*\|_2^2 - \frac{\mu(t+1)}{4} \|\theta_t - \theta_*\|_2^2$$

$$\sum_{u=1}^{t} u \left[ g(\theta_{u-1}) - g(\theta_{*}) \right] \leqslant \sum_{t=1}^{u} \frac{B^{2}u}{\mu(u+1)} + \frac{1}{4} \sum_{u=1}^{t} \left[ u(u-1) \|\theta_{u-1} - \theta_{*}\|_{2}^{2} - u(u+1) \|\theta_{u} - \theta_{*}\|_{2}^{2} \right]$$

$$\leqslant \frac{B^{2}t}{\mu} + \frac{1}{4} \left[ 0 - t(t+1) \|\theta_{t} - \theta_{*}\|_{2}^{2} \right] \leqslant \frac{B^{2}t}{\mu}$$

• Using convexity: 
$$g\left(\frac{2}{t(t+1)}\sum_{u=1}^{t}u\theta_{u-1}\right)-g(\theta_*)\leqslant \frac{2B^2}{t+1}$$

• NB: with step-size  $\gamma_n = 1/(n\mu)$ , extra logarithmic factor

# **Summary: minimizing convex functions**

- **Assumption**: *g* convex
- Gradient descent:  $\theta_t = \theta_{t-1} \gamma_t g'(\theta_{t-1})$ 
  - $O(1/\sqrt{t})$  convergence rate for non-smooth convex functions
  - O(1/t) convergence rate for smooth convex functions
  - $O(e^{-\rho t})$  convergence rate for strongly smooth convex functions
- Newton method:  $\theta_t = \theta_{t-1} g''(\theta_{t-1})^{-1}g'(\theta_{t-1})$ 
  - $-O(e^{-\rho 2^t})$  convergence rate

# **Summary: minimizing convex functions**

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- Newton method:  $\theta_t = \theta_{t-1} g''(\theta_{t-1})^{-1}g'(\theta_{t-1})$ 
  - $-O(e^{-\rho 2^t})$  convergence rate
- Key insights from Bottou and Bousquet (2008)
  - 1. In machine learning, no need to optimize below statistical error
  - 2. In machine learning, cost functions are averages
    - **⇒ Stochastic approximation**

### **Summary of rates of convergence**

- Problem parameters
  - D diameter of the domain
  - -B Lipschitz-constant
  - -L smoothness constant
  - $\mu$  strong convexity constant

	convex	strongly convex
nonsmooth	deterministic: $BD/\sqrt{t}$	deterministic: $B^2/(t\mu)$
smooth	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
quadratic	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
		· ·

#### **Outline** - I

#### 1. Introduction

- Large-scale machine learning and optimization
- Classes of functions (convex, smooth, etc.)
- Traditional statistical analysis through Rademacher complexity

#### 2. Classical methods for convex optimization

- Smooth optimization (gradient descent, Newton method)
- Non-smooth optimization (subgradient descent)

### 3. Classical stochastic approximation (not covered)

• Robbins-Monro algorithm (1951)

### **Outline** - II

### 4. Non-smooth stochastic approximation

- Stochastic (sub)gradient and averaging
- Non-asymptotic results and lower bounds

### 5. Smooth stochastic approximation algorithms

- Non-asymptotic analysis for smooth functions
- Least-squares regression without decaying step-sizes

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## **Stochastic approximation**

- Goal: Minimizing a function f defined on  $\mathbb{R}^d$ 
  - given only unbiased estimates  $f_n'(\theta_n)$  of its gradients  $f'(\theta_n)$  at certain points  $\theta_n \in \mathbb{R}^d$

# Stochastic approximation

- Goal: Minimizing a function f defined on  $\mathbb{R}^d$ 
  - given only unbiased estimates  $f'_n(\theta_n)$  of its gradients  $f'(\theta_n)$  at certain points  $\theta_n \in \mathbb{R}^d$
- Machine learning statistics
  - loss for a single pair of observations:  $|f_n(\theta)| = \ell(y_n, \theta^\top \Phi(x_n))$

$$f_n(\theta) = \ell(y_n, \theta^{\top} \Phi(x_n))$$

- $-f(\theta) = \mathbb{E} f_n(\theta) = \mathbb{E} \ell(y_n, \theta^{\top} \Phi(x_n)) =$ generalization error
- Expected gradient:  $f'(\theta) = \mathbb{E}f'_n(\theta) = \mathbb{E}\left\{\ell'(y_n, \theta^\top \Phi(x_n)) \Phi(x_n)\right\}$
- Non-asymptotic results
- Number of iterations = number of observations

## **Stochastic approximation**

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  - given only unbiased estimates  $f_n'(\theta_n)$  of its gradients  $f'(\theta_n)$  at certain points  $\theta_n \in \mathbb{R}^d$

### • Stochastic approximation

- (much) broader applicability beyond convex optimization

$$\theta_n = \theta_{n-1} - \gamma_n h_n(\theta_{n-1})$$
 with  $\mathbb{E}[h_n(\theta_{n-1})|\theta_{n-1}] = h(\theta_{n-1})$ 

- Beyond convex problems, i.i.d assumption, finite dimension, etc.
- Typically asymptotic results
- See, e.g., Kushner and Yin (2003); Benveniste et al. (2012)

### Relationship to online learning

### • Stochastic approximation

- Minimize  $f(\theta) = \mathbb{E}_z \ell(\theta, z) =$  generalization error of  $\theta$
- Using the gradients of single i.i.d. observations

### Relationship to online learning

### • Stochastic approximation

- Minimize  $f(\theta) = \mathbb{E}_z \ell(\theta, z) =$  generalization error of  $\theta$
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#### Batch learning

- Finite set of observations:  $z_1, \ldots, z_n$
- Empirical risk:  $\hat{f}(\theta) = \frac{1}{n} \sum_{k=1}^{n} \ell(\theta, z_i)$
- Estimator  $\hat{\theta} = \text{Minimizer of } \hat{f}(\theta)$  over a certain class  $\Theta$
- Generalization bound using uniform concentration results

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- Generalization bound using uniform concentration results

### Online learning

- Update  $\hat{\theta}_n$  after each new (potentially adversarial) observation  $z_n$
- Cumulative loss:  $\frac{1}{n} \sum_{k=1}^{n} \ell(\hat{\theta}_{k-1}, z_k)$
- Online to batch through averaging (Cesa-Bianchi et al., 2004)

### **Convex stochastic approximation**

- Key properties of f and/or  $f_n$ 
  - Smoothness: f B-Lipschitz continuous, f' L-Lipschitz continuous
  - Strong convexity:  $f \mu$ -strongly convex

## Convex stochastic approximation

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- **Key algorithm:** Stochastic gradient descent (a.k.a. Robbins-Monro)

$$\theta_n = \theta_{n-1} - \gamma_n f'_n(\theta_{n-1})$$

- Polyak-Ruppert averaging:  $\bar{\theta}_n = \frac{1}{n} \sum_{k=0}^{n-1} \theta_k$
- Which learning rate sequence  $\gamma_n$ ? Classical setting:  $\gamma_n = Cn^{-\alpha}$

$$\gamma_n = C n^{-\alpha}$$

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$$\gamma_n = C n^{-\alpha}$$

### Desirable practical behavior

- Applicable (at least) to classical supervised learning problems
- Robustness to (potentially unknown) constants  $(L,B,\mu)$
- Adaptivity to difficulty of the problem (e.g., strong convexity)

## Stochastic subgradient "descent"/method

### Assumptions

- $f_n$  convex and B-Lipschitz-continuous on  $\{\|\theta\|_2 \leq D\}$
- $(f_n)$  i.i.d. functions such that  $\mathbb{E}f_n=f$
- $-\theta_*$  global optimum of f on  $\mathcal{C} = \{\|\theta\|_2 \leqslant D\}$
- Algorithm:  $\theta_n = \Pi_D \left( \theta_{n-1} \frac{2D}{B\sqrt{n}} f_n'(\theta_{n-1}) \right)$

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- Algorithm:  $\theta_n = \Pi_D \left( \theta_{n-1} \frac{2D}{B\sqrt{n}} f_n'(\theta_{n-1}) \right)$
- Bound:

$$\mathbb{E}f\left(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\right) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$$

- "Same" three-line proof as in the deterministic case
- Minimax rate (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
- ullet Running-time complexity: O(dn) after n iterations

# Stochastic subgradient method - proof - I

- Iteration:  $\theta_n = \Pi_D(\theta_{n-1} \gamma_n f_n'(\theta_{n-1}))$  with  $\gamma_n = \frac{2D}{B\sqrt{n}}$
- $\mathcal{F}_n$ : information up to time n
- $||f'_n(\theta)||_2 \leq B$  and  $||\theta||_2 \leq D$ , unbiased gradients/functions  $\mathbb{E}(f_n|\mathcal{F}_{n-1}) = f$

$$\|\theta_{n} - \theta_{*}\|_{2}^{2} \leq \|\theta_{n-1} - \theta_{*} - \gamma_{n} f'_{n}(\theta_{n-1})\|_{2}^{2} \text{ by contractivity of projections}$$

$$\leq \|\theta_{n-1} - \theta_{*}\|_{2}^{2} + B^{2} \gamma_{n}^{2} - 2\gamma_{n}(\theta_{n-1} - \theta_{*})^{\top} f'_{n}(\theta_{n-1}) \text{ because } \|f'_{n}(\theta_{n-1})\|_{2} \leq B$$

$$\mathbb{E}\left[\|\theta_{n}-\theta_{*}\|_{2}^{2}|\mathcal{F}_{n-1}\right] \leqslant \|\theta_{n-1}-\theta_{*}\|_{2}^{2}+B^{2}\gamma_{n}^{2}-2\gamma_{n}(\theta_{n-1}-\theta_{*})^{\top}f'(\theta_{n-1})$$

$$\leqslant \|\theta_{n-1}-\theta_{*}\|_{2}^{2}+B^{2}\gamma_{n}^{2}-2\gamma_{n}\left[f(\theta_{n-1})-f(\theta_{*})\right] \text{ (subgradient property)}$$

$$\mathbb{E}\|\theta_{n}-\theta_{*}\|_{2}^{2} \leqslant \mathbb{E}\|\theta_{n-1}-\theta_{*}\|_{2}^{2}+B^{2}\gamma_{n}^{2}-2\gamma_{n}\left[\mathbb{E}f(\theta_{n-1})-f(\theta_{*})\right]$$

$$\bullet \ \ \text{leading to} \ \mathbb{E} f(\theta_{n-1}) - f(\theta_*) \leqslant \frac{B^2 \gamma_n}{2} + \frac{1}{2\gamma_n} \big[ \mathbb{E} \|\theta_{n-1} - \theta_*\|_2^2 - \mathbb{E} \|\theta_n - \theta_*\|_2^2 \big]$$

# Stochastic subgradient method - proof - II

 $\bullet \ \ \text{Starting from} \ \ \underline{\mathbb{E}} f(\theta_{n-1}) - f(\theta_*) \leqslant \frac{B^2 \gamma_n}{2} + \frac{1}{2\gamma_n} \big[\underline{\mathbb{E}} \|\theta_{n-1} - \theta_*\|_2^2 - \underline{\mathbb{E}} \|\theta_n - \theta_*\|_2^2 \big]$ 

$$\sum_{u=1}^{n} \left[ \mathbb{E} f(\theta_{u-1}) - f(\theta_*) \right] \leqslant \sum_{u=1}^{n} \frac{B^2 \gamma_u}{2} + \sum_{u=1}^{n} \frac{1}{2 \gamma_u} \left[ \mathbb{E} \|\theta_{u-1} - \theta_*\|_2^2 - \mathbb{E} \|\theta_u - \theta_*\|_2^2 \right]$$

$$\leqslant \sum_{u=1}^{n} \frac{B^2 \gamma_u}{2} + \frac{4D^2}{2 \gamma_n} \leqslant 2DB\sqrt{n} \text{ with } \gamma_n = \frac{2D}{B\sqrt{n}}$$

• Using convexity:  $\mathbb{E} f \left( \frac{1}{n} \sum_{k=0}^{n-1} \theta_k \right) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$ 

## Stochastic subgradient descent - strong convexity - I

### Assumptions

- $f_n$  convex and B-Lipschitz-continuous
- $(f_n)$  i.i.d. functions such that  $\mathbb{E} f_n = f$
- $f \mu$ -strongly convex on  $\{\|\theta\|_2 \leqslant D\}$
- $-\theta_*$  global optimum of f over  $\{\|\theta\|_2 \leq D\}$

• Algorithm: 
$$\theta_n = \Pi_D \left( \theta_{n-1} - \frac{2}{\mu(n+1)} f'_n(\theta_{n-1}) \right)$$

• Bound:

$$\mathbb{E}f\left(\frac{2}{n(n+1)}\sum_{k=1}^{n}k\theta_{k-1}\right) - f(\theta_{*}) \leqslant \frac{2B^{2}}{\mu(n+1)}$$

- "Same" proof than deterministic case (Lacoste-Julien et al., 2012)
- Minimax rate (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)

# Stochastic subgradient - strong convexity - proof - I

- Iteration:  $\theta_n = \Pi_D(\theta_{n-1} \gamma_n f'_n(\theta_{t-1}))$  with  $\gamma_n = \frac{2}{\mu(n+1)}$
- Assumption:  $||f'_n(\theta)||_2 \leq B$  and  $||\theta||_2 \leq D$  and  $\mu$ -strong convexity of f

$$\begin{split} \|\theta_{n} - \theta_{*}\|_{2}^{2} & \leqslant \quad \|\theta_{n-1} - \theta_{*} - \gamma_{n} f_{n}'(\theta_{t-1})\|_{2}^{2} \text{ by contractivity of projections} \\ & \leqslant \quad \|\theta_{n-1} - \theta_{*}\|_{2}^{2} + B^{2} \gamma_{n}^{2} - 2 \gamma_{n} (\theta_{n-1} - \theta_{*})^{\top} f_{n}'(\theta_{t-1}) \text{ because } \|f_{n}'(\theta_{t-1})\|_{2} \leqslant B \\ \mathbb{E}(\cdot | \mathcal{F}_{n-1}) & \leqslant \quad \|\theta_{n-1} - \theta_{*}\|_{2}^{2} + B^{2} \gamma_{n}^{2} - 2 \gamma_{n} \left[ f(\theta_{n-1}) - f(\theta_{*}) + \frac{\mu}{2} \|\theta_{n-1} - \theta_{*}\|_{2}^{2} \right] \end{split}$$

(property of subgradients and strong convexity)

leading to

$$\mathbb{E}f(\theta_{n-1}) - f(\theta_*) \leqslant \frac{B^2 \gamma_n}{2} + \frac{1}{2} \left[ \frac{1}{\gamma_n} - \mu \right] \|\theta_{n-1} - \theta_*\|_2^2 - \frac{1}{2\gamma_n} \|\theta_n - \theta_*\|_2^2$$

$$\leqslant \frac{B^2}{\mu(n+1)} + \frac{\mu}{2} \left[ \frac{n-1}{2} \right] \|\theta_{n-1} - \theta_*\|_2^2 - \frac{\mu(n+1)}{4} \|\theta_n - \theta_*\|_2^2$$

# Stochastic subgradient - strong convexity - proof - II

$$\bullet \ \operatorname{From} \mathbb{E} f(\theta_{n-1}) - f(\theta_*) \leqslant \frac{B^2}{\mu(n+1)} + \frac{\mu}{2} \big[ \frac{n-1}{2} \big] \mathbb{E} \|\theta_{n-1} - \theta_*\|_2^2 - \frac{\mu(n+1)}{4} \mathbb{E} \|\theta_n - \theta_*\|_2^2$$

$$\sum_{u=1}^{n} u \left[ \mathbb{E} f(\theta_{u-1}) - f(\theta_{*}) \right] \leqslant \sum_{u=1}^{n} \frac{B^{2}u}{\mu(u+1)} + \frac{1}{4} \sum_{u=1}^{n} \left[ u(u-1)\mathbb{E} \|\theta_{u-1} - \theta_{*}\|_{2}^{2} - u(u+1)\mathbb{E} \|\theta_{u} - \theta_{*}\|_{2}^{2} \right]$$

$$\leqslant \frac{B^{2}n}{\mu} + \frac{1}{4} \left[ 0 - n(n+1)\mathbb{E} \|\theta_{n} - \theta_{*}\|_{2}^{2} \right] \leqslant \frac{B^{2}n}{\mu}$$

- Using convexity:  $\mathbb{E} f\left(\frac{2}{n(n+1)}\sum_{u=1}^n u\theta_{u-1}\right) g(\theta_*) \leqslant \frac{2B^2}{n+1}$
- NB: with step-size  $\gamma_n=1/(n\mu)$ , extra logarithmic factor (see later)

# Stochastic subgradient descent - strong convexity - II

### Assumptions

- $f_n$  convex and B-Lipschitz-continuous
- $(f_n)$  i.i.d. functions such that  $\mathbb{E} f_n = f$
- $\theta_*$  global optimum of  $g = f + \frac{\mu}{2} \| \cdot \|_2^2$
- No compactness assumption no projections

#### • Algorithm:

$$\theta_n = \theta_{n-1} - \frac{2}{\mu(n+1)} g'_n(\theta_{n-1}) = \theta_{n-1} - \frac{2}{\mu(n+1)} [f'_n(\theta_{n-1}) + \mu \theta_{n-1}]$$

• Bound: 
$$\mathbb{E}g\left(\frac{2}{n(n+1)}\sum_{k=1}^{n}k\theta_{k-1}\right)-g(\theta_*)\leqslant \frac{2B^2}{\mu(n+1)}$$

Minimax convergence rate

### Beyond convergence in expectation

• Typical result: 
$$\mathbb{E} f \left( \frac{1}{n} \sum_{k=0}^{n-1} \theta_k \right) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$$

- Obtained with simple conditioning arguments

### High-probability bounds

- Markov inequality: 
$$\mathbb{P}\Big(f\Big(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\Big) - f(\theta_*) \geqslant \varepsilon\Big) \leqslant \frac{2DB}{\sqrt{n}\varepsilon}$$

### Beyond convergence in expectation

• Typical result: 
$$\mathbb{E} f\left(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\right) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$$

- Obtained with simple conditioning arguments

#### High-probability bounds

- Markov inequality:  $\mathbb{P}\Big(f\Big(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\Big)-f(\theta_*)\geqslant \varepsilon\Big)\leqslant \frac{2DB}{\sqrt{n}\varepsilon}$
- Concentration inequality (Nemirovski et al., 2009; Nesterov and Vial, 2008)

$$\mathbb{P}\left(f\left(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\right) - f(\theta_*) \geqslant \frac{2DB}{\sqrt{n}}(2+4t)\right) \leqslant 2\exp(-t^2)$$

• See also Bach (2013) for logistic regression

## Beyond stochastic gradient method

#### Adding a proximal step

- Goal:  $\min_{\theta \in \mathbb{R}^d} f(\theta) + \Omega(\theta) = \mathbb{E} f_n(\theta) + \Omega(\theta)$
- Replace recursion  $\theta_n = \theta_{n-1} \gamma_n f_n'(\theta_n)$  by

$$\theta_n = \min_{\theta \in \mathbb{R}^d} \left\| \theta - \theta_{n-1} + \gamma_n f'_n(\theta_n) \right\|_2^2 + C\Omega(\theta)$$

- Xiao (2010); Hu et al. (2009)
- May be accelerated (Ghadimi and Lan, 2013)

#### Related frameworks

- Regularized dual averaging (Nesterov, 2009; Xiao, 2010)
- Mirror descent (Nemirovski et al., 2009; Lan et al., 2012)

# Minimax rates (Agarwal et al., 2012)

- Model of computation (i.e., algorithms): first-order oracle
  - Queries a function f by obtaining  $f(\theta_k)$  and  $f'(\theta_k)$  with zero-mean bounded variance noise, for  $k=0,\ldots,n-1$  and outputs  $\theta_n$

#### Class of functions

– convex B-Lipschitz-continuous (w.r.t.  $\ell_2$ -norm) on a compact convex set  $\mathcal C$  containing an  $\ell_\infty$ -ball

#### Performance measure

- for a given algorithm and function  $\varepsilon_n(\mathsf{algo},f) = f(\theta_n) \inf_{\theta \in \mathcal{C}} f(\theta)$
- for a given algorithm:  $\sup \varepsilon_n(\mathsf{algo}, f)$  functions f
- Minimax performance:  $\inf_{\mathsf{algo}} \sup_{\mathsf{functions}} \varepsilon_n(\mathsf{algo}, f)$

# Minimax rates (Agarwal et al., 2012)

• Convex functions: domain  $\mathcal C$  that contains an  $\ell_\infty$ -ball of radius D

$$\inf_{\text{algo}} \sup_{\text{functions } f} \varepsilon(\text{algo}, f) \geqslant \operatorname{cst} \times \min \left\{ \frac{BD}{\sqrt{\frac{d}{n}}}, BD \right\}$$

- Consequences for  $\ell_2$ -ball of radius D:  $BD/\sqrt{n}$
- Upper-bound through stochastic subgradient
- $\mu$ -strongly-convex functions:

$$\inf_{\text{algo}} \sup_{\text{functions } f} \varepsilon_n(\text{algo}, f) \geqslant \operatorname{cst} \times \min \Big\{ \frac{B^2}{\mu n}, \frac{B^2}{\mu d}, BD \sqrt{\frac{d}{n}}, BD \Big\}$$

### **Summary of rates of convergence**

- Problem parameters
  - D diameter of the domain
  - -B Lipschitz-constant
  - L smoothness constant
  - $\mu$  strong convexity constant

	convex	strongly convex
nonsmooth	deterministic: $BD/\sqrt{t}$	deterministic: $B^2/(t\mu)$
	stochastic: $BD/\sqrt{n}$	stochastic: $B^2/(n\mu)$
smooth	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
quadratic	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$

#### **Outline** - I

#### 1. Introduction

- Large-scale machine learning and optimization
- Classes of functions (convex, smooth, etc.)
- Traditional statistical analysis through Rademacher complexity

### 2. Classical methods for convex optimization

- Smooth optimization (gradient descent, Newton method)
- Non-smooth optimization (subgradient descent)

### 3. Classical stochastic approximation (not covered)

• Robbins-Monro algorithm (1951)

### **Outline** - II

### 4. Non-smooth stochastic approximation

- Stochastic (sub)gradient and averaging
- Non-asymptotic results and lower bounds

### 5. Smooth stochastic approximation algorithms

- Non-asymptotic analysis for smooth functions
- Least-squares regression without decaying step-sizes

#### 6. Finite data sets

Gradient methods with exponential convergence rates

- Known global minimax rates of convergence for non-smooth problems (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
  - Strongly convex:  $O((\mu n)^{-1})$ Attained by averaged stochastic gradient descent with  $\gamma_n \propto (\mu n)^{-1}$
  - Non-strongly convex:  $O(n^{-1/2})$  Attained by averaged stochastic gradient descent with  $\gamma_n \propto n^{-1/2}$

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- Many contributions in optimization and online learning: Bottou and Le Cun (2005); Bottou and Bousquet (2008); Hazan et al. (2007); Shalev-Shwartz and Srebro (2008); Shalev-Shwartz et al. (2007, 2009); Xiao (2010); Duchi and Singer (2009); Nesterov and Vial (2008); Nemirovski et al. (2009)

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- Asymptotic analysis of averaging (Polyak and Juditsky, 1992; Ruppert, 1988)
  - All step sizes  $\gamma_n=Cn^{-\alpha}$  with  $\alpha\in(1/2,1)$  lead to  $O(n^{-1})$  for smooth strongly convex problems

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  - All step sizes  $\gamma_n = C n^{-\alpha}$  with  $\alpha \in (1/2,1)$  lead to  $O(n^{-1})$  for smooth strongly convex problems
- Non-asymptotic analysis for smooth problems?

# **Smoothness/convexity assumptions**

- Iteration:  $\theta_n = \theta_{n-1} \gamma_n f_n'(\theta_{n-1})$ 
  - Polyak-Ruppert averaging:  $\bar{\theta}_n = \frac{1}{n} \sum_{k=0}^{n-1} \theta_k$
- Smoothness of  $f_n$ : For each  $n \ge 1$ , the function  $f_n$  is a.s. convex, differentiable with L-Lipschitz-continuous gradient  $f'_n$ :
  - Smooth loss and bounded data
- **Strong convexity of** f: The function f is strongly convex with respect to the norm  $\|\cdot\|$ , with convexity constant  $\mu > 0$ :
  - Invertible population covariance matrix
  - or regularization by  $\frac{\mu}{2} \|\theta\|^2$

# Summary of new results (Bach and Moulines, 2011)

• Stochastic gradient descent with learning rate  $\gamma_n = C n^{-\alpha}$ 

#### Strongly convex smooth objective functions

- Old:  $O(n^{-1})$  rate achieved without averaging for  $\alpha = 1$
- New:  $O(n^{-1})$  rate achieved with averaging for  $\alpha \in [1/2, 1]$
- Non-asymptotic analysis with explicit constants
- Forgetting of initial conditions
- Robustness to the choice of C

# Summary of new results (Bach and Moulines, 2011)

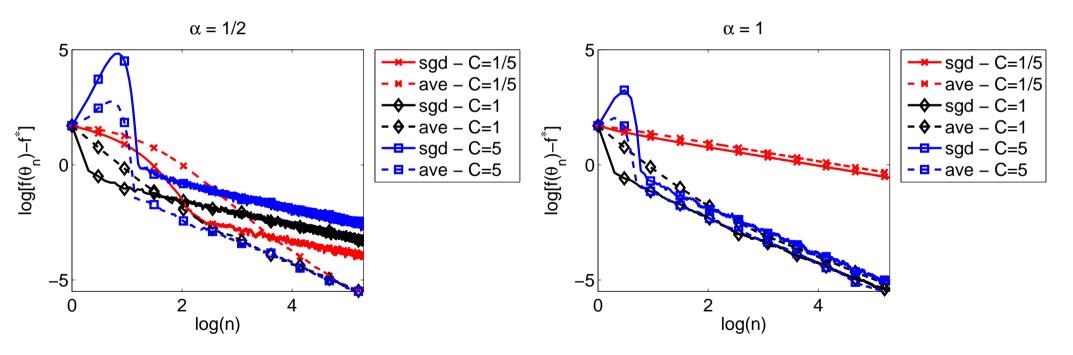
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- Non-asymptotic analysis with explicit constants
- Forgetting of initial conditions
- Robustness to the choice of C
- ullet Convergence rates for  $\mathbb{E}\| heta_n- heta_*\|^2$  and  $\mathbb{E}\|ar{ heta}_n- heta_*\|^2$ 
  - no averaging:  $O\left(\frac{\sigma^2 \gamma_n}{\mu}\right) + O(e^{-\mu n \gamma_n}) \|\theta_0 \theta_*\|^2$
  - $-\text{ averaging: } \frac{\operatorname{tr} H(\theta_*)^{-1}}{n} + \mu^{-1} O(n^{-2\alpha} + n^{-2+\alpha}) + O\Big(\frac{\|\theta_0 \theta_*\|^2}{\mu^2 n^2}\Big)$

# Robustness to wrong constants for $\gamma_n = C n^{-\alpha}$

- $f(\theta) = \frac{1}{2} |\theta|^2$  with i.i.d. Gaussian noise (d=1)
- Left:  $\alpha = 1/2$
- Right:  $\alpha = 1$



• See also http://leon.bottou.org/projects/sgd

# Summary of new results (Bach and Moulines, 2011)

- Stochastic gradient descent with learning rate  $\gamma_n = C n^{-\alpha}$
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#### Strongly convex smooth objective functions

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#### Non-strongly convex smooth objective functions

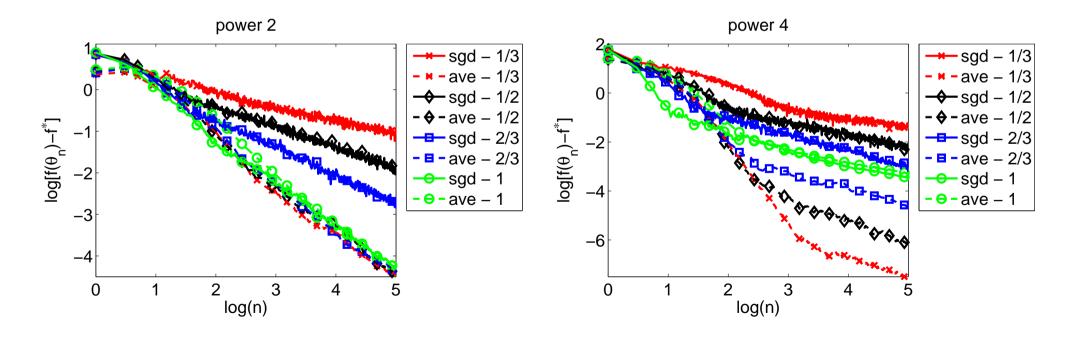
- Old:  $O(n^{-1/2})$  rate achieved with averaging for  $\alpha = 1/2$
- New:  $O(\max\{n^{1/2-3\alpha/2},n^{-\alpha/2},n^{\alpha-1}\})$  rate achieved without averaging for  $\alpha \in [1/3,1]$

#### • Take-home message

- Use  $\alpha = 1/2$  with averaging to be adaptive to strong convexity

## Robustness to lack of strong convexity

- Left:  $f(\theta) = |\theta|^2$  between -1 and 1
- Right:  $f(\theta) = |\theta|^4$  between -1 and 1
- $\bullet$  affine outside of [-1,1], continuously differentiable.

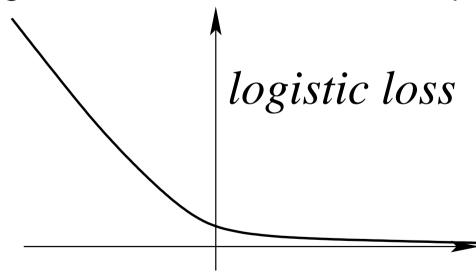


# Convex stochastic approximation Existing work

- Known global minimax rates of convergence for non-smooth problems (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
  - Strongly convex:  $O((\mu n)^{-1})$ Attained by averaged stochastic gradient descent with  $\gamma_n \propto (\mu n)^{-1}$
  - Non-strongly convex:  $O(n^{-1/2})$  Attained by averaged stochastic gradient descent with  $\gamma_n \propto n^{-1/2}$
- Asymptotic analysis of averaging (Polyak and Juditsky, 1992;
   Ruppert, 1988)
  - All step sizes  $\gamma_n=Cn^{-\alpha}$  with  $\alpha\in(1/2,1)$  lead to  $O(n^{-1})$  for smooth strongly convex problems
- A single adaptive algorithm for smooth problems with convergence rate  $O(\min\{1/\mu n, 1/\sqrt{n}\})$  in all situations?

- Logistic regression:  $(\Phi(x_n), y_n) \in \mathbb{R}^d \times \{-1, 1\}$ 
  - Single data point:  $f_n(\theta) = \log(1 + \exp(-y_n \theta^{\top} \Phi(x_n)))$
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  - with R = radius of data (Bach, 2013):

$$\mathbb{E}f(\bar{\theta}_n) - f(\theta_*) \leqslant \min\left\{\frac{1}{\sqrt{n}}, \frac{R^2}{n\mu}\right\} \left(15 + 5R\|\theta_0 - \theta_*\|\right)^4$$

Proof based on self-concordance (Nesterov and Nemirovski, 1994)

#### **Self-concordance**

- Usual definition for convex  $\varphi : \mathbb{R} \to \mathbb{R}$ :  $|\varphi'''(t)| \leq 2\varphi''(t)^{3/2}$ 
  - Affine invariant
  - Extendable to all convex functions on  $\mathbb{R}^d$  by looking at rays
  - Used for the sharp proof of quadratic convergence of Newton method (Nesterov and Nemirovski, 1994)
- Generalized notion:  $|\varphi'''(t)| \leqslant \varphi''(t)$ 
  - Applicable to logistic regression (with extensions)
  - $-\varphi(t) = \log(1 + e^{-t}), \ \varphi'(t) = (1 + e^{t})^{-1}, \ \text{etc...}$
- Important properties
  - Allows global Taylor expansions
  - Relates expansions of derivatives of different orders

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– A single adaptive algorithm for smooth problems with convergence rate O(1/n) in all situations?

## Least-mean-square algorithm

- Least-squares:  $f(\theta) = \frac{1}{2}\mathbb{E}\big[(y_n \langle \Phi(x_n), \theta \rangle)^2\big]$  with  $\theta \in \mathbb{R}^d$ 
  - SGD = least-mean-square algorithm (see, e.g., Macchi, 1995)
  - usually studied without averaging and decreasing step-sizes
  - with strong convexity assumption  $\mathbb{E}\big[\Phi(x_n)\otimes\Phi(x_n)\big]=H\succcurlyeq\mu\cdot\mathrm{Id}$

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- New analysis for averaging and constant step-size  $\gamma = 1/(4R^2)$ 
  - Assume  $\|\Phi(x_n)\| \leqslant R$  and  $|y_n \langle \Phi(x_n), \theta_* \rangle| \leqslant \sigma$  almost surely
  - No assumption regarding lowest eigenvalues of H
  - Main result:  $\left| \mathbb{E} f(\bar{\theta}_{n-1}) f(\theta_*) \leqslant \frac{4\sigma^2 d}{n} + \frac{4R^2 \|\theta_0 \theta_*\|^2}{n} \right|$
- Matches statistical lower bound (Tsybakov, 2003)
  - Non-asymptotic robust version of Györfi and Walk (1996)

## Least-squares - Proof technique - I

• LMS recursion:

$$\theta_n - \theta_* = [I - \gamma \Phi(x_n) \otimes \Phi(x_n)](\theta_{n-1} - \theta_*) + \gamma \varepsilon_n \Phi(x_n)$$

• Simplified LMS recursion: with  $H = \mathbb{E} \big[ \Phi(x_n) \otimes \Phi(x_n) \big]$ 

$$\theta_n - \theta_* = [I - \gamma \mathbf{H}](\theta_{n-1} - \theta_*) + \gamma \varepsilon_n \Phi(x_n)$$

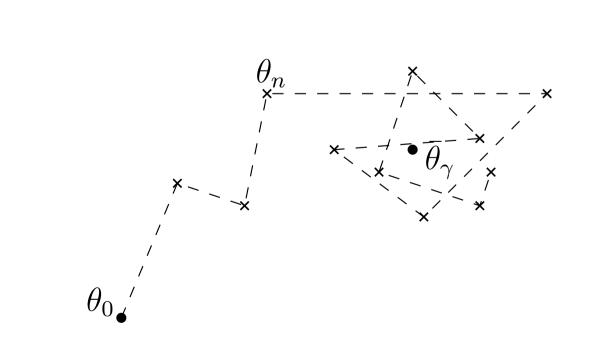
- Direct proof technique of Polyak and Juditsky (1992), e.g.,

$$\theta_n - \theta_* = \left[I - \gamma \mathbf{H}\right]^n (\theta_0 - \theta_*) + \gamma \sum_{k=1}^n \left[I - \gamma \mathbf{H}\right]^{n-k} \varepsilon_k \Phi(x_k)$$

 $\bullet$  Infinite expansion of Aguech, Moulines, and Priouret (2000) in powers of  $\gamma$ 

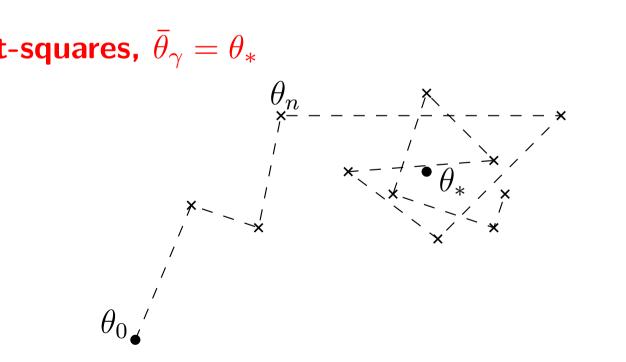
$$\theta_n = \theta_{n-1} - \gamma (\langle \Phi(x_n), \theta_{n-1} \rangle - y_n) \Phi(x_n)$$

- The sequence  $(\theta_n)_n$  is a homogeneous Markov chain
  - convergence to a stationary distribution  $\pi_{\gamma}$
  - with expectation  $\bar{\theta}_{\gamma} \stackrel{\text{def}}{=} \int \theta \pi_{\gamma}(\mathrm{d}\theta)$



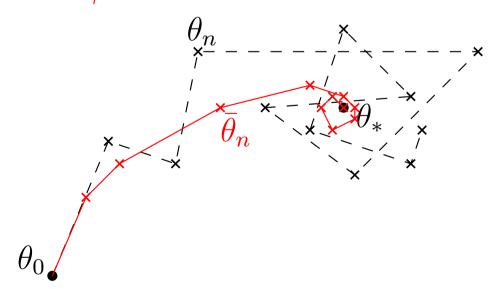
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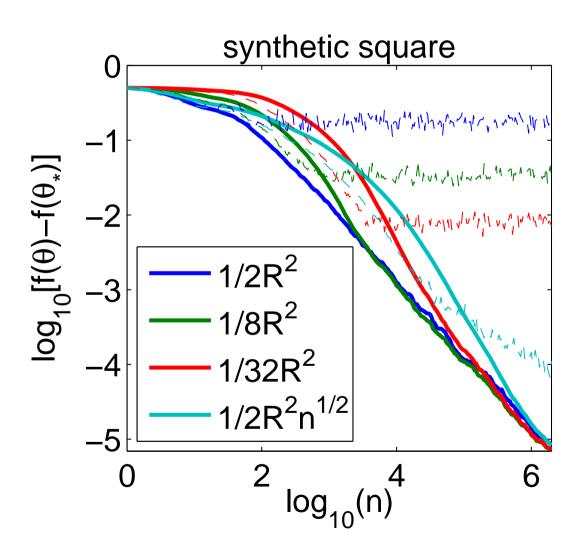


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  - $\theta_n$  does not converge to  $\theta_*$  but oscillates around it
  - oscillations of order  $\sqrt{\gamma}$
- Ergodic theorem:
  - Averaged iterates converge to  $ar{ heta}_{\gamma}= heta_*$  at rate O(1/n)

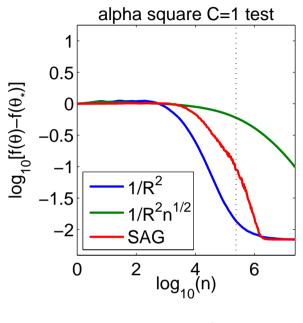
# Simulations - synthetic examples

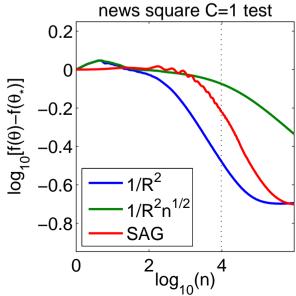
ullet Gaussian distributions - d=20

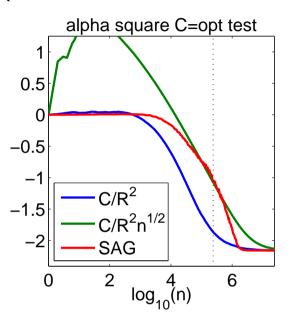


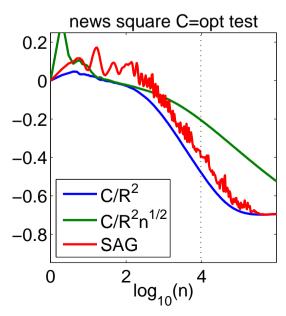
#### **Simulations - benchmarks**

• alpha (d = 500, n = 500 000), news (d = 1 300 000, n = 20 000)









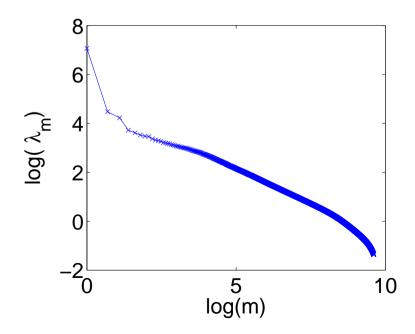
## **Optimal bounds for least-squares?**

- **Least-squares**: cannot beat  $\sigma^2 d/n$  (Tsybakov, 2003). Really?
  - What if  $d \gg n$ ?
- Refined assumptions with adaptivity (Dieuleveut and Bach, 2014)
  - Beyond strong convexity or lack thereof

# Finer assumptions (Dieuleveut and Bach, 2014)

#### • Covariance eigenvalues

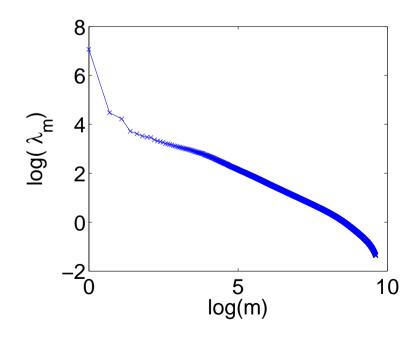
- Pessimistic assumption: all eigenvalues  $\lambda_m$  less than a constant
- Actual decay as  $\lambda_m = o(m^{-\alpha})$  with  $\operatorname{tr} H^{1/\alpha} = \sum_m \lambda_m^{1/\alpha}$  small

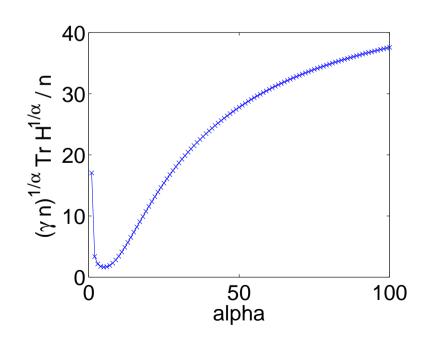


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#### Optimal predictor

- Pessimistic assumption:  $\|\theta_0 \theta_*\|^2$  finite
- Finer assumption:  $||H^{1/2-r}(\theta_0-\theta_*)||_2$  small
- $\ \text{Replace} \ \frac{\|\theta_0 \theta_*\|^2}{\gamma n} \ \text{by} \ \frac{4\|H^{1/2-r}(\theta_0 \theta_*)\|_2}{\gamma^{2r} n^{2\min\{r,1\}}}$

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$$f(\bar{\theta}_n) - f(\theta_*) \leqslant \frac{16\sigma^2 \operatorname{tr} H^{1/\alpha}}{n} (\gamma n)^{1/\alpha} + \frac{4\|H^{1/2 - r}(\theta_0 - \theta_*)\|_2}{\gamma^{2r} n^{2\min\{r, 1\}}}$$

- Previous results:  $\alpha = +\infty$  and r = 1/2
- Valid for all lpha and r
- Optimal step-size potentially decaying with n
- Extension to non-parametric estimation (kernels) with optimal rates

## From least-squares to non-parametric estimation - I

• Extension to Hilbert spaces:  $\Phi(x), \theta \in \mathcal{H}$ 

$$\theta_n = \theta_{n-1} - \gamma (\langle \Phi(x_n), \theta_{n-1} \rangle - y_n) \Phi(x_n)$$

• If  $\theta_0 = 0$ ,  $\theta_n$  is a linear combination of  $\Phi(x_1), \ldots, \Phi(x_n)$ 

$$\theta_n = \sum_{k=1}^n \alpha_k \Phi(x_k) \quad \text{and} \quad \alpha_n = -\gamma \sum_{k=1}^{n-1} \alpha_k \langle \Phi(x_k), \Phi(x_n) \rangle + \gamma y_n$$

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- Kernel trick:  $k(x, x') = \langle \Phi(x), \Phi(x') \rangle$ 
  - Reproducing kernel Hilbert spaces and non-parametric estimation
  - See, e.g., Schölkopf and Smola (2001); Shawe-Taylor and Cristianini (2004); Dieuleveut and Bach (2014)
  - Still  $O(n^2)$

## From least-squares to non-parametric estimation - II

- Simple example: Sobolev space on  $\mathcal{X} = [0, 1]$ 
  - $-\Phi(x) =$  weighted Fourier basis  $\Phi(x)_j = \varphi_j \cos(2j\pi x)$  (plus sine)
  - kernel  $k(x, x') = \sum_{j} \varphi_{j}^{2} \cos \left[2j\pi(x x')\right]$
  - Optimal prediction function  $\theta_*$  has norm  $\|\theta_*\|^2 = \sum_i |\mathcal{F}(\theta_*)_j|^2 \varphi_j^{-2}$
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## From least-squares to non-parametric estimation - II

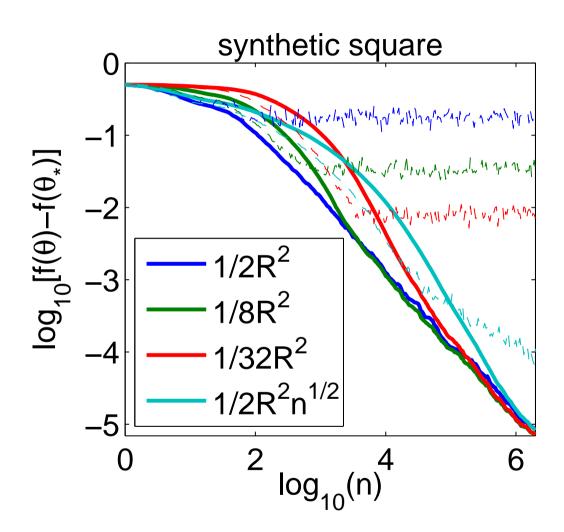
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  - Optimal prediction function  $\theta_*$  has norm  $\|\theta_*\|^2 = \sum_i |\mathcal{F}(\theta_*)_j|^2 \varphi_i^{-2}$
  - Depending on smoothness, may or may not be finite
- Adapted norm  $||H^{1/2-r}\theta_*||^2 = \sum_j |\mathcal{F}(\theta_*)_j|^2 \varphi_j^{-4r}$  may be finite

$$f(\bar{\theta}_n) - f(\theta_*) \leqslant \frac{16\sigma^2 \operatorname{tr} H^{1/\alpha}}{n} (\gamma n)^{1/\alpha} + \frac{4\|H^{1/2-r}(\theta_0 - \theta_*)\|_2}{\gamma^{2r} n^{2\min\{r,1\}}}$$

ullet Same effect than  $\ell_2$ -regularization with weight  $\lambda$  equal to  $\frac{1}{\gamma n}$ 

# Simulations - synthetic examples

ullet Gaussian distributions - d=20



ullet Explaining actual behavior for all n

# Bias-variance decomposition (Défossez and Bach, 2015)

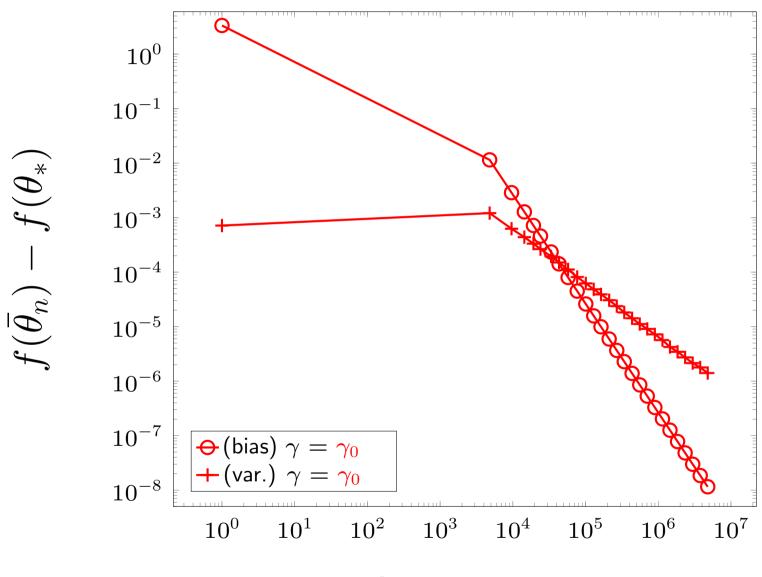
- Simplification: dominating (but exact) term when  $n \to \infty$  and  $\gamma \to 0$
- Variance (e.g., starting from the solution)

$$f(\bar{\theta}_n) - f(\theta_*) \sim \frac{1}{n} \mathbb{E} \left[ \varepsilon^2 \Phi(x)^\top H^{-1} \Phi(x) \right]$$

- NB: if noise  $\varepsilon$  is independent, then we obtain  $\frac{d\sigma^2}{n}$
- Exponentially decaying remainder terms (strongly convex problems)
- Bias (e.g., no noise)

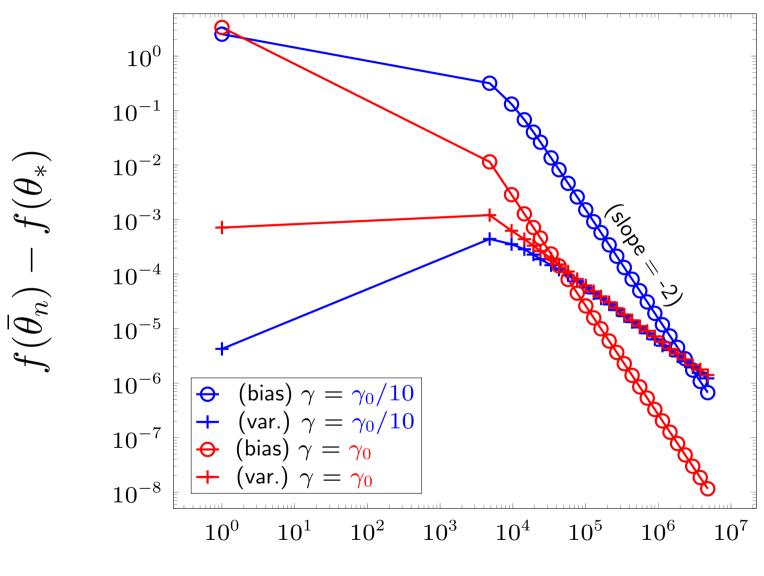
$$f(\bar{\theta}_n) - f(\theta_*) \sim \frac{1}{n^2 \gamma^2} (\theta_0 - \theta_*)^\top H^{-1} (\theta_0 - \theta_*)$$

# Bias-variance decomposition (synthetic data d=25)



Iteration n

# Bias-variance decomposition (synthetic data d=25)



Iteration n

Sampling from a different distribution with importance weights

$$\mathbb{E}_{\boldsymbol{p}(\boldsymbol{x})\boldsymbol{p}(\boldsymbol{y}|\boldsymbol{x})}|\boldsymbol{y} - \boldsymbol{\Phi}(\boldsymbol{x})^{\top}\boldsymbol{\theta}|^{2} = \mathbb{E}_{\boldsymbol{q}(\boldsymbol{x})\boldsymbol{p}(\boldsymbol{y}|\boldsymbol{x})}\frac{d\boldsymbol{p}(\boldsymbol{x})}{d\boldsymbol{q}(\boldsymbol{x})}|\boldsymbol{y} - \boldsymbol{\Phi}(\boldsymbol{x})^{\top}\boldsymbol{\theta}|^{2}$$

- Recursion:  $\theta_n = \theta_{n-1} - \gamma \frac{dp(x_n)}{dq(x_n)} (\Phi(x_n)^{\top} \theta_{n-1} - y_n) \Phi(x_n)$ 

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- Specific to least-squares =  $\mathbb{E}_{q(x)p(y|x)} \left| \sqrt{\frac{dp(x)}{dq(x)}} y \sqrt{\frac{dp(x)}{dq(x)}} \Phi(x)^{\top} \theta \right|^2$
- Reweighting of the data: same bounds apply!

• Sampling from a different distribution with importance weights

$$\mathbb{E}_{\mathbf{p}(\mathbf{x})p(y|x)}|y - \Phi(x)^{\top}\theta|^2 = \mathbb{E}_{\mathbf{q}(\mathbf{x})p(y|x)}\frac{dp(x)}{dq(x)}|y - \Phi(x)^{\top}\theta|^2$$

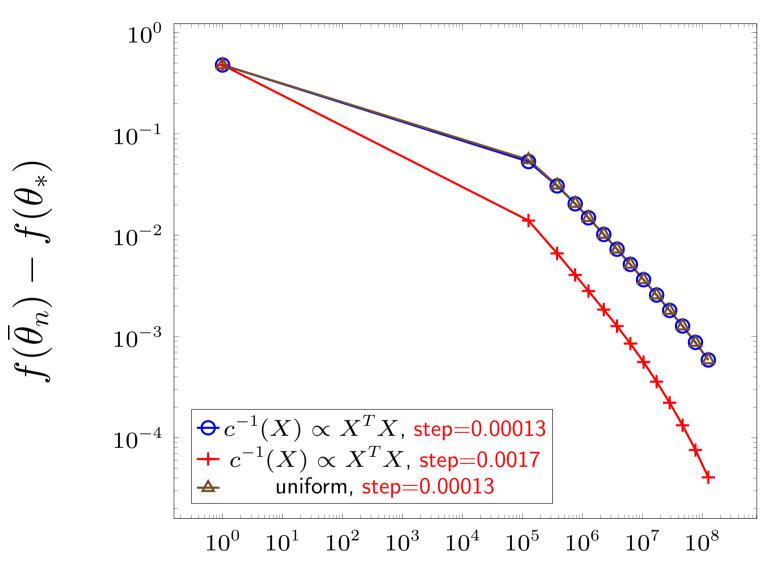
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- Reweighting of the data: same bounds apply!
- Optimal for variance:  $\frac{dq(x)}{dp(x)} \propto \sqrt{\Phi(x)^{\top} H^{-1} \Phi(x)}$ 
  - Same density as active learning (Kanamori and Shimodaira, 2003)
  - Limited gains: different between first and second moments
  - Caveat: need to know H

• Sampling from a different distribution with importance weights

$$\mathbb{E}_{\mathbf{p}(\mathbf{x})p(y|x)}|y - \Phi(x)^{\top}\theta|^2 = \mathbb{E}_{\mathbf{q}(\mathbf{x})p(y|x)}\frac{dp(x)}{dq(x)}|y - \Phi(x)^{\top}\theta|^2$$

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- Reweighting of the data: same bounds apply!
- Optimal for bias:  $\frac{dq(x)}{dp(x)} \propto \|\Phi(x)\|^2$ 
  - Simpy allows biggest possible step size  $\gamma < \frac{2}{\operatorname{tr} H}$
  - Large gains in practice
  - Corresponds to normalized least-mean-squares

# Convergence on Sido dataset (d = 4932)



Iteration n

Current results with averaged SGD

- Variance (starting from optimal 
$$\theta_*$$
) =  $\frac{\sigma^2 d}{n}$ 

- Bias (no noise) = 
$$\min \left\{ \frac{R^2 \|\theta_0 - \theta_*\|^2}{n}, \frac{R^4 \langle \theta_0 - \theta_*, \frac{H^{-1}(\theta_0 - \theta_*) \rangle}{n^2} \right\}$$

• Current results with averaged SGD (ill-conditioned problems)

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	Bias	Variance
Averaged gradient descent	2	0
(Bach and Moulines, 2013)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n}$	$\frac{\sigma^2 d}{n}$

	Bias	Variance
Averaged gradient descent		
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Averaged gradient descent		
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Accelerated gradient descent		
(Nesterov, 1983)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n^2}$	$\sigma^2 d$

- Acceleration is notoriously non-robust to noise (d'Aspremont, 2008; Schmidt et al., 2011)
  - For non-structured noise, see Lan (2012)

	Bias	Variance
Averaged gradient descent		
(Bach and Moulines, 2013)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n}$	$\frac{\sigma^2 d}{n}$
Accelerated gradient descent		
(Nesterov, 1983)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n^2}$	$\sigma^2 d$
"Between" averaging and acceleration		
(Flammarion and Bach, 2015)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n^{1+\alpha}}$	$\frac{\sigma^2 d}{n^{1-\alpha}}$

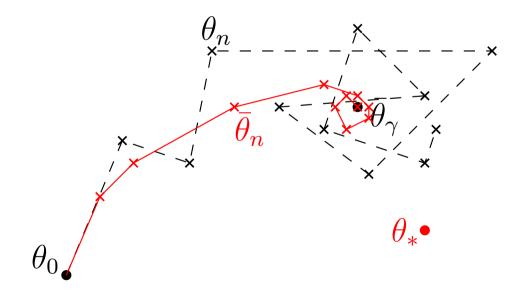
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Averaging and acceleration		
(Dieuleveut, Flammarion, and Bach, 2016)	$\frac{R^2 \ \theta_0 - \theta_*\ ^2}{n^2}$	$\frac{\sigma^2 d}{n}$

## Beyond least-squares - Markov chain interpretation

- Recursion  $\theta_n = \theta_{n-1} \gamma f_n'(\theta_{n-1})$  also defines a Markov chain
  - Stationary distribution  $\pi_{\gamma}$  such that  $\int f'(\theta)\pi_{\gamma}(\mathrm{d}\theta)=0$
  - When f' is not linear,  $f'(\int \theta \pi_{\gamma}(d\theta)) \neq \int f'(\theta) \pi_{\gamma}(d\theta) = 0$

## Beyond least-squares - Markov chain interpretation

- Recursion  $\theta_n = \theta_{n-1} \gamma f_n'(\theta_{n-1})$  also defines a Markov chain
  - Stationary distribution  $\pi_{\gamma}$  such that  $\int f'(\theta)\pi_{\gamma}(\mathrm{d}\theta)=0$
  - When f' is not linear,  $f'(\int \theta \pi_{\gamma}(d\theta)) \neq \int f'(\theta) \pi_{\gamma}(d\theta) = 0$
- $\theta_n$  oscillates around the wrong value  $\bar{\theta}_{\gamma} \neq \theta_*$



## Beyond least-squares - Markov chain interpretation

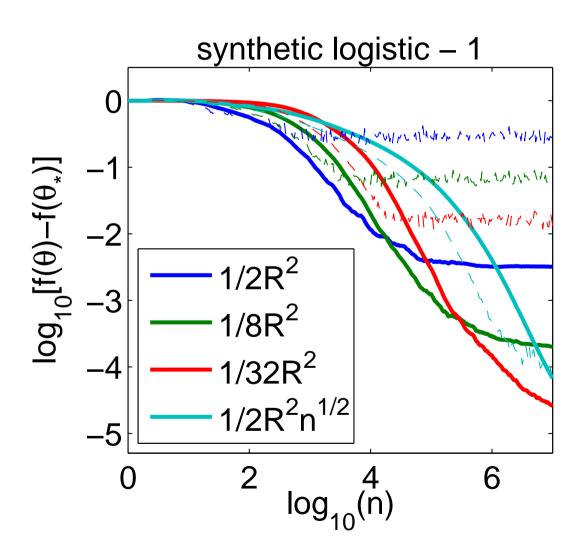
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  - Stationary distribution  $\pi_{\gamma}$  such that  $\int f'(\theta)\pi_{\gamma}(\mathrm{d}\theta)=0$
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- $\theta_n$  oscillates around the wrong value  $\bar{\theta}_{\gamma} \neq \theta_*$ 
  - moreover,  $\|\theta_* \theta_n\| = O_p(\sqrt{\gamma})$
  - Linear convergence up to the noise level for strongly-convex problems (Nedic and Bertsekas, 2000)

#### Ergodic theorem

- averaged iterates converge to  $\bar{\theta}_{\gamma} \neq \theta_{*}$  at rate O(1/n)
- moreover,  $\|\theta_* \overline{\theta}_{\gamma}\| = O(\gamma)$  (Bach, 2013)

## **Simulations - synthetic examples**

ullet Gaussian distributions - d=20



#### Known facts

- 1. Averaged SGD with  $\gamma_n \propto n^{-1/2}$  leads to *robust* rate  $O(n^{-1/2})$  for all convex functions
- 2. Averaged SGD with  $\gamma_n$  constant leads to *robust* rate  $O(n^{-1})$  for all convex *quadratic* functions
- 3. Newton's method squares the error at each iteration for smooth functions
- 4. A single step of Newton's method is equivalent to minimizing the quadratic Taylor expansion

#### Known facts

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- 3. Newton's method squares the error at each iteration for smooth functions  $\Rightarrow O((n^{-1/2})^2)$
- 4. A single step of Newton's method is equivalent to minimizing the quadratic Taylor expansion

#### Online Newton step

- Rate:  $O((n^{-1/2})^2 + n^{-1}) = O(n^{-1})$
- Complexity: O(d) per iteration

• The Newton step for  $f=\mathbb{E} f_n(\theta)\stackrel{\mathrm{def}}{=}\mathbb{E} \big[\ell(y_n,\langle\theta,\Phi(x_n)\rangle)\big]$  at  $\tilde{\theta}$  is equivalent to minimizing the quadratic approximation

$$g(\theta) = f(\tilde{\theta}) + \langle f'(\tilde{\theta}), \theta - \tilde{\theta} \rangle + \frac{1}{2} \langle \theta - \tilde{\theta}, f''(\tilde{\theta})(\theta - \tilde{\theta}) \rangle$$

$$= f(\tilde{\theta}) + \langle \mathbb{E}f'_n(\tilde{\theta}), \theta - \tilde{\theta} \rangle + \frac{1}{2} \langle \theta - \tilde{\theta}, \mathbb{E}f''_n(\tilde{\theta})(\theta - \tilde{\theta}) \rangle$$

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ullet Complexity of least-mean-square recursion for g is O(d)

$$\theta_n = \theta_{n-1} - \gamma \left[ f'_n(\tilde{\theta}) + f''_n(\tilde{\theta})(\theta_{n-1} - \tilde{\theta}) \right]$$

- $-f_n''(\tilde{\theta}) = \ell''(y_n, \langle \tilde{\theta}, \Phi(x_n) \rangle) \Phi(x_n) \otimes \Phi(x_n)$  has rank one
- New online Newton step without computing/inverting Hessians

## Choice of support point for online Newton step

#### Two-stage procedure

- (1) Run n/2 iterations of averaged SGD to obtain  $\tilde{\theta}$
- (2) Run n/2 iterations of averaged constant step-size LMS
  - Reminiscent of one-step estimators (see, e.g., Van der Vaart, 2000)
  - Provable convergence rate of O(d/n) for logistic regression
  - Additional assumptions but no strong convexity

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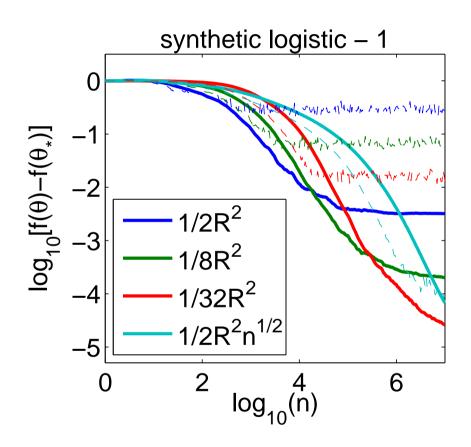
#### Update at each iteration using the current averaged iterate

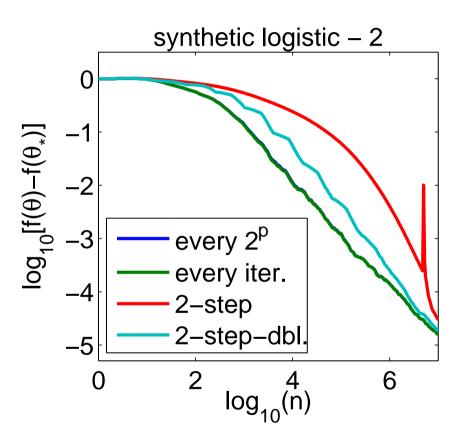
- Recursion: 
$$\theta_n = \theta_{n-1} - \gamma \left[ f_n'(\bar{\theta}_{n-1}) + f_n''(\bar{\theta}_{n-1})(\theta_{n-1} - \bar{\theta}_{n-1}) \right]$$

- No provable convergence rate (yet) but best practical behavior
- Note (dis)similarity with regular SGD:  $\theta_n = \theta_{n-1} \gamma f'_n(\theta_{n-1})$

## **Simulations - synthetic examples**

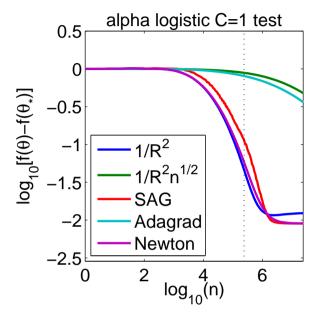
• Gaussian distributions - d=20

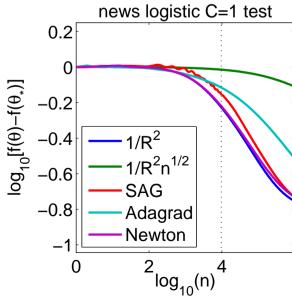


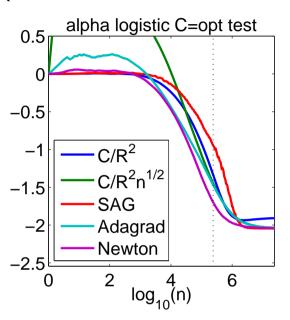


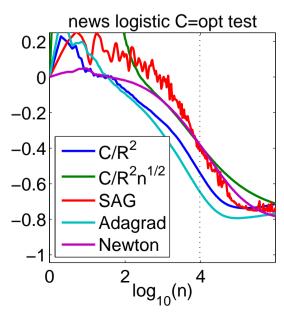
## **Simulations - benchmarks**

• alpha (d = 500, n = 500 000), news (d = 1 300 000, n = 20 000)









## **Summary of rates of convergence**

- Problem parameters
  - D diameter of the domain
  - -B Lipschitz-constant
  - -L smoothness constant
  - $\mu$  strong convexity constant

	convex	strongly convex
nonsmooth	deterministic: $BD/\sqrt{t}$	deterministic: $B^2/(t\mu)$
	stochastic: $BD/\sqrt{n}$	stochastic: $B^2/(n\mu)$
smooth	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
	stochastic: $LD^2/\sqrt{n}$	stochastic: $L/(n\mu)$
quadratic	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
	stochastic: $d/n + LD^2/n$	stochastic: $d/n + LD^2/n$

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	stochastic: $LD^2/\sqrt{n}$	stochastic: $L/(n\mu)$
	finite sum: $n/t$	finite sum: $\exp(-\min\{1/n, \mu/L\}t)$
quadratic	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
	stochastic: $d/n + LD^2/n$	stochastic: $d/n + LD^2/n$

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#### 2. Classical methods for convex optimization

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- Non-smooth optimization (subgradient descent)

## 3. Classical stochastic approximation (not covered)

• Robbins-Monro algorithm (1951)

#### **Outline** - II

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## Going beyond a single pass over the data

### • Stochastic approximation

- Assumes infinite data stream
- Observations are used only once
- Directly minimizes testing cost  $\mathbb{E}_{(x,y)} \ell(y, \theta^{\top} \Phi(x))$

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#### Machine learning practice

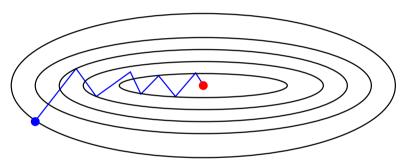
- Finite data set  $(x_1, y_1, \ldots, x_n, y_n)$
- Multiple passes
- Minimizes training cost  $\frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^{\top} \Phi(x_i))$
- Need to regularize (e.g., by the  $\ell_2$ -norm) to avoid overfitting

• Goal: minimize 
$$g(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)$$

- Minimizing  $g(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$  with  $f_i(\theta) = \ell \big( y_i, \theta^\top \Phi(x_i) \big) + \mu \Omega(\theta)$
- Batch gradient descent:  $\theta_t = \theta_{t-1} \gamma_t g'(\theta_{t-1}) = \theta_{t-1} \frac{\gamma_t}{n} \sum_{i=1}^n f_i'(\theta_{t-1})$ 
  - Linear (e.g., exponential) convergence rate in  $O(e^{-\alpha t})$
  - Iteration complexity is linear in n (with line search)

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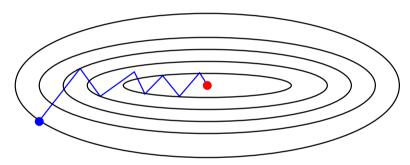


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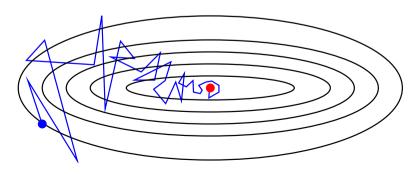
- Stochastic gradient descent:  $\theta_t = \theta_{t-1} \gamma_t f'_{i(t)}(\theta_{t-1})$ 
  - Sampling with replacement: i(t) random element of  $\{1,\ldots,n\}$
  - Convergence rate in O(1/t)
  - Iteration complexity is independent of n (step size selection?)

• Minimizing 
$$g(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$$
 with  $f_i(\theta) = \ell \left( y_i, \theta^\top \Phi(x_i) \right) + \mu \Omega(\theta)$ 

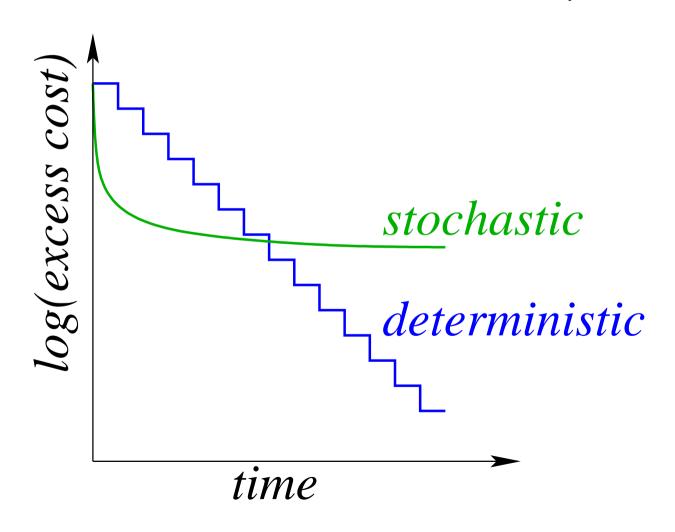
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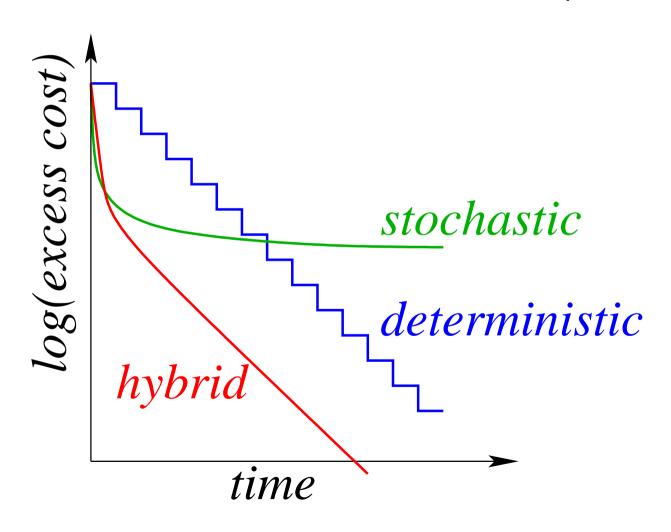
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 $\bullet$  Goal = best of both worlds: Linear rate with O(1) iteration cost Robustness to step size



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# Stochastic average gradient (Le Roux, Schmidt, and Bach, 2012)

- Stochastic average gradient (SAG) iteration
  - Keep in memory the gradients of all functions  $f_i$ ,  $i = 1, \ldots, n$
  - Random selection  $i(t) \in \{1, \dots, n\}$  with replacement
  - $\text{ Iteration: } \theta_t = \theta_{t-1} \frac{\gamma_t}{n} \sum_{i=1}^n y_i^t \text{ with } y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$

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- Stochastic version of incremental average gradient (Blatt et al., 2008)
- Extra memory requirement
  - Supervised machine learning
    - If  $f_i(\theta) = \ell_i(y_i, \Phi(x_i)^\top \theta)$ , then  $f_i'(\theta) = \ell_i'(y_i, \Phi(x_i)^\top \theta) \Phi(x_i)$
    - Only need to store n real numbers

## Stochastic average gradient - Convergence analysis

#### Assumptions

- Each  $f_i$  is  $R^2$ -smooth,  $i = 1, \ldots, n$
- $-g = \frac{1}{n} \sum_{i=1}^{n} f_i$  is  $\mu$ -strongly convex (with potentially  $\mu = 0$ )
- constant step size  $\gamma_t = 1/(16R^2)$
- initialization with one pass of averaged SGD

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- initialization with one pass of averaged SGD
- Strongly convex case (Le Roux et al., 2012, 2013)

$$\mathbb{E}\big[g(\theta_t) - g(\theta_*)\big] \leqslant \left(\frac{8\sigma^2}{n\mu} + \frac{4R^2\|\theta_0 - \theta_*\|^2}{n}\right) \exp\left(-t \min\left\{\frac{1}{8n}, \frac{\mu}{16R^2}\right\}\right)$$

- Linear (exponential) convergence rate with O(1) iteration cost
- After one pass, reduction of cost by  $\exp\left(-\min\left\{\frac{1}{8},\frac{n\mu}{16R^2}\right\}\right)$

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- Non-strongly convex case (Le Roux et al., 2013)

$$\mathbb{E}\left[g(\theta_t) - g(\theta_*)\right] \leqslant 48 \frac{\sigma^2 + R^2 \|\theta_0 - \theta_*\|^2}{\sqrt{n}} \frac{n}{t}$$

- Improvement over regular batch and stochastic gradient
- Adaptivity to potentially hidden strong convexity

## Convergence analysis - Proof sketch

- Main step: find "good" Lyapunov function  $J(\theta_t, y_1^t, \dots, y_n^t)$ 
  - such that  $\mathbb{E}[J(\theta_t, y_1^t, \dots, y_n^t) | \mathcal{F}_{t-1}] < J(\theta_{t-1}, y_1^{t-1}, \dots, y_n^{t-1})$
  - no natural candidates

### Computer-aided proof

- Parameterize function  $J(\theta_t, y_1^t, \dots, y_n^t) = g(\theta_t) g(\theta_*) + \text{quadratic}$
- Solve semidefinite program to obtain candidates (that depend on  $n,\mu,L$ )
- Check validity with symbolic computations

## Rate of convergence comparison

- Assume that L=100,  $\mu=.01$ , and n=80000 ( $L\neq R^2$ )
  - Full gradient method has rate

$$\left(1 - \frac{\mu}{L}\right) = 0.9999$$

Accelerated gradient method has rate

$$(1 - \sqrt{\frac{\mu}{L}}) = 0.9900$$

- Running n iterations of SAG for the same cost has rate

$$\left(1 - \frac{1}{8n}\right)^n = 0.8825$$

- Fastest possible first-order method has rate

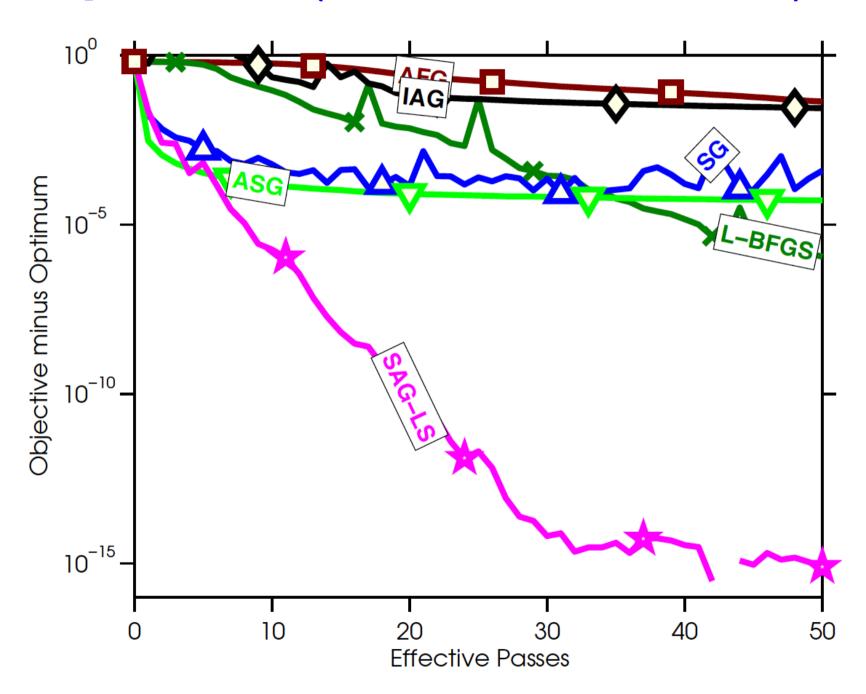
$$\left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^2 = 0.9608$$

- Beating two lower bounds (with additional assumptions)
  - (1) stochastic gradient and (2) full gradient

## Stochastic average gradient Implementation details and extensions

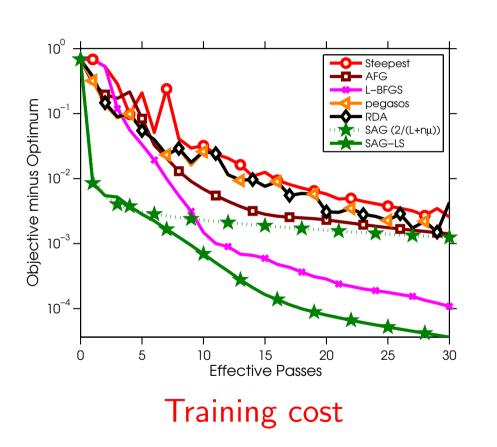
- The algorithm can use sparsity in the features to reduce the storage and iteration cost
- Grouping functions together can further reduce the memory requirement
- ullet We have obtained good performance when  $R^2$  is not known with a heuristic line-search
- Algorithm allows non-uniform sampling
- Possibility of making proximal, coordinate-wise, and Newton-like variants

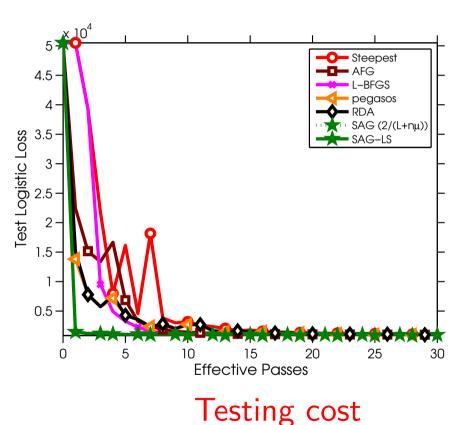
## spam dataset (n = 92 189, d = 823 470)



## protein dataset (n = 145751, d = 74)

Dataset split in two (training/testing)





#### **Extensions and related work**

- Exponential convergence rate for strongly convex problems
- Need to store gradients
  - SVRG (Johnson and Zhang, 2013)
- Adaptivity to non-strong convexity
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014)
- Simple proof
  - SVRG, SAGA, random coordinate descent (Nesterov, 2012; Shalev-Shwartz and Zhang, 2012)
- Lower bounds
  - Agarwal and Bottou (2014)

#### Variance reduction

ullet Principle: reducing variance of sample of X by using a sample from another random variable Y with known expectation

$$Z_{\alpha} = \alpha(X - Y) + \mathbb{E}Y$$

- $-\mathbb{E}Z_{\alpha} = \alpha \mathbb{E}X + (1 \alpha)\mathbb{E}Y$
- $-\operatorname{var} Z_{\alpha} = \alpha^{2} \left[\operatorname{var} X + \operatorname{var} Y 2\operatorname{cov}(X, Y)\right]$
- $-\alpha=1$ : no bias,  $\alpha<1$ : potential bias (but reduced variance)
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- Useful if Y positively correlated with X
- Application to gradient estimation : SVRG (Johnson and Zhang, 2013)
  - Estimating the averaged gradient  $g'(\theta) = \frac{1}{n} \sum_{i=1}^{n} f'_i(\theta)$
  - Using the gradients of a previous iterate  $\theta$

## Stochastic variance reduced gradient (SVRG)

- Algorithm divide into "epochs"
- ullet At each epoch, starting from  $heta_0 = ilde{ heta}$ , perform the iteration
  - Sample  $i_t$  uniformly at random
  - Gradient step:  $\theta_t = \theta_{t-1} \gamma \left[ f'_{i_t}(\theta_{t-1}) f'_{i_t}(\tilde{\theta}) + g'(\tilde{\theta}) \right]$
- **Proposition**: If each  $f_i$  is  $R^2$ -smooth and  $g = \frac{1}{n} \sum_{i=1}^n f_i$  is  $\mu$ -strongly convex, then after  $k = 20R^2/\mu$  steps and with  $\gamma = 1/10R^2$ , then  $f(\theta) f(\theta_*)$  is reduced by 10%

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## Subgradient descent for machine learning

- Assumptions (f is the expected risk,  $\hat{f}$  the empirical risk)
  - "Linear" predictors:  $\theta(x) = \theta^{\top} \Phi(x)$ , with  $\|\Phi(x)\|_2 \leqslant R$  a.s.
  - $-\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \Phi(x_i)^{\top} \theta)$
  - G-Lipschitz loss: f and  $\hat{f}$  are GR-Lipschitz on  $\Theta = \{\|\theta\|_2 \leqslant D\}$
- ullet Statistics: with probability greater than  $1-\delta$

$$\sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| \leqslant \frac{GRD}{\sqrt{n}} \left[ 2 + \sqrt{2 \log \frac{2}{\delta}} \right]$$

• Optimization: after t iterations of subgradient method

$$\hat{f}(\hat{\theta}) - \min_{\eta \in \Theta} \hat{f}(\eta) \leqslant \frac{GRD}{\sqrt{t}}$$

• t=n iterations, with total running-time complexity of  $O(n^2d)$ 

## Stochastic subgradient "descent"/method

## Assumptions

- $f_n$  convex and B-Lipschitz-continuous on  $\{\|\theta\|_2 \leq D\}$
- $(f_n)$  i.i.d. functions such that  $\mathbb{E} f_n = f$
- $\theta_*$  global optimum of f on  $\{\|\theta\|_2 \leq D\}$
- Algorithm:  $\theta_n = \Pi_D \left( \theta_{n-1} \frac{2D}{B\sqrt{n}} f_n'(\theta_{n-1}) \right)$
- Bound:

$$\mathbb{E}f\left(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\right) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$$

- "Same" three-line proof as in the deterministic case
- Minimax rate (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
- Running-time complexity: O(dn) after n iterations

## Summary of new results (Bach and Moulines, 2011)

• Stochastic gradient descent with learning rate  $\gamma_n = C n^{-\alpha}$ 

## Strongly convex smooth objective functions

- Old:  $O(n^{-1})$  rate achieved without averaging for  $\alpha = 1$
- New:  $O(n^{-1})$  rate achieved with averaging for  $\alpha \in [1/2, 1]$
- Non-asymptotic analysis with explicit constants
- Forgetting of initial conditions
- Robustness to the choice of C
- Convergence rates for  $\mathbb{E}\|\theta_n-\theta_*\|^2$  and  $\mathbb{E}\|\bar{\theta}_n-\theta_*\|^2$ 
  - no averaging:  $O\left(\frac{\sigma^2 \gamma_n}{\mu}\right) + O(e^{-\mu n \gamma_n}) \|\theta_0 \theta_*\|^2$
  - $-\text{ averaging: } \frac{\operatorname{tr} H(\theta_*)^{-1}}{n} + \mu^{-1} O(n^{-2\alpha} + n^{-2+\alpha}) + O\Big(\frac{\|\theta_0 \theta_*\|^2}{\mu^2 n^2}\Big)$

## Least-mean-square algorithm

- Least-squares:  $f(\theta) = \frac{1}{2}\mathbb{E}\big[(y_n \langle \Phi(x_n), \theta \rangle)^2\big]$  with  $\theta \in \mathbb{R}^d$ 
  - SGD = least-mean-square algorithm (see, e.g., Macchi, 1995)
  - usually studied without averaging and decreasing step-sizes
  - with strong convexity assumption  $\mathbb{E}\big[\Phi(x_n)\otimes\Phi(x_n)\big]=H\succcurlyeq\mu\cdot\mathrm{Id}$
- New analysis for averaging and constant step-size  $\gamma = 1/(4R^2)$ 
  - Assume  $\|\Phi(x_n)\| \leqslant R$  and  $|y_n \langle \Phi(x_n), \theta_* \rangle| \leqslant \sigma$  almost surely
  - No assumption regarding lowest eigenvalues of H
  - Main result:  $\left| \mathbb{E} f(\bar{\theta}_{n-1}) f(\theta_*) \leqslant \frac{4\sigma^2 d}{n} + \frac{4R^2 \|\theta_0 \theta_*\|^2}{n} \right|$
- Matches statistical lower bound (Tsybakov, 2003)
  - Non-asymptotic robust version of Györfi and Walk (1996)

## Choice of support point for online Newton step

### Two-stage procedure

- (1) Run n/2 iterations of averaged SGD to obtain  $\tilde{\theta}$
- (2) Run n/2 iterations of averaged constant step-size LMS
  - Reminiscent of one-step estimators (see, e.g., Van der Vaart, 2000)
  - Provable convergence rate of O(d/n) for logistic regression
  - Additional assumptions but no strong convexity

### Update at each iteration using the current averaged iterate

- Recursion: 
$$\theta_n = \theta_{n-1} - \gamma \left[ f_n'(\bar{\theta}_{n-1}) + f_n''(\bar{\theta}_{n-1})(\theta_{n-1} - \bar{\theta}_{n-1}) \right]$$

- No provable convergence rate (yet) but best practical behavior
- Note (dis)similarity with regular SGD:  $\theta_n = \theta_{n-1} \gamma f'_n(\theta_{n-1})$

# Stochastic average gradient (Le Roux, Schmidt, and Bach, 2012)

- Stochastic average gradient (SAG) iteration
  - Keep in memory the gradients of all functions  $f_i$ ,  $i = 1, \ldots, n$
  - Random selection  $i(t) \in \{1, \dots, n\}$  with replacement

$$- \text{ Iteration: } \theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^n y_i^t \text{ with } y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$$

- Stochastic version of incremental average gradient (Blatt et al., 2008)
- Extra memory requirement
  - Supervised machine learning
    - If  $f_i(\theta) = \ell_i(y_i, \Phi(x_i)^\top \theta)$ , then  $f_i'(\theta) = \ell_i'(y_i, \Phi(x_i)^\top \theta) \Phi(x_i)$
    - Only need to store n real numbers

## **Summary of rates of convergence**

- Problem parameters
  - D diameter of the domain
  - -B Lipschitz-constant
  - L smoothness constant
  - $\mu$  strong convexity constant

	convex	strongly convex
nonsmooth	deterministic: $BD/\sqrt{t}$	deterministic: $B^2/(t\mu)$
	stochastic: $BD/\sqrt{n}$	stochastic: $B^2/(n\mu)$
smooth	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
	stochastic: $LD^2/\sqrt{n}$	stochastic: $L/(n\mu)$
	finite sum: $n/t$	finite sum: $\exp(-\min\{1/n, \mu/L\}t)$
quadratic	deterministic: $LD^2/t^2$	deterministic: $\exp(-t\sqrt{\mu/L})$
	stochastic: $d/n + LD^2/n$	stochastic: $d/n + LD^2/n$

## **Conclusions**Machine learning and convex optimization

## • Statistics with or without optimization?

- Significance of mixing algorithms with analysis
- Benefits of mixing algorithms with analysis

### Open problems

- Non-parametric stochastic approximation
- Characterization of implicit regularization of online methods
- Structured prediction
- Going beyond a single pass over the data (testing performance)
- Further links between convex optimization and online learning/bandits
- Parallel and distributed optimization

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