Statistical machine learning and convex optimization

Francis Bach - Aymeric Dieuleveut

Mastère M2 - Paris-Sud - Spring 2022

Slides available: `www.di.ens.fr/~fbach/fbach_orsay_2022.pdf`

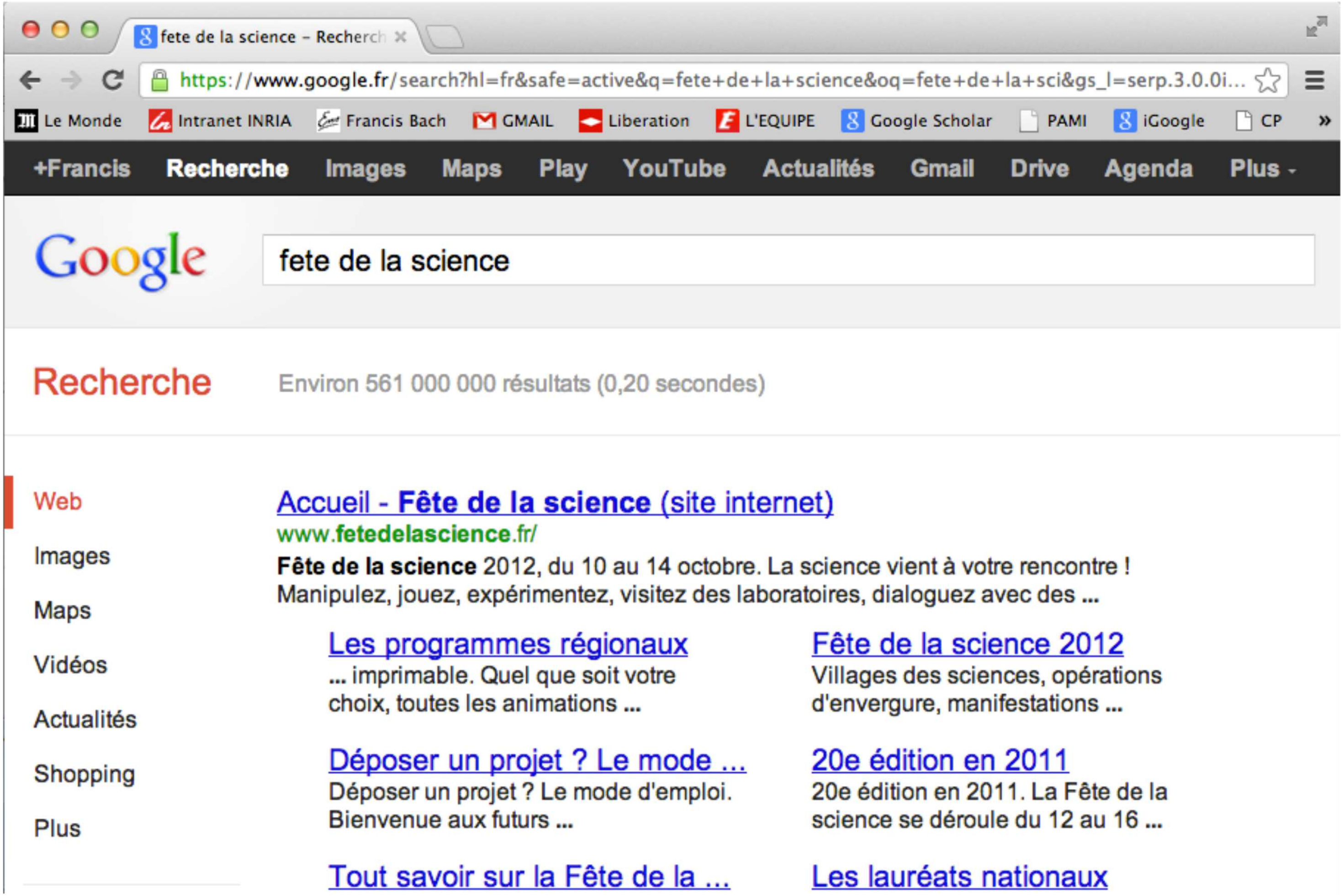
Statistical machine learning and convex optimization

- **Six classes** (lecture notes and slides online), Gotomeeting/live
  1. FB: Monday January 24, 2pm to 5pm
  2. FB: Monday January 31, 2pm to 5pm
  3. AD: Monday February 07, 2pm to 5pm
  4. AD: Monday February 14, 2pm to 5pm
  5. AD: Monday February 2~~1~~8, 2pm to 5pm
  6. FB: Monday March 07, 2pm to 5pm
- **Evaluation**
  1. Basic implementations (Matlab / Python / R)
  2. Attending 4 out of 6 classes is mandatory
  3. Short exam (Monday March 28, 2pm to 4/5pm)
- **Register online** (`https://www.di.ens.fr/~fbach/orsay2022.html`)
- Book in preparation: `https://www.di.ens.fr/~fbach/ltfp_book.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



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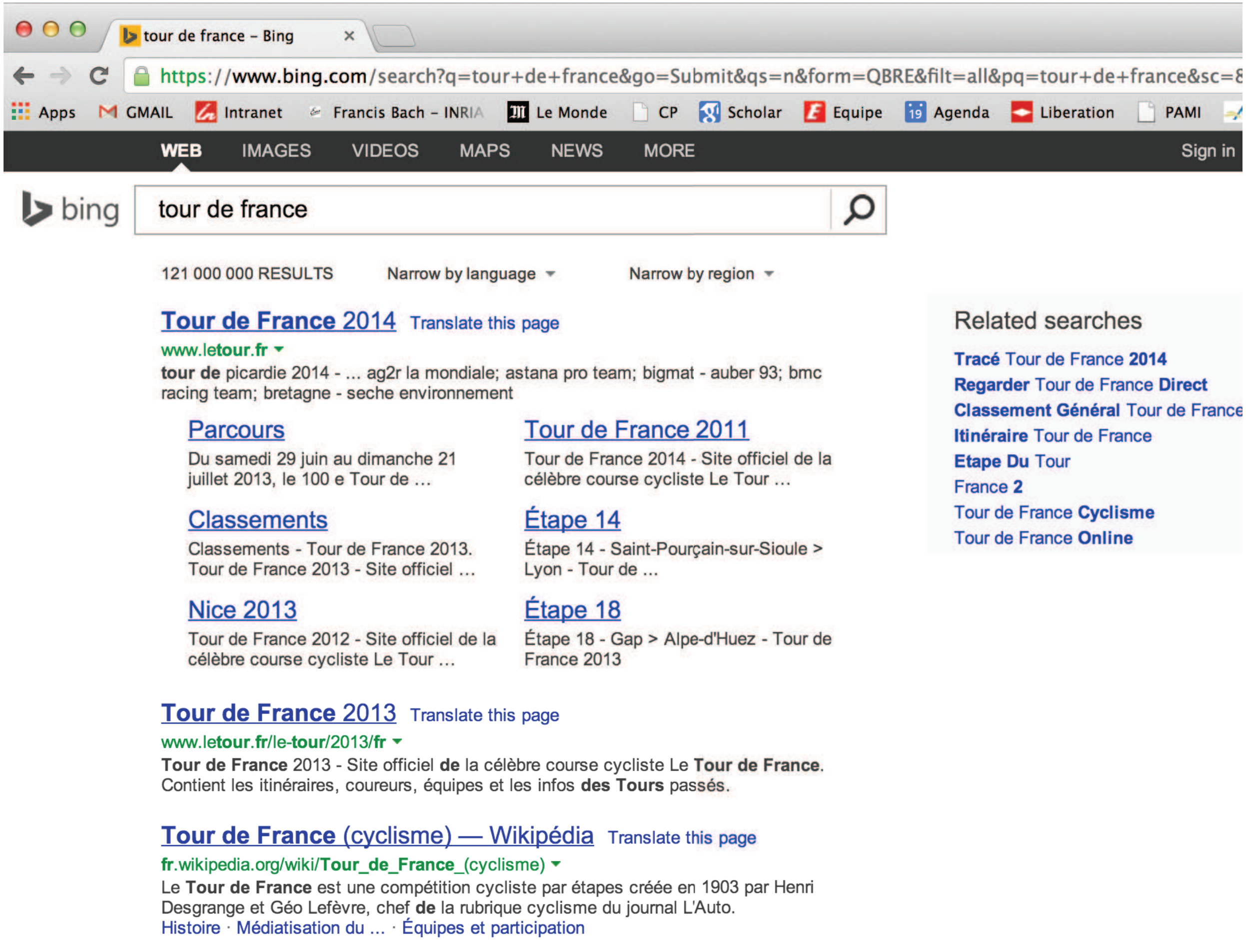
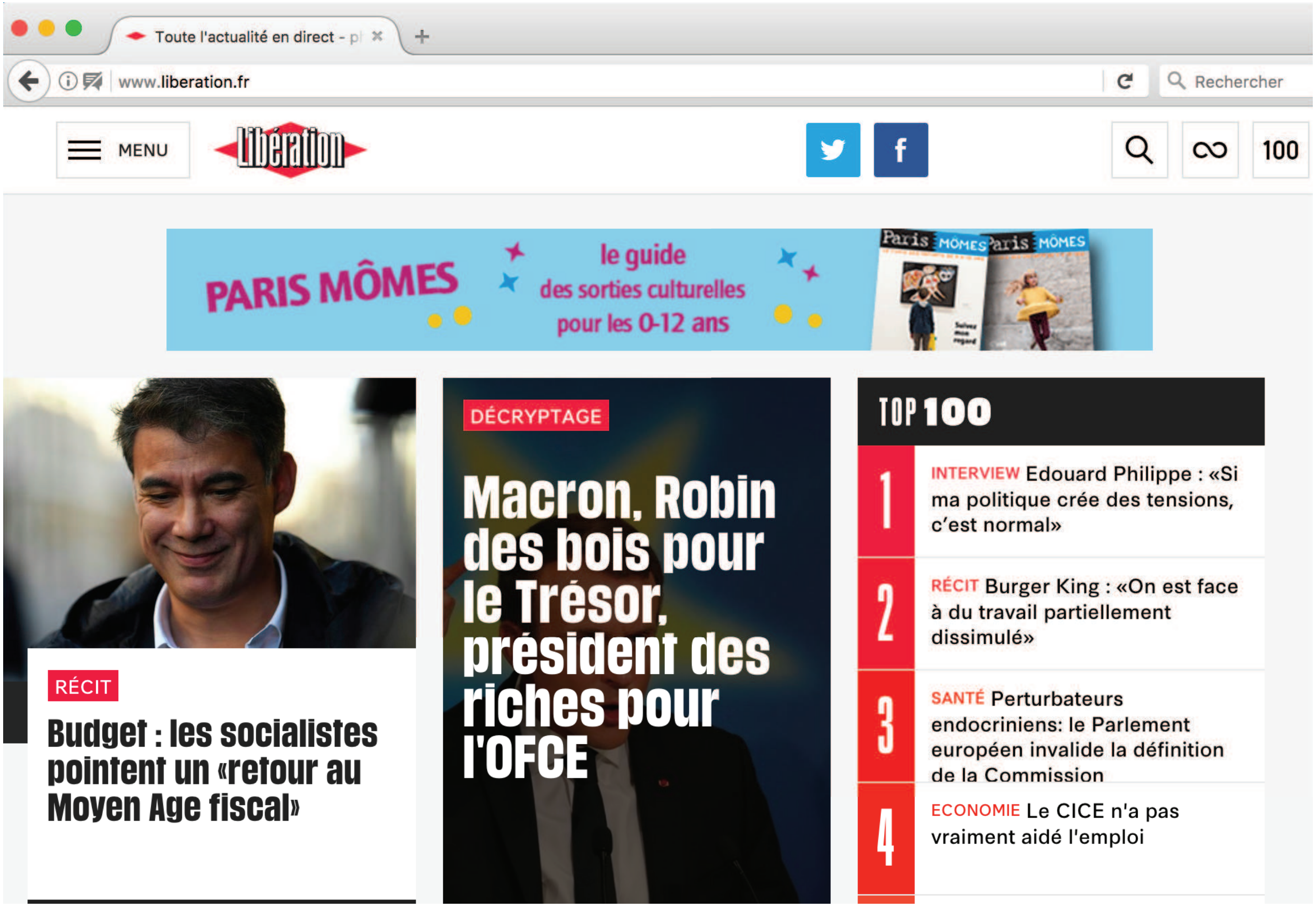
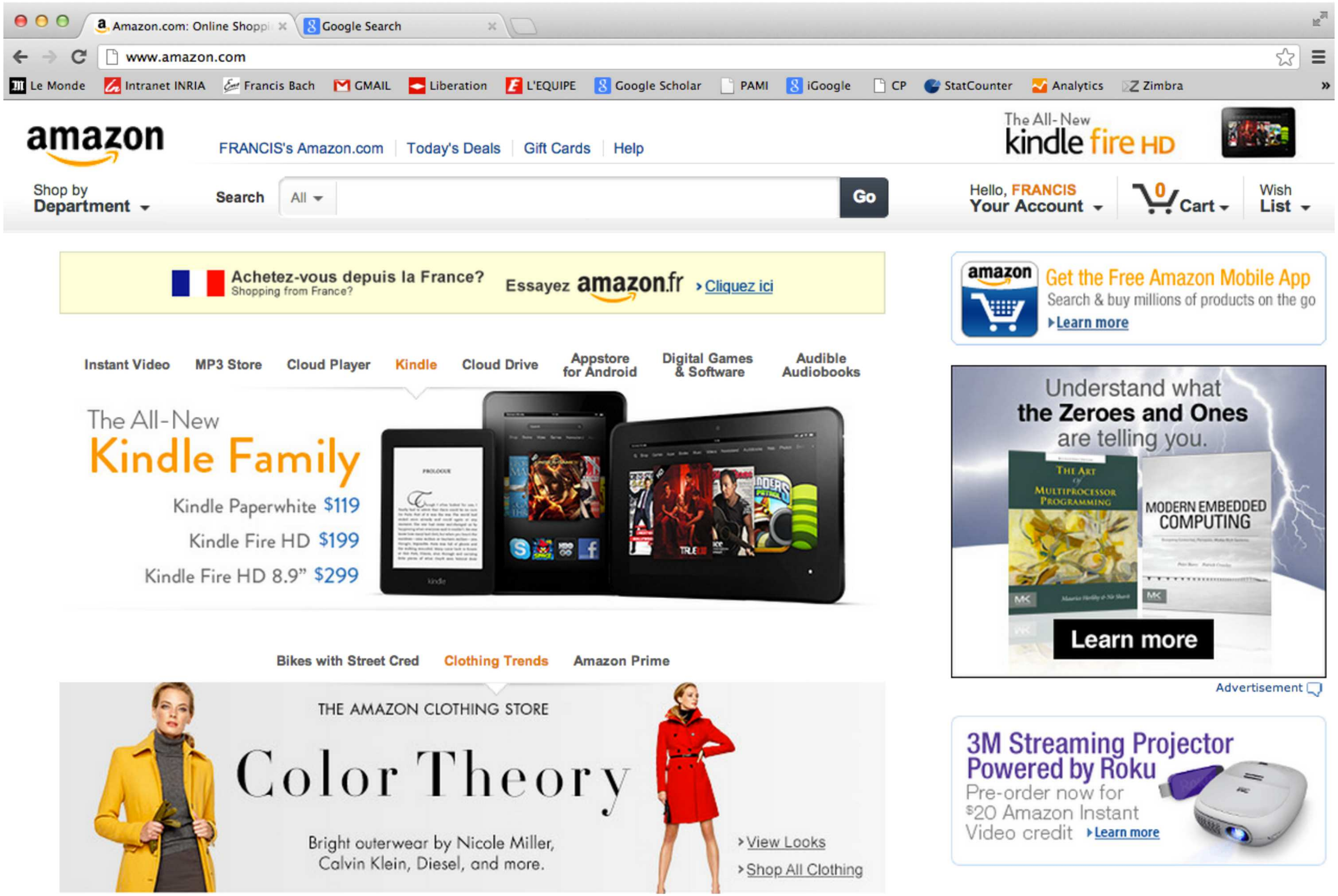


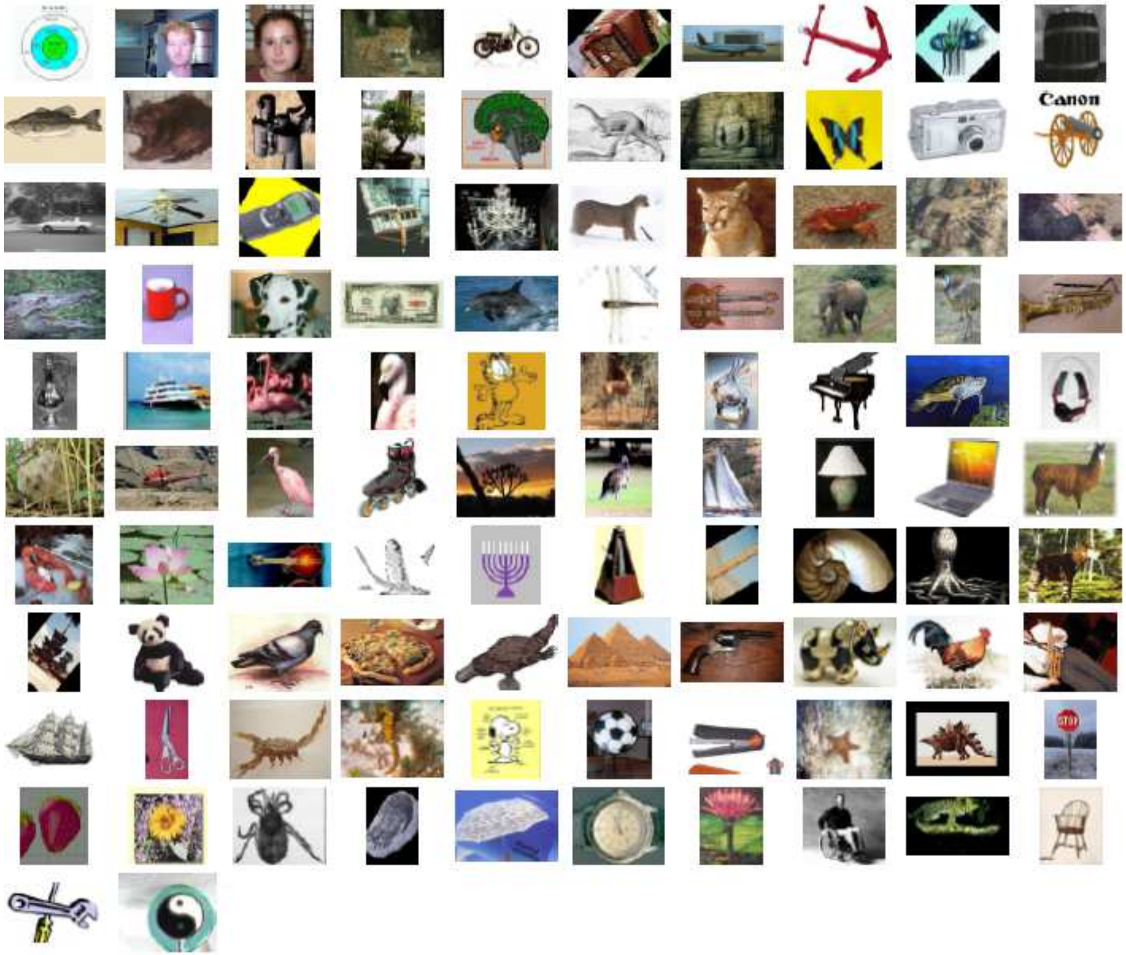
Advertising



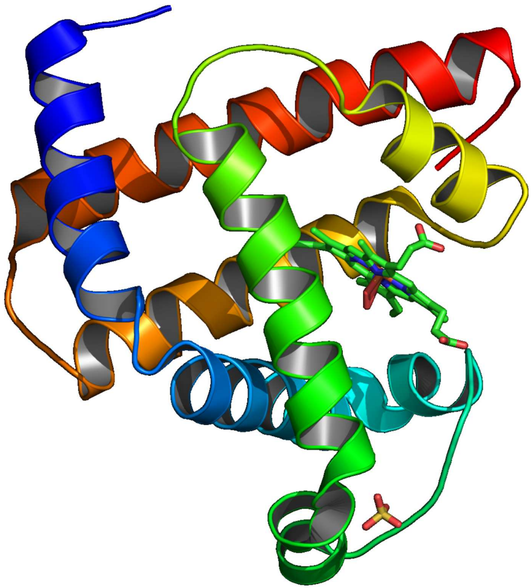
Marketing - Personalized recommendation



Visual object recognition



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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- **Ideal running-time complexity**: $O(dn)$

Context
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- **Examples**: computer vision, bioinformatics, advertising

- **Ideal running-time complexity**: $O(dn)$

- **Going back to simple methods**
  - Stochastic gradient methods (Robbins and Monro, 1951b)
  - Mixing statistics and optimization

Scaling to large problems
"Retour aux sources"

- **1950's**: Computers not powerful enough

IBM "1620", 1959
CPU frequency: 50 KHz
Price $>$ 100 000 dollars

- **2010's**: Data too massive

Scaling to large problems
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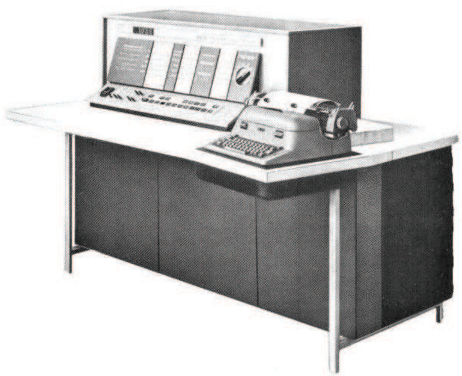

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- **2010's**: Data too massive

- **Stochastic gradient methods** (Robbins and Monro, 1951a)
  - Going back to simple methods

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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**
   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging

5. **Smooth stochastic approximation algorithms**
   - Non-asymptotic analysis for smooth functions
   - Logistic regression
   - Least-squares regression without decaying step-sizes

6. **Finite data sets**
   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

Supervised machine learning

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **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

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

convex data fitting term + regularizer

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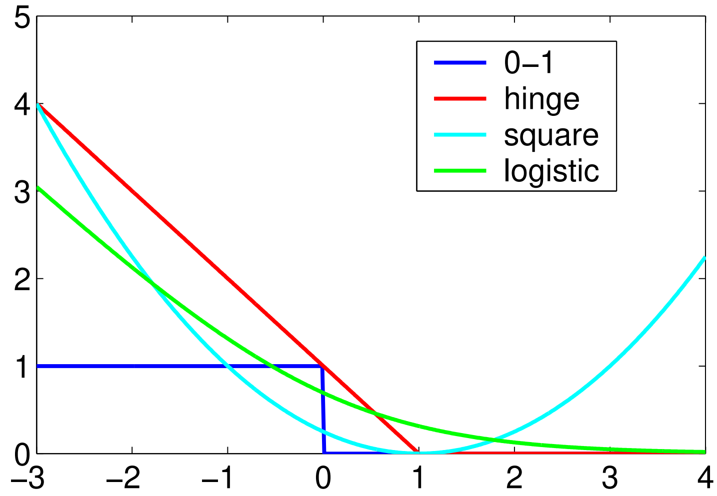
- **Classification** : $y \in \{-1, 1\}$, prediction $\hat{y} = \text{sign}(\theta^\top \Phi(x))$
  - loss of the form $\ell(y\,\theta^\top \Phi(x))$
  - "True" 0-1 loss: $\ell(y\,\theta^\top \Phi(x)) = 1_{y\,\theta^\top \Phi(x) < 0}$
  - Usual convex losses:



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: ℓ_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)

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convex data fitting term $+$ regularizer

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convex data fitting term + regularizer

- 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 $\hat{\theta}$

Supervised machine learning

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

convex data fitting term $+$ constraint

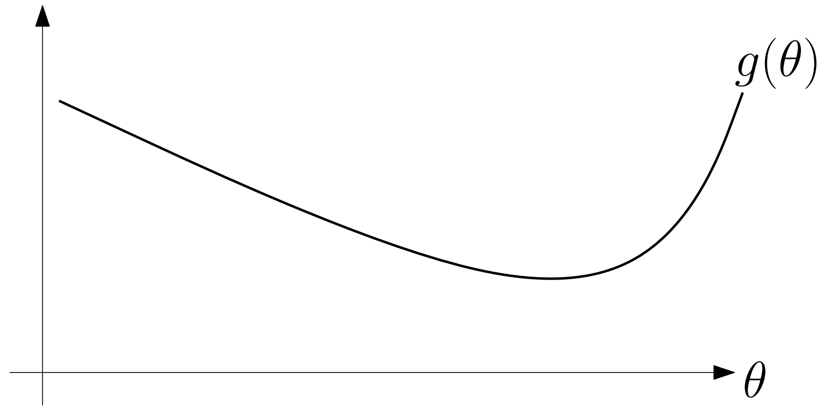
- Empirical risk: $\hat{f}(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, \theta^\top \Phi(x_i))$ training cost
- Expected risk: $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \theta^\top \Phi(x))$ testing cost
- **Two fundamental questions**: (1) computing $\hat{\theta}$ and (2) analyzing $\hat{\theta}$
 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

General assumptions

- **Data**: n observations $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}$, $i = 1, \dots, n$, **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

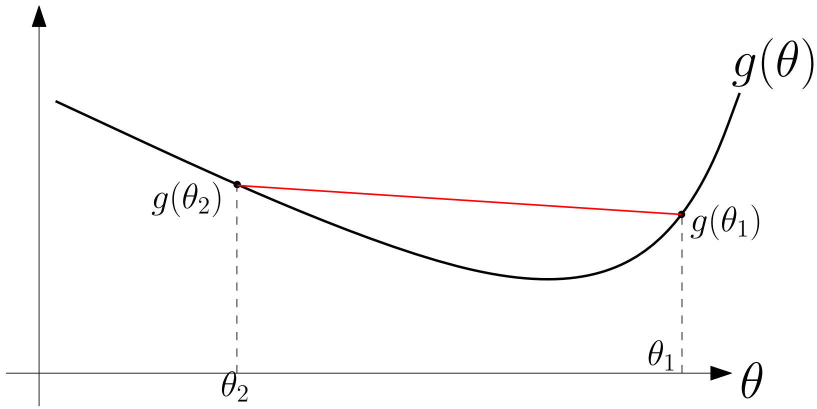
Convexity

- **Global definitions**



Convexity

- **Global definitions (full domain)**



  - Not assuming differentiability:

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

Convexity

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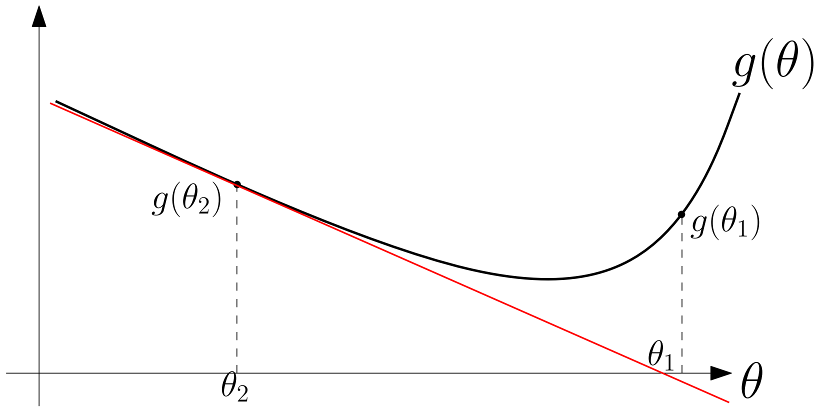


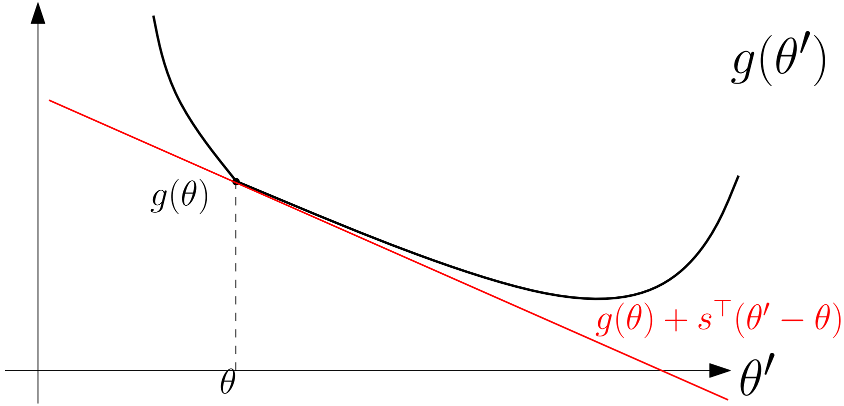
  - Assuming differentiability:

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

- **Extensions to all functions with subgradients / subdifferential**

Subgradients and subdifferentials

- Given $g : \mathbb{R}^d \to \mathbb{R}$ convex



  – $s \in \mathbb{R}^d$ is a subgradient of g at θ if and only if

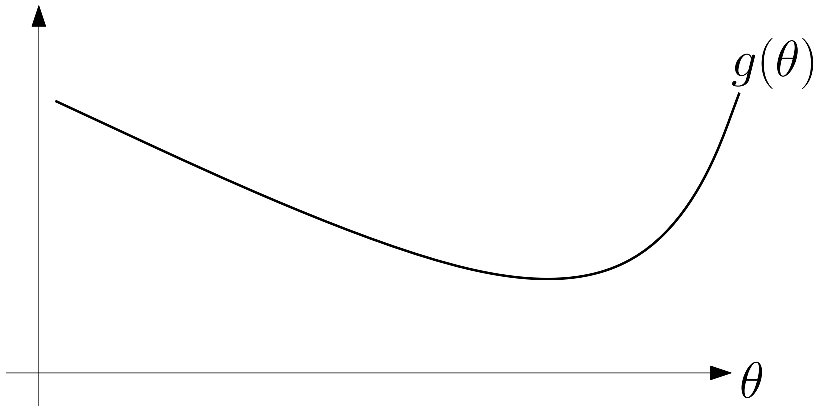
$$\forall \theta' \in \mathbb{R}^d, g(\theta') \geqslant g(\theta) + s^\top(\theta' - \theta)$$

  – Subdifferential $\partial g(\theta)$ = set of all subgradients at θ
  – If g is differentiable at θ, then $\partial g(\theta) = \{g'(\theta)\}$
  – Example: absolute value

- **The subdifferential is never empty!** See Rockafellar (1997)

Convexity

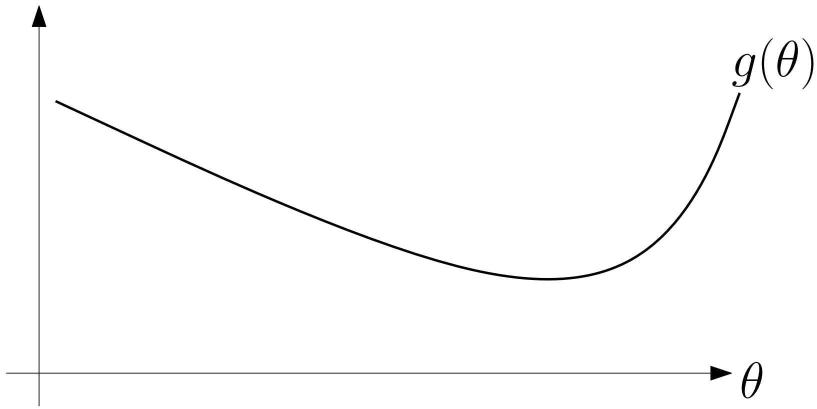
- **Global definitions (full domain)**



- **Local definitions**
  - Twice differentiable functions
  - $\forall \theta,\ g''(\theta) \succcurlyeq 0$ (positive semi-definite Hessians)

Convexity

- **Global definitions (full domain)**



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- **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:

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

$$\Leftrightarrow$$

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

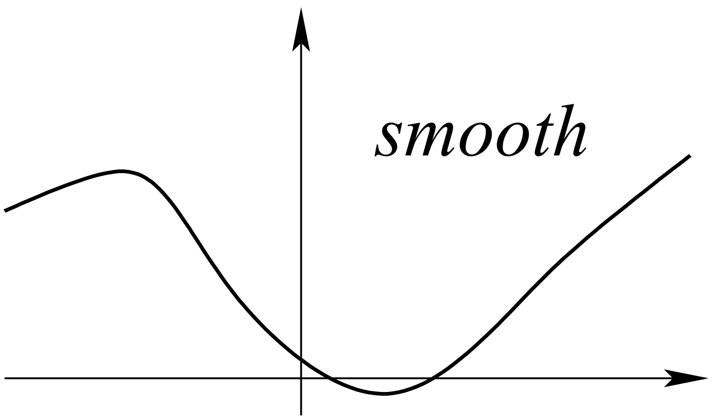
- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
  - G-Lipschitz loss and R-bounded data: $B = GR$

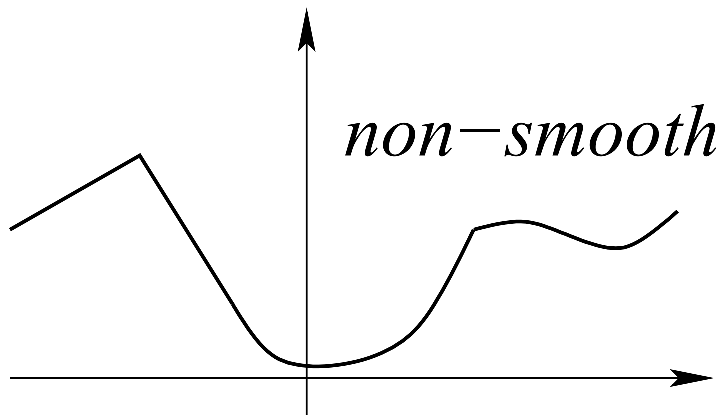
Smoothness and strong convexity

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

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

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





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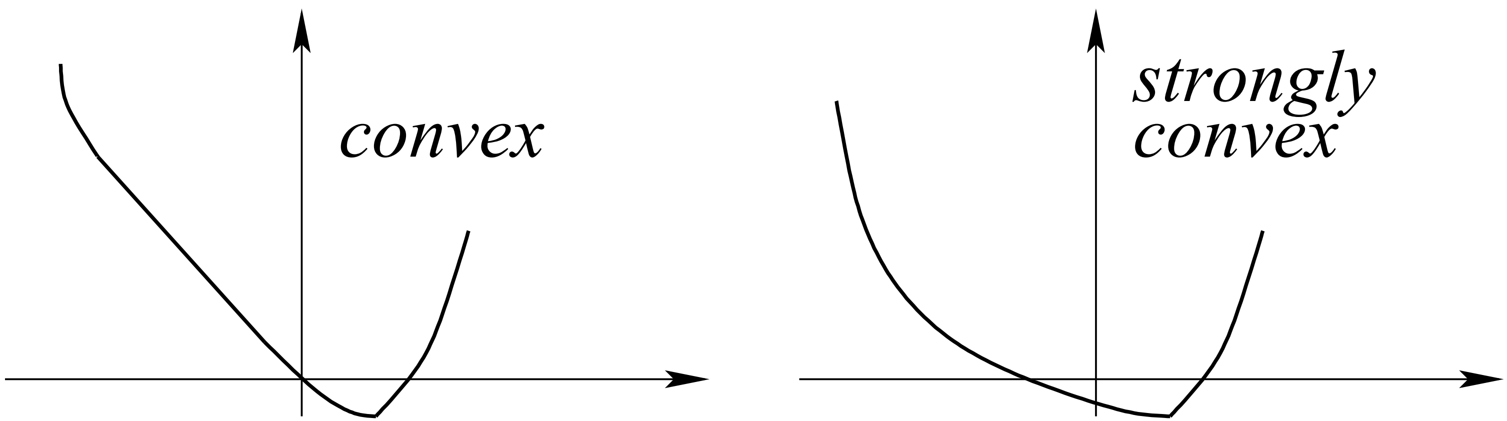
  - Hessian $\approx$ covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top$
  - $L_{\rm loss}$-smooth loss and R-bounded data: $L = L_{\rm loss}R^2$

Smoothness and strong convexity

- A function $g : \mathbb{R}^d \to \mathbb{R}$ is μ-strongly convex if and only if

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

- If g is twice differentiable: $\forall \theta \in \mathbb{R}^d,\ \ g''(\theta) \succcurlyeq \mu \cdot \mathrm{Id}$



- If g is convex, then $g + \frac{\mu}{2}\|\cdot\|_2^2$ is μ-strongly convex

Smoothness and strong convexity

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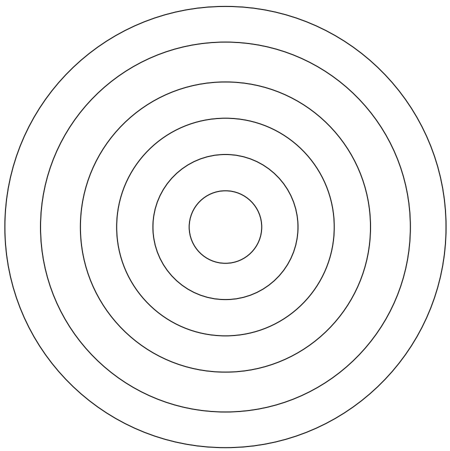
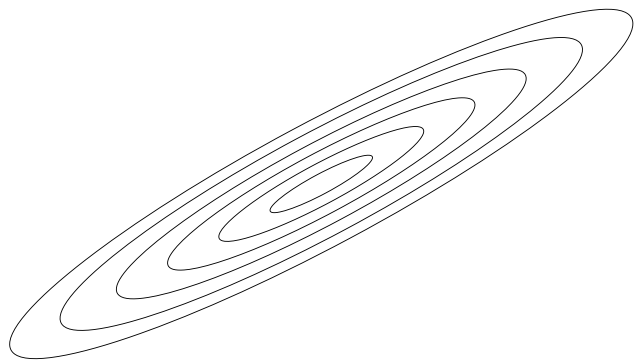


(large μ/L)



(small μ/L)

Smoothness and strong convexity

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- If g is twice differentiable: $\forall \theta \in \mathbb{R}^d, \;\; g''(\theta) \succcurlyeq \mu \cdot \mathrm{Id}$

- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
  - Hessian $\approx$ covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top$
  - Data with invertible covariance matrix (low correlation/dimension)

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  - Data with invertible covariance matrix (low correlation/dimension)

- **Adding regularization by** $\frac{\mu}{2}\|\theta\|^2$
  - creates additional bias unless μ 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):

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

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

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

Analysis of empirical risk minimization

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

$$f(\hat{\theta}) - \min_{\theta \in \mathbb{R}^d} f(\theta) = \underbrace{\left[f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) \right]}_{\text{Estimation error}} + \underbrace{\left[\min_{\theta \in \Theta} f(\theta) - \min_{\theta \in \mathbb{R}^d} f(\theta) \right]}_{\text{Approximation error}}$$

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

Analysis of empirical risk minimization

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

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

Estimation error Approximation error

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

$$f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) = \big[f(\hat{\theta}) - \hat{f}(\hat{\theta}) \big] + \big[\hat{f}(\hat{\theta}) - \hat{f}((\theta_*)_\Theta) \big] + \big[\hat{f}((\theta_*)_\Theta) - f((\theta_*)_\Theta) \big]$$

$$\leqslant \sup_{\theta \in \Theta} f(\theta) - \hat{f}(\theta) + \qquad 0 \qquad + \sup_{\theta \in \Theta} \hat{f}(\theta) - f(\theta)$$

Analysis of empirical risk minimization

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Estimation error Approximation error

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   – Typically slow rate $O\big(1/\sqrt{n}\big)$

2. **More refined concentration results** with faster rates $O(1/n)$

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Estimation error   Approximation error

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

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

   – Typically slow rate $O\big(1/\sqrt{n}\big)$

2. **More refined concentration results** with faster rates $O(1/n)$

Motivation from least-squares

- For least-squares, we have $\ell(y,\theta^\top\Phi(x)) = \frac{1}{2}(y-\theta^\top\Phi(x))^2$, and

$$\begin{aligned}
\hat f(\theta) - f(\theta) &= \frac{1}{2}\theta^\top\bigg(\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top - \mathbb{E}\Phi(X)\Phi(X)^\top\bigg)\theta \\
&\quad -\theta^\top\bigg(\frac{1}{n}\sum_{i=1}^n y_i\Phi(x_i) - \mathbb{E}Y\Phi(X)\bigg) + \frac{1}{2}\bigg(\frac{1}{n}\sum_{i=1}^n y_i^2 - \mathbb{E}Y^2\bigg), \\
\sup_{\|\theta\|_2\leqslant D} |f(\theta)-\hat f(\theta)| &\leqslant \frac{D^2}{2}\bigg\|\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top - \mathbb{E}\Phi(X)\Phi(X)^\top\bigg\|_{\rm op} \\
&\quad +D\bigg\|\frac{1}{n}\sum_{i=1}^n y_i\Phi(x_i) - \mathbb{E}Y\Phi(X)\bigg\|_2 + \frac{1}{2}\bigg|\frac{1}{n}\sum_{i=1}^n y_i^2 - \mathbb{E}Y^2\bigg|, \\
\sup_{\|\theta\|_2\leqslant D} |f(\theta)-\hat f(\theta)| &\leqslant O(1/\sqrt{n}) \text{ with high probability from 3 concentrations}
\end{aligned}$$

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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  - No assumptions regarding convexity

- With probability greater than $1 - \delta$

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

- Expectated estimation error: $\mathbb{E}\big[\sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)|\big] \leqslant \dfrac{4\ell_0 + 4GRD}{\sqrt{n}}$

- Using Rademacher averages (see, e.g., Boucheron et al., 2005)

- **Lipschitz functions $\Rightarrow$ slow rate**

Symmetrization with Rademacher variables

- Let $\mathcal{D}' = \{x_1', y_1', \dots, x_n', y_n'\}$ an independent copy of the data $\mathcal{D} = \{x_1, y_1, \dots, x_n, y_n\}$, with corresponding loss functions $f_i'(\theta)$

$$
\begin{aligned}
\mathbb{E}\big[\sup_{\theta\in\Theta} f(\theta) - \hat{f}(\theta)\big] &= \mathbb{E}\Big[\sup_{\theta\in\Theta}\Big(f(\theta) - \frac{1}{n}\sum_{i=1}^n f_i(\theta)\Big)\Big] \\
&= \mathbb{E}\bigg[\sup_{\theta\in\Theta}\frac{1}{n}\sum_{i=1}^n \mathbb{E}\big(f_i'(\theta) - f_i(\theta)|\mathcal{D}\big)\bigg] \\
&\leqslant \mathbb{E}\bigg[\mathbb{E}\bigg[\sup_{\theta\in\Theta}\frac{1}{n}\sum_{i=1}^n \big(f_i'(\theta) - f_i(\theta)\big)\ \bigg|\mathcal{D}\bigg]\bigg] \\
&= \mathbb{E}\bigg[\sup_{\theta\in\Theta}\frac{1}{n}\sum_{i=1}^n \big(f_i'(\theta) - f_i(\theta)\big)\bigg] \\
&= \mathbb{E}\bigg[\sup_{\theta\in\Theta}\frac{1}{n}\sum_{i=1}^n \varepsilon_i\big(f_i'(\theta) - f_i(\theta)\big)\bigg] \text{ with } \varepsilon_i \text{ uniform in } \{-1,1\} \\
&\leqslant 2\mathbb{E}\bigg[\sup_{\theta\in\Theta}\frac{1}{n}\sum_{i=1}^n \varepsilon_i f_i(\theta)\bigg] = \text{Rademacher complexity}
\end{aligned}
$$

Rademacher complexity

- Rademacher complexity of the class of functions $(X, Y) \mapsto \ell(Y, \theta^\top \Phi(X))$

$$R_n = \mathbb{E}\bigg[\sup_{\theta\in\Theta} \frac{1}{n}\sum_{i=1}^n \varepsilon_i f_i(\theta)\bigg]$$

  – with $f_i(\theta) = \ell(x_i, \theta^\top \Phi(x_i))$, (x_i, y_i), i.i.d

- NB 1: two expectations, with respect to $\mathcal{D}$ *and* with respect to ε
  – "Empirical" Rademacher average $\hat{R}_n$ by conditioning on $\mathcal{D}$

- NB 2: sometimes defined as $\sup_{\theta\in\Theta}\left|\frac{1}{n}\sum_{i=1}^n \varepsilon_i f_i(\theta)\right|$

- **Main property**:

$$\mathbb{E}\big[\sup_{\theta\in\Theta} f(\theta) - \hat{f}(\theta)\big] \text{ and } \mathbb{E}\big[\sup_{\theta\in\Theta} \hat{f}(\theta) - f(\theta)\big] \leqslant 2R_n$$

From Rademacher complexity to uniform bound

- Let $Z = \sup_{\theta \in \Theta} |f(\theta) - \hat{f}(\theta)|$

- By changing the pair (x_i, y_i), Z may only change by

$$\frac{2}{n} \sup |\ell(Y, \theta^\top \Phi(X))| \leqslant \frac{2}{n}\big(\sup |\ell(Y, 0)| + GRD\big) \leqslant \frac{2}{n}\big(\ell_0 + GRD\big) = c$$

with $\sup |\ell(Y, 0)| = \ell_0$

- **MacDiarmid inequality**: with probability greater than $1 - \delta$,

$$Z \leqslant \mathbb{E} Z + \sqrt{\frac{n}{2}} c \cdot \sqrt{\log \frac{1}{\delta}} \leqslant 2 R_n + \frac{\sqrt{2}}{\sqrt{n}}\big(\ell_0 + GRD\big)\sqrt{\log \frac{1}{\delta}}$$

Bounding the Rademacher average - I

- We have, with $\varphi_i(u) = \ell(y_i, u) - \ell(y_i, 0)$ is almost surely G-Lipschitz:

$$\begin{aligned}
\hat{R}_n &= \mathbb{E}_\varepsilon \Big[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i f_i(\theta) \Big] \\
&= \mathbb{E}_\varepsilon \Big[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i f_i(0) \Big] + \mathbb{E}_\varepsilon \Big[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \big[f_i(\theta) - f_i(0) \big] \Big] \\
&= 0 + \mathbb{E}_\varepsilon \Big[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \big[f_i(\theta) - f_i(0) \big] \Big] \\
&= 0 + \mathbb{E}_\varepsilon \Big[\sup_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \varphi_i(\theta^\top \Phi(x_i)) \Big]
\end{aligned}$$

- Using Ledoux-Talagrand contraction results for Rademacher averages (since φ_i is G-Lipschitz), we get (Meir and Zhang, 2003):

$$\hat{R}_n \leqslant G \cdot \mathbb{E}_\varepsilon \Big[\sup_{\|\theta\|_2 \leqslant D} \frac{1}{n} \sum_{i=1}^n \varepsilon_i \theta^\top \Phi(x_i) \Big]$$

Proof of Ledoux-Talagrand lemma (Meir and Zhang, 2003, Lemma 5)

- Given any b, $a_i : \Theta \to \mathbb{R}$ (no assumption) and $\varphi_i : \mathbb{R} \to \mathbb{R}$ any 1-Lipschitz-functions, $i = 1, \dots, n$

$$\mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} b(\theta) + \sum_{i=1}^n \varepsilon_i \varphi_i(a_i(\theta)) \right] \leqslant \mathbb{E}_\varepsilon \left[\sup_{\theta \in \Theta} b(\theta) + \sum_{i=1}^n \varepsilon_i a_i(\theta) \right]$$

- **Proof by induction on** n
  - $n = 0$: trivial

- From n to $n+1$: see next slide

From n to $n+1$

$$
\begin{aligned}
& \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_{n+1}}\left[\sup_{\theta\in\Theta} b(\theta) + \sum_{i=1}^{n+1} \varepsilon_i \varphi_i(a_i(\theta))\right] \\
= \; & \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_n}\left[\sup_{\theta,\theta'\in\Theta} \frac{b(\theta)+b(\theta')}{2} + \sum_{i=1}^{n} \varepsilon_i \frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2} + \frac{\varphi_{n+1}(a_{n+1}(\theta)) - \varphi_{n+1}(a_{n+1}(\theta'))}{2}\right] \\
= \; & \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_n}\left[\sup_{\theta,\theta'\in\Theta} \frac{b(\theta)+b(\theta')}{2} + \sum_{i=1}^{n} \varepsilon_i \frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2} + \frac{|\varphi_{n+1}(a_{n+1}(\theta)) - \varphi_{n+1}(a_{n+1}(\theta'))|}{2}\right] \\
\leqslant \; & \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_n}\left[\sup_{\theta,\theta'\in\Theta} \frac{b(\theta)+b(\theta')}{2} + \sum_{i=1}^{n} \varepsilon_i \frac{\varphi_i(a_i(\theta))+\varphi_i(a_i(\theta'))}{2} + \frac{|a_{n+1}(\theta) - a_{n+1}(\theta')|}{2}\right] \\
= \; & \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_n}\mathbb{E}_{\varepsilon_{n+1}}\left[\sup_{\theta\in\Theta} b(\theta) + \varepsilon_{n+1} a_{n+1}(\theta) + \sum_{i=1}^{n} \varepsilon_i \varphi_i(a_i(\theta))\right] \\
\leqslant \; & \mathbb{E}_{\varepsilon_1,\dots,\varepsilon_n,\varepsilon_{n+1}}\left[\sup_{\theta\in\Theta} b(\theta) + \varepsilon_{n+1} a_{n+1}(\theta) + \sum_{i=1}^{n} \varepsilon_i a_i(\theta)\right] \text{ by recursion}
\end{aligned}
$$

Bounding the Rademacher average - II

- We have:

$$
\begin{aligned}
R_n &\leqslant 2G\mathbb{E}\Big[\sup_{\|\theta\|_2\leqslant D}\frac{1}{n}\sum_{i=1}^n \varepsilon_i\theta^\top\Phi(x_i)\Big] \\
&= 2G\mathbb{E}\Big\|D\frac{1}{n}\sum_{i=1}^n \varepsilon_i\Phi(x_i)\Big\|_2 \\
&\leqslant 2GD\sqrt{\mathbb{E}\Big\|\frac{1}{n}\sum_{i=1}^n \varepsilon_i\Phi(x_i)\Big\|_2^2} \text{ by Jensen's inequality} \\
&\leqslant \frac{2GRD}{\sqrt{n}} \text{ by using } \|\Phi(x)\|_2\leqslant R \text{ and independence}
\end{aligned}
$$

- Overall, we get, with probability $1-\delta$:

$$
\sup_{\theta\in\Theta}\big|f(\theta)-\hat{f}(\theta)\big| \leqslant \frac{1}{\sqrt{n}}(\ell_0+GRD)(4+\sqrt{2\log\frac{1}{\delta}})
$$

Putting it all together

- We have, with probability $1-\delta$
  - For exact minimizer $\hat{\theta} \in \arg\min_{\theta \in \Theta} \hat{f}(\theta)$, we have

$$f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) \leqslant \sup_{\theta \in \Theta} \hat{f}(\theta) - f(\theta) + \sup_{\theta \in \Theta} f(\theta) - \hat{f}(\theta)$$

$$\leqslant \frac{2}{\sqrt{n}}(\ell_0 + GRD)(4 + \sqrt{2 \log \frac{1}{\delta}})$$

  - For inexact minimizer $\eta \in \Theta$

$$f(\eta) - \min_{\theta \in \Theta} f(\theta) \leqslant 2 \cdot \sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| + \left[\hat{f}(\eta) - \hat{f}(\hat{\theta})\right]$$

- **Only need to optimize with precision** $\frac{2}{\sqrt{n}}(\ell_0 + GRD)$

Putting it all together

- We have, with probability $1 - \delta$
  - For exact minimizer $\hat{\theta} \in \arg\min_{\theta \in \Theta} \hat{f}(\theta)$, we have

$$
\begin{aligned}
f(\hat{\theta}) - \min_{\theta \in \Theta} f(\theta) &\leqslant 2 \cdot \sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| \\
&\leqslant \frac{2}{\sqrt{n}}(\ell_0 + GRD)(4 + \sqrt{2 \log \frac{1}{\delta}})
\end{aligned}
$$

  - For inexact minimizer $\eta \in \Theta$

$$
f(\eta) - \min_{\theta \in \Theta} f(\theta) \leqslant 2 \cdot \sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)| + \left[\hat{f}(\eta) - \hat{f}(\hat{\theta})\right]
$$

- **Only need to optimize with precision** $\frac{2}{\sqrt{n}}(\ell_0 + GRD)$

Slow rate for supervised learning (summary)

- **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

- With probability greater than $1 - \delta$

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

- Expectated estimation error: $\mathbb{E}\big[\sup_{\theta \in \Theta} |\hat{f}(\theta) - f(\theta)|\big] \leqslant \dfrac{4(\ell_0 + GRD)}{\sqrt{n}}$

- Using Rademacher averages (see, e.g., Boucheron et al., 2005)

- **Lipschitz functions $\Rightarrow$ slow rate**

Motivation from mean estimation

- Estimator $\hat{\theta} = \frac{1}{n}\sum_{i=1}^n z_i = \arg\min_{\theta \in \mathbb{R}} \frac{1}{2n}\sum_{i=1}^n (\theta - z_i)^2 = \hat{f}(\theta)$
  - $\theta_* = \mathbb{E}z = \arg\min_{\theta \in \mathbb{R}} \frac{1}{2}\mathbb{E}(\theta - z)^2 = f(\theta)$
  - From before (estimation error): $f(\hat{\theta}) - f(\theta_*) = O(1/\sqrt{n})$

Motivation from mean estimation

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  - $\theta_* = \mathbb{E}z = \arg\min_{\theta\in\mathbb{R}} \frac{1}{2}\mathbb{E}(\theta - z)^2 = f(\theta)$
  - From before (estimation error): $f(\hat{\theta}) - f(\theta_*) = O(1/\sqrt{n})$

- Direct computation:
  - $f(\theta) = \frac{1}{2}\mathbb{E}(\theta - z)^2 = \frac{1}{2}(\theta - \mathbb{E}z)^2 + \frac{1}{2}\,\mathrm{var}(z)$

- More refined/direct bound:

$$
\begin{aligned}
f(\hat{\theta}) - f(\mathbb{E}z) &= \frac{1}{2}(\hat{\theta} - \mathbb{E}z)^2 \\
\mathbb{E}\big[f(\hat{\theta}) - f(\mathbb{E}z)\big] &= \frac{1}{2}\mathbb{E}\bigg(\frac{1}{n}\sum_{i=1}^n z_i - \mathbb{E}z\bigg)^2 = \frac{1}{2n}\,\mathrm{var}(z)
\end{aligned}
$$

- 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

- For any $a > 0$, with probability greater than $1 - \delta$, for all $\theta \in \mathbb{R}^d$,

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

- Results from Sridharan, Srebro, and Shalev-Shwartz (2008)
  - see also Boucheron and Massart (2011) and references therein

- **Strongly convex functions $\Rightarrow$ fast rate**
  - Warning: μ should decrease with n to reduce approximation error

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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**

   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging

5. **Smooth stochastic approximation algorithms**

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

6. **Finite data sets**

   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

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

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
- **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)

Several criteria for characterizing convergence

- **Objective function values**

$$g(\theta) - \inf_{\eta \in \mathbb{R}^d} g(\eta)$$

  – Usually weaker condition

- **Iterates**

$$\inf_{\eta \in \arg\min g} \big\| \theta - \eta \big\|^2$$

  – Typically used for strongly-convex problems

- NB 1: relationships between the two types in several situations (see later)

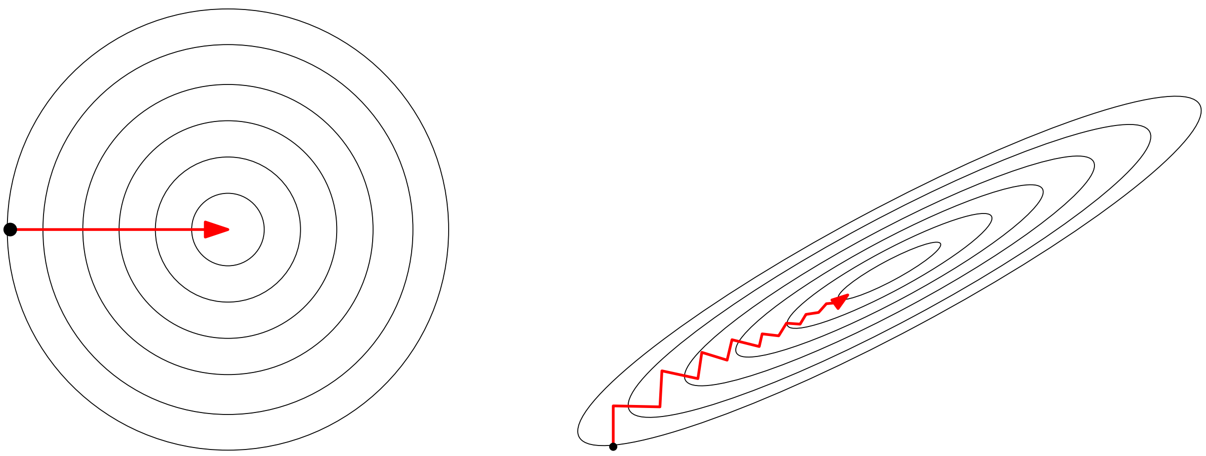
- NB 2: similarity with prediction vs. estimation in statistics

(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 μ-strongly convex

- **Algorithm**:

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

- **Bound**:

$$g(\theta_t) - g(\theta_*) \leqslant (1 - \mu/L)^t \big[g(\theta_0) - g(\theta_*)\big]$$

- 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 θ_*

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

- Gradient descent:

$$\begin{aligned}
\theta_t &= \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - c) = \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - H\theta_*) \\
\theta_t - \theta_* &= (I - \frac{1}{L}H)(\theta_{t-1} - \theta_*) = (I - \frac{1}{L}H)^t(\theta_0 - \theta_*)
\end{aligned}$$

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

Gradient descent - Proof for quadratic functions

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

- Gradient descent:

$$\begin{aligned} \theta_t &= \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - c) = \theta_{t-1} - \frac{1}{L}(H\theta_{t-1} - H\theta_*) \\ \theta_t - \theta_* &= (I - \frac{1}{L}H)(\theta_{t-1} - \theta_*) = (I - \frac{1}{L}H)^t(\theta_0 - \theta_*) \end{aligned}$$

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

Properties of smooth convex functions

- Let $g : \mathbb{R}^d \to \mathbb{R}$ a convex L-smooth function. Then for all $\theta, \eta \in \mathbb{R}^d$:
  - Definition: $\|g'(\theta) - g'(\eta)\| \leqslant L\|\theta - \eta\|$
  - If twice differentiable: $0 \preccurlyeq g''(\theta) \preccurlyeq LI$

- Quadratic upper-bound: $0 \leqslant g(\theta) - g(\eta) - g'(\eta)^\top(\theta - \eta) \leqslant \frac{L}{2}\|\theta - \eta\|^2$
  - Taylor expansion with integral remainder

- Co-coercivity: $\frac{1}{L}\|g'(\theta) - g'(\eta)\|^2 \leqslant \big[g'(\theta) - g'(\eta)\big]^\top(\theta - \eta)$

- If g is μ-strongly convex (no need for smoothness), then

$$g(\theta) \leqslant g(\eta) + g'(\eta)^\top(\theta - \eta) + \frac{1}{2\mu}\|g'(\theta) - g'(\eta)\|^2$$

- "Distance" to optimum: $g(\theta) - g(\theta_*) \leqslant g'(\theta)^\top(\theta - \theta_*)$

Proof of co-coercivity

- Quadratic upper-bound: $0 \leqslant g(\theta) - g(\eta) - g'(\eta)^\top(\theta - \eta) \leqslant \frac{L}{2}\|\theta - \eta\|^2$
  - Taylor expansion with integral remainder

- Lower bound: $g(\theta) \geqslant g(\eta) + g'(\eta)^\top(\theta - \eta) + \frac{1}{2L}\|g'(\theta) - g'(\eta)\|^2$
  - Define $h(\theta) = g(\theta) - \theta^\top g'(\eta)$, convex with global minimum at η
  - $h(\eta) \leqslant h(\theta - \frac{1}{L}h'(\theta)) \leqslant h(\theta) + h'(\theta)^\top(-\frac{1}{L}h'(\theta))) + \frac{L}{2}\| - \frac{1}{L}h'(\theta))\|^2$, which is thus less than $h(\theta) - \frac{1}{2L}\|h'(\theta)\|^2$
  - Thus $g(\eta) - \eta^\top g'(\eta) \leqslant g(\theta) - \theta^\top g'(\eta) - \frac{1}{2L}\|g'(\theta) - g'(\eta)\|^2$

- Proof of co-coercivity
  - Apply lower bound twice for (η, θ) and (θ, η), and sum to get $0 \geqslant [g'(\eta) - g'(\theta)]^\top(\theta - \eta) + \frac{1}{L}\|g'(\theta) - g'(\eta)\|^2$

- NB: simple proofs with second-order derivatives

Proof of $g(\theta) \leqslant g(\eta) + g'(\eta)^\top(\theta - \eta) + \frac{1}{2\mu}\|g'(\theta) - g'(\eta)\|^2$

- Define $h(\theta) = g(\theta) - \theta^\top g'(\eta)$, convex with global minimum at η

- $h(\eta) = \min_\theta h(\theta) \geqslant \min_\zeta h(\theta) + h'(\theta)^\top(\zeta - \theta) + \frac{\mu}{2}\|\zeta - \theta\|^2$, which is attained for $\zeta - \theta = -\frac{1}{\mu}h'(\theta)$
  - This leads to $h(\eta) \geqslant h(\theta) - \frac{1}{2\mu}\|h'(\theta)\|^2$
  - Hence, $g(\eta) - \eta^\top g'(\eta) \geqslant g(\theta) - \theta^\top g'(\eta) - \frac{1}{2\mu}\|g'(\eta) -' (\theta)\|^2$
  - NB: no need for smooothness

- NB: simple proofs with second-order derivatives

- With $\eta = \theta_*$ global minimizer, another "distance" to optimum

$$g(\theta) - g(\theta_*) \leqslant \frac{1}{2\mu}\|g'(\theta)\|^2 \quad \text{“Polyak-Lojasiewicz”}$$

Convergence proofs through Lyapunov functions

- Given sequence of iterates (θ_t), find a function $V \geqslant 0$ such that

$$V(\theta_t) \leqslant (1-\alpha) V(\theta_{t-1})$$

  – Then $V(\theta_t) \leqslant (1-\alpha)^t V(\alpha_0)$

- Many variations

  – Time-dependence: $V_t(\theta_t) \leqslant (1-\alpha_t) V_{t-1}(\theta_{t-1})$
  – Weak decrease: $V(\theta_t) \leqslant V(\theta_{t-1}) - U(\theta_t)$
  Then $U(\theta_t) \leqslant V(\theta_{t-1}) - V(\theta_t)$ and $\frac{1}{T}\sum_{t=1}^T U(\theta_t) \leqslant \frac{V(\theta_0)}{T}$

- Noise term: $V(\theta_t) \leqslant V(\theta_{t-1}) - U(\theta_t) + M(\theta_{t-1})$

- Classical candidates: $\|\theta - \theta_*\|_2^2$ and $g(\theta) - g(\theta_*)$

Convergence proof - gradient descent smooth strongly convex functions

- Iteration: $\theta_t = \theta_{t-1} - \gamma g'(\theta_{t-1})$ with $\gamma = 1/L$

$$
\begin{aligned}
g(\theta_t) &= g\big[\theta_{t-1} - \gamma g'(\theta_{t-1})\big] \leqslant g(\theta_{t-1}) + g'(\theta_{t-1})^\top \big[-\gamma g'(\theta_{t-1})\big] + \frac{L}{2}\| -\gamma g'(\theta_{t-1})\|^2 \\
&= g(\theta_{t-1}) - \gamma(1-\gamma L/2)\|g'(\theta_{t-1})\|^2 \\
&= g(\theta_{t-1}) - \frac{1}{2L}\|g'(\theta_{t-1})\|^2 \text{ if } \gamma = 1/L, \\
&\leqslant g(\theta_{t-1}) - \frac{\mu}{L}\big[g(\theta_{t-1}) - g(\theta_*)\big] \text{ using strongly-convex “distance” to optimum}
\end{aligned}
$$

Thus, $g(\theta_t) - g(\theta_*) \leqslant (1-\mu/L)\big[g(\theta_{t-1}) - g(\theta_*)\big] \leqslant (1-\mu/L)^t\big[g(\theta_0) - g(\theta_*)\big]$

- May also get (Nesterov, 2004): $\|\theta_t - \theta_*\|^2 \leqslant \big(1 - \frac{2\gamma\mu L}{\mu+L}\big)^t \|\theta_0 - \theta_*\|^2$ as soon as $\gamma \leqslant \frac{2}{\mu+L}$

Convergence proof - gradient descent smooth convex functions - I

- Iteration: $\theta_t = \theta_{t-1} - \gamma g'(\theta_{t-1})$ with $\gamma = 1/L$

$$
\begin{aligned}
\|\theta_t - \theta_*\|^2 &= \|\theta_{t-1} - \theta_* - \gamma g'(\theta_{t-1})\|^2 \\
&= \|\theta_{t-1} - \theta_*\|^2 + \gamma^2 \|g'(\theta_{t-1})\|^2 - 2\gamma(\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \\
&\leqslant \|\theta_{t-1} - \theta_*\|^2 + \gamma^2 \|g'(\theta_{t-1})\|^2 - 2\frac{\gamma}{L}\|g'(\theta_{t-1})\|^2 \text{ using co-coercivity} \\
&= \|\theta_{t-1} - \theta_*\|^2 - \gamma(2/L - \gamma)\|g'(\theta_{t-1})\|^2 \leqslant \|\theta_{t-1} - \theta_*\|^2 \text{ if } \gamma \leqslant 2/L \\
&\leqslant \|\theta_0 - \theta_*\|^2 : \text{ bounded iterates} \\
g(\theta_t) &\leqslant g(\theta_{t-1}) - \frac{1}{2L}\|g'(\theta_{t-1})\|^2 \text{ (see previous slide)} \\
g(\theta_{t-1}) - g(\theta_*) &\leqslant g'(\theta_{t-1})^\top(\theta_{t-1} - \theta_*) \leqslant \|g'(\theta_{t-1})\| \cdot \|\theta_{t-1} - \theta_*\| \text{ (Cauchy-Schwarz)} \\
g(\theta_t) - g(\theta_*) &\leqslant g(\theta_{t-1}) - g(\theta_*) - \frac{1}{2L\|\theta_0 - \theta_*\|^2}\big[g(\theta_{t-1}) - g(\theta_*)\big]^2
\end{aligned}
$$

Convergence proof - gradient descent smooth convex functions - II

- Iteration: $\theta_t = \theta_{t-1} - \gamma g'(\theta_{t-1})$ with $\gamma = 1/L$

$$
\begin{aligned}
g(\theta_t) - g(\theta_*) &\leqslant g(\theta_{t-1}) - g(\theta_*) - \frac{1}{2L\|\theta_0 - \theta_*\|^2}\big[g(\theta_{t-1}) - g(\theta_*)\big]^2 \\
\text{of the form } \Delta_k &\leqslant \Delta_{k-1} - \alpha \Delta_{k-1}^2 \text{ with } 0 \leqslant \Delta_k = g(\theta_k) - g(\theta_*) \leqslant \frac{L}{2}\|\theta_k - \theta_*\|^2 \\
\frac{1}{\Delta_{k-1}} &\leqslant \frac{1}{\Delta_k} - \alpha \frac{\Delta_{k-1}}{\Delta_k} \text{ by dividing by } \Delta_k \Delta_{k-1} \\
\frac{1}{\Delta_{k-1}} &\leqslant \frac{1}{\Delta_k} - \alpha \text{ because } (\Delta_k) \text{ is non-increasing} \\
\frac{1}{\Delta_0} &\leqslant \frac{1}{\Delta_t} - \alpha t \text{ by summing from } k = 1 \text{ to } t \\
\Delta_t &\leqslant \frac{\Delta_0}{1 + \alpha t \Delta_0} \text{ by inverting} \\
&\leqslant \frac{2L\|\theta_0 - \theta_*\|^2}{t+4} \text{ since } \Delta_0 \leqslant \frac{L}{2}\|\theta_k - \theta_*\|^2 \text{ and } \alpha = \frac{1}{2L\|\theta_0 - \theta_*\|^2}
\end{aligned}
$$

Limits on convergence rate of first-order methods

- **First-order method**: any iterative algorithm that selects θ_t in $\theta_0 + \mathrm{span}(g'(\theta_0), \dots, g'(\theta_{t-1}))$

- **Problem class**: convex L-smooth functions with a global minimizer θ_*

- **Theorem**: for every integer $t \leqslant (d-1)/2$ and every θ_0, there exist functions in the problem class such that for any first-order method,

$$g(\theta_t) - g(\theta_*) \geqslant \frac{3}{32} \frac{L\|\theta_0 - \theta_*\|^2}{(t+1)^2}$$

– $O(1/t)$ rate for gradient method may not be optimal!

Limits on convergence rate of first-order methods
Proof sketch

- Define quadratic function

$$g_t(\theta) = \frac{L}{8}\Big[(\theta^1)^2 + \sum_{i=1}^{t-1}(\theta^i - \theta^{i+1})^2 + (\theta^t)^2 - 2\theta^1\Big]$$

  – Fact 1: g_t is L-smooth
  – Fact 2: minimizer supported by first t coordinates (closed form)
  – Fact 3: any first-order method starting from zero will be supported in the first k coordinates after iteration k
  – Fact 4: the minimum over this support in $\{1, \dots, k\}$ may be computed in closed form

- Given iteration k, take $g = g_{2k+1}$ and compute lower-bound on $\frac{g(\theta_k) - g(\theta_*)}{\|\theta_0 - \theta_*\|^2}$

Accelerated gradient methods (Nesterov, 1983)

- **Assumptions**
  - g convex with L-Lipschitz-cont. gradient , min. attained at θ_*

- **Algorithm**:

$$\begin{aligned}\theta_t &= \eta_{t-1} - \frac{1}{L} g'(\eta_{t-1}) \\ \eta_t &= \theta_t + \frac{t-1}{t+2}(\theta_t - \theta_{t-1})\end{aligned}$$

- **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 θ_*
  - g μ-strongly convex

- **Algorithm**:

$$\begin{aligned} \theta_t &= \eta_{t-1} - \frac{1}{L} g'(\eta_{t-1}) \\ \eta_t &= \theta_t + \frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}} (\theta_t - \theta_{t-1}) \end{aligned}$$

- **Bound**: $g(\theta_t) - g(\theta_*) \leqslant L\|\theta_0 - \theta_*\|^2 (1 - \sqrt{\mu/L})^t$
  - 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)
  - $\theta_{t+1} = \arg\min_{\theta \in \mathbb{R}^d} f(\theta_t) + (\theta - \theta_t)^\top \nabla f(\theta_t) + \frac{L}{2} \|\theta - \theta_t\|_2^2$
  - $\theta_{t+1} = \theta_t - \frac{1}{L} \nabla f(\theta_t)$

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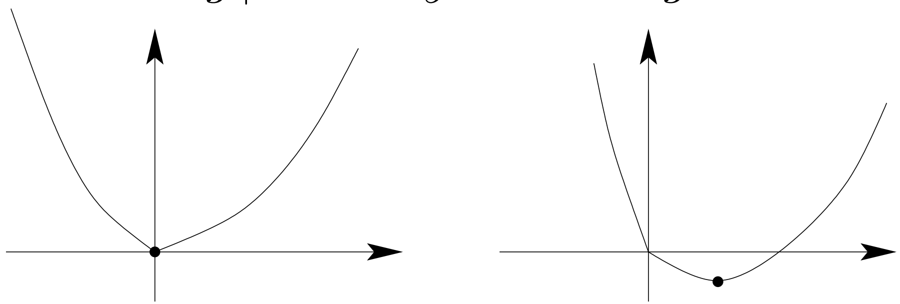
  - $\theta_{t+1} = \theta_t - \frac{1}{L} \nabla f(\theta_t)$

- Problems of the form: $\boxed{\min_{\theta \in \mathbb{R}^d} f(\theta) + \mu \Omega(\theta)}$
  - $\theta_{t+1} = \arg\min_{\theta \in \mathbb{R}^d} f(\theta_t) + (\theta - \theta_t)^\top \nabla f(\theta_t) + \mu \Omega(\theta) + \frac{L}{2} \|\theta - \theta_t\|_2^2$
  - $\Omega(\theta) = \|\theta\|_1 \Rightarrow$ **Thresholded gradient descent**

- Similar convergence rates than smooth optimization
  - Acceleration methods (Nesterov, 2007; Beck and Teboulle, 2009)

Soft-thresholding for the ℓ_1-norm

- **Example 1**: quadratic problem in 1D, i.e. $\boxed{\min_{x \in \mathbb{R}} \frac{1}{2}x^2 - xy + \lambda|x|}$
- 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., $y \geqslant \lambda$) $\Rightarrow x^* = y - \lambda$
  - $x \leqslant 0$ is the solution iff $g_- \geqslant 0$ (i.e., $y \leqslant -\lambda$) $\Rightarrow x^* = y + \lambda$

- Solution $\boxed{x^* = \operatorname{sign}(y)(|y| - \lambda)_+}$ = soft thresholding

Soft-thresholding for the ℓ_1-norm

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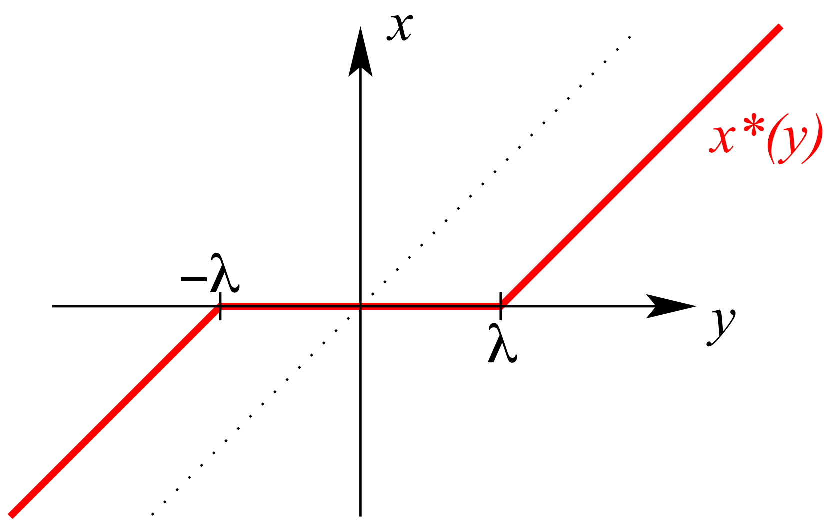

Projected gradient descent

- Problems of the form: $\boxed{\min_{\theta \in \mathcal{K}} f(\theta)}$
  - $\theta_{t+1} = \arg\min_{\theta \in \mathcal{K}} f(\theta_t) + (\theta - \theta_t)^\top \nabla f(\theta_t) + \frac{L}{2}\|\theta - \theta_t\|_2^2$
  - $\theta_{t+1} = \arg\min_{\theta \in \mathcal{K}} \frac{1}{2}\Big\|\theta - \big(\theta_t - \frac{1}{L}\nabla f(\theta_t)\big)\Big\|_2^2$
  - Projected gradient descent
- Similar convergence rates than smooth optimization
  - Acceleration methods (Nesterov, 2007; Beck and Teboulle, 2009)

Newton method

- Given θ_{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**: $\theta_t = \theta_{t-1} - f''(\theta_{t-1})^{-1} f'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ convergence rate

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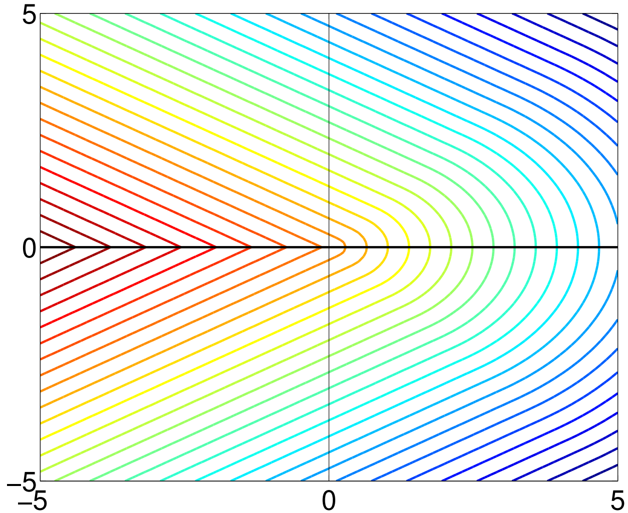
  - Optimal rates $O(1/t^2)$ and $O(e^{-t\sqrt{\mu/L}})$
- **Newton method**: $\theta_t = \theta_{t-1} - f''(\theta_{t-1})^{-1} f'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ convergence rate
- **From smooth to non-smooth**
  - Subgradient method and ellipsoid

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

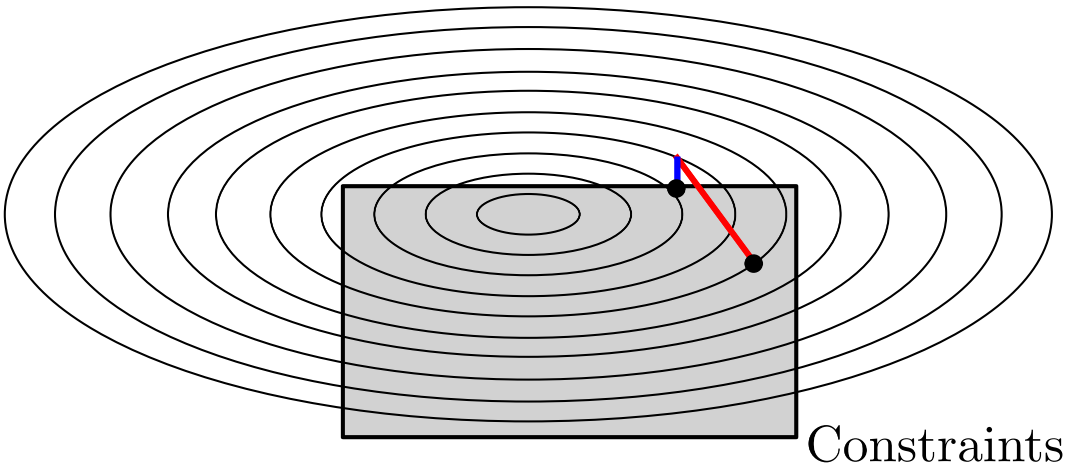
- $g(\theta_1, \theta_2) = \begin{cases} -5(9\theta_1^2 + 16\theta_2^2)^{1/2} & \text{if } \theta_1 > |\theta_2| \\ -(9\theta_1 + 16|\theta_2|)^{1/2} & \text{if } \theta_1 \leqslant |\theta_2| \end{cases}$

- Steepest descent starting from any θ 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**: $\theta_t = \Pi_D\left(\theta_{t-1} - \frac{2D}{B\sqrt{t}} g'(\theta_{t-1})\right)$
  - Π_D : orthogonal projection onto $\{\|\theta\|_2 \leqslant D\}$



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- **Algorithm**: $\theta_t = \Pi_D\Big(\theta_{t-1} - \dfrac{2D}{B\sqrt{t}} g'(\theta_{t-1})\Big)$
  - Π_D : orthogonal projection onto $\{\|\theta\|_2 \leqslant D\}$
- **Bound**:

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

- 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 $\|\theta\|_2 \leqslant D$

$$\begin{aligned}
\|\theta_t - \theta_*\|_2^2 &\leqslant \|\theta_{t-1} - \theta_* - \gamma_t g'(\theta_{t-1})\|_2^2 \text{ by contractivity of projections} \\
&\leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2\gamma_t^2 - 2\gamma_t(\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \text{ because } \|g'(\theta_{t-1})\|_2 \leqslant B \\
&\leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2\gamma_t^2 - 2\gamma_t\big[g(\theta_{t-1}) - g(\theta_*)\big] \text{ (property of subgradients)}
\end{aligned}$$

- leading to

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

Subgradient method/“descent” - proof - II

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

- Constant step-size $\gamma_t = \gamma$

$$\begin{aligned}\sum_{u=1}^{t}\big[g(\theta_{u-1}) - g(\theta_*)\big] &\leqslant \sum_{u=1}^{t}\frac{B^2\gamma}{2} + \sum_{u=1}^{t}\frac{1}{2\gamma}\big[\|\theta_{u-1} - \theta_*\|_2^2 - \|\theta_u - \theta_*\|_2^2\big] \\ &\leqslant t\frac{B^2\gamma}{2} + \frac{1}{2\gamma}\|\theta_0 - \theta_*\|_2^2 \leqslant t\frac{B^2\gamma}{2} + \frac{2}{\gamma}D^2\end{aligned}$$

- Optimized step-size $\gamma_T = \frac{2D}{B\sqrt{T}}$ depends on “horizon” T
  - Leads to bound of $2DB\sqrt{T}$

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

Subgradient method/"descent" - proof - III

- Starting from $\quad g(\theta_{t-1}) - g(\theta_*) \leqslant \dfrac{B^2\gamma_t}{2} + \dfrac{1}{2\gamma_t}\big[\|\theta_{t-1}-\theta_*\|_2^2 - \|\theta_t-\theta_*\|_2^2\big]$

- Decreasing step-size

$$\sum_{u=1}^{t}\big[g(\theta_{u-1}) - g(\theta_*)\big] \leqslant \sum_{u=1}^{t}\frac{B^2\gamma_u}{2} + \sum_{u=1}^{t}\frac{1}{2\gamma_u}\big[\|\theta_{u-1}-\theta_*\|_2^2 - \|\theta_u-\theta_*\|_2^2\big]$$

$$= \sum_{u=1}^{t}\frac{B^2\gamma_u}{2} + \sum_{u=1}^{t-1}\|\theta_u-\theta_*\|_2^2\Big(\frac{1}{2\gamma_{u+1}} - \frac{1}{2\gamma_u}\Big) + \frac{\|\theta_0-\theta_*\|_2^2}{2\gamma_1} - \frac{\|\theta_t-\theta_*\|_2^2}{2\gamma_t}$$

$$\leqslant \sum_{u=1}^{t}\frac{B^2\gamma_u}{2} + \sum_{u=1}^{t-1}4D^2\Big(\frac{1}{2\gamma_{u+1}} - \frac{1}{2\gamma_u}\Big) + \frac{4D^2}{2\gamma_1}$$

$$= \sum_{u=1}^{t}\frac{B^2\gamma_u}{2} + \frac{4D^2}{2\gamma_t} \leqslant 3DB\sqrt{t} \text{ with } \gamma_t = \frac{2D}{B\sqrt{t}}$$

- Using convexity: $\quad g\big(\frac{1}{t}\sum_{k=0}^{t-1}\theta_k\big) - g(\theta_*) \leqslant \frac{3DB}{\sqrt{t}}$

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 $\Theta = \{\|\theta\|_2 \leqslant D\}$

- **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 $O(n^2 d)$

Subgradient descent - strong convexity

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

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

- **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 μ-strong convexity of f

$$
\begin{aligned}
\|\theta_t - \theta_*\|_2^2 & \leqslant \|\theta_{t-1} - \theta_* - \gamma_t g'(\theta_{t-1})\|_2^2 \text{ by contractivity of projections} \\
& \leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2\gamma_t^2 - 2\gamma_t(\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \text{ because } \|g'(\theta_{t-1})\|_2 \leqslant \\
& \leqslant \|\theta_{t-1} - \theta_*\|_2^2 + B^2\gamma_t^2 - 2\gamma_t\big[g(\theta_{t-1}) - g(\theta_*) + \frac{\mu}{2}\|\theta_{t-1} - \theta_*\|_2^2\big] \\
& \qquad \text{(property of subgradients and strong convexity)}
\end{aligned}
$$

- leading to

$$
\begin{aligned}
g(\theta_{t-1}) - g(\theta_*) & \leqslant \frac{B^2\gamma_t}{2} + \frac{1}{2}\Big[\frac{1}{\gamma_t} - \mu\Big]\|\theta_{t-1} - \theta_*\|_2^2 - \frac{1}{2\gamma_t}\|\theta_t - \theta_*\|_2^2 \\
& \leqslant \frac{B^2}{\mu(t+1)} + \frac{\mu}{2}\Big[\frac{t-1}{2}\Big]\|\theta_{t-1} - \theta_*\|_2^2 - \frac{\mu(t+1)}{4}\|\theta_t - \theta_*\|_2^2
\end{aligned}
$$

Subgradient method - strong convexity - proof - II

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

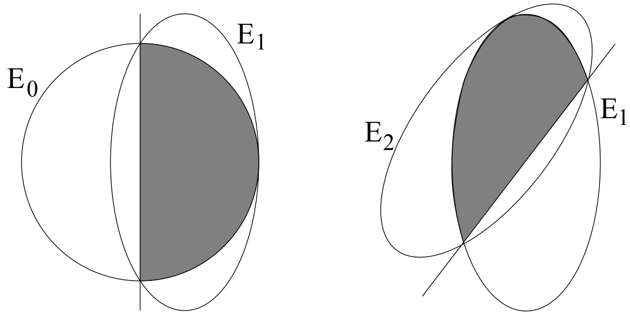
$$
\begin{aligned}
\sum_{u=1}^{t} u\big[g(\theta_{u-1}) - g(\theta_*)\big] &\leqslant \sum_{t=1}^{u} \frac{B^2 u}{\mu(u+1)} + \frac{1}{4}\sum_{u=1}^{t}\big[u(u-1)\|\theta_{u-1}-\theta_*\|_2^2 - u(u+1)\|\theta_u-\theta_*\|_2^2\big] \\
&\leqslant \quad \frac{B^2 t}{\mu} + \frac{1}{4}\big[0 - t(t+1)\|\theta_t-\theta_*\|_2^2\big] \leqslant \frac{B^2 t}{\mu}
\end{aligned}
$$

- Using convexity: $g\bigg(\dfrac{2}{t(t+1)}\displaystyle\sum_{u=1}^{t} u\theta_{u-1}\bigg) - g(\theta_*) \leqslant \dfrac{2B^2}{t+1}$

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

Ellipsoid method

- Minimizing convex function $g : \mathbb{R}^d \to \mathbb{R}$
  - Builds a sequence of ellipsoids that contains the global minima.



- Represent $E_t = \{\theta \in \mathbb{R}^d, (\theta - \theta_t)^\top P_t^{-1}(\theta - \theta_t) \leqslant 1\}$

- Fact 1: $\theta_{t+1} = \theta_t - \frac{1}{d+1} P_t h_t$ and $P_{t+1} = \frac{d^2}{d^2-1}(P_t - \frac{2}{d+1} P_t h_t h_t^\top P_t)$ with $h_t = \frac{1}{\sqrt{g'(\theta_t)^\top P_t g'(x_t)}} g'(\theta_t)$

- Fact 2: $\text{vol}(\mathcal{E}_t) \approx \text{vol}(\mathcal{E}_{t-1}) e^{-1/2d} \Rightarrow$ CV rate in $O(e^{-t/d^2})$

Summary: minimizing convex functions

- **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**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ convergence rate

Summary: minimizing convex functions

- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
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  - $O\big(e^{-\rho 2^t}\big)$ 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
  3. Testing errors are more important than training errors

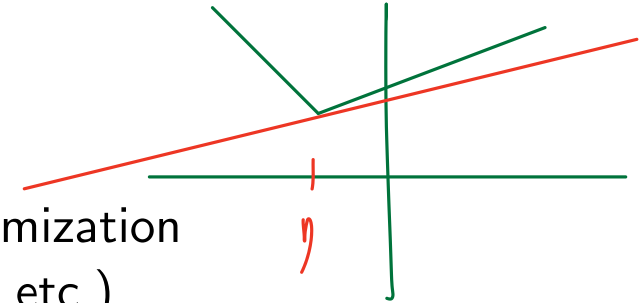
$\Rightarrow$ **Stochastic approximation**

Summary of rates of convergence

- Problem parameters
  - D diameter of the domain
  - B Lipschitz-constant
  - L smoothness constant
  - μ 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

$\forall \theta \in \mathbb{R}^d \quad f(\theta) \geqslant f(\eta) + \langle g_\eta, \theta - \eta \rangle$

2. **Classical methods for convex optimization**
   - Smooth optimization (gradient descent, Newton method)
   - Non-smooth optimization (subgradient descent)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**
   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging

5. **Smooth stochastic approximation algorithms**
   - Non-asymptotic analysis for smooth functions
   - Logistic regression
   - Least-squares regression without decaying step-sizes

6. **Finite data sets**
   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

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 $\theta_n \in \mathbb{R}^d$

$$\hat{R}_n(\theta) = \frac{1}{n} \sum_{i=1}^{n} \underbrace{f_i(\theta)}_{\text{loss of model } \theta \text{, on obs } x_i, y_i}$$

$$f_i(\theta) = \ell(\theta, (x_i, y_i)) = \tilde{\ell}(\theta(x_i), y_i)$$

$$R(\theta) = \mathbb{E}_p \left[\ell(\theta, (x, y)) \right]$$

$\hat{\theta}$ model built from data.

$\nabla \ell(\hat{\theta}, (x_i, y_i))$ unbiased est of $\nabla \mathbb{E}_{\rho}\left[\ell(\hat{\theta}, (x,y)) \,|\, \hat{\theta}\right]$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \parallel$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \nabla R(\hat{\theta})$

sup cdt°

$x_i, y_i \,|\, \hat{\theta} \sim \rho$

$$\left(\begin{array}{l} x_i, y_i \sim \rho \\ (x_i, y_i) \perp\!\!\!\perp \hat{\theta} \end{array} \right) \text{ sup cdt°}$$

given 1 new data point (x_n, y_n), I can build a stochastic oracle (unbiased) of the gradient of $R(\hat{\theta})$

generalization risk

$\hat{\theta} \perp\!\!\!\perp (x_n, y_n)$

Stochastic approximation

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

- **Machine learning - statistics**
  - **loss for a single pair of observations**: $\boxed{f_n(\theta) = \ell(y_n, \theta^\top \Phi(x_n))}$
  - $f(\theta) = \mathbb{E} f_n(\theta) = \mathbb{E}\, \ell(y_n, \theta^\top \Phi(x_n))$ = **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

- **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**
  - (much) broader applicability beyond convex optimization

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

  - Beyond convex problems, i.i.d assumption, finite dimension, etc.
  - Typically asymptotic results (see next lecture)
  - 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 θ
  - 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 θ
  - Using the gradients of single i.i.d. observations

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

Relationship to online learning

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

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  - Estimator $\hat{\theta}$ = Minimizer of $\hat{f}(\theta)$ over a certain class Θ
  - 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**
  - L- Smoothness: ~~f B-Lipschitz continuous~~, f' L-Lipschitz continuous
  - Strong convexity: f μ-strongly convex
  - B - Lipschitz : f B - Lipschitz

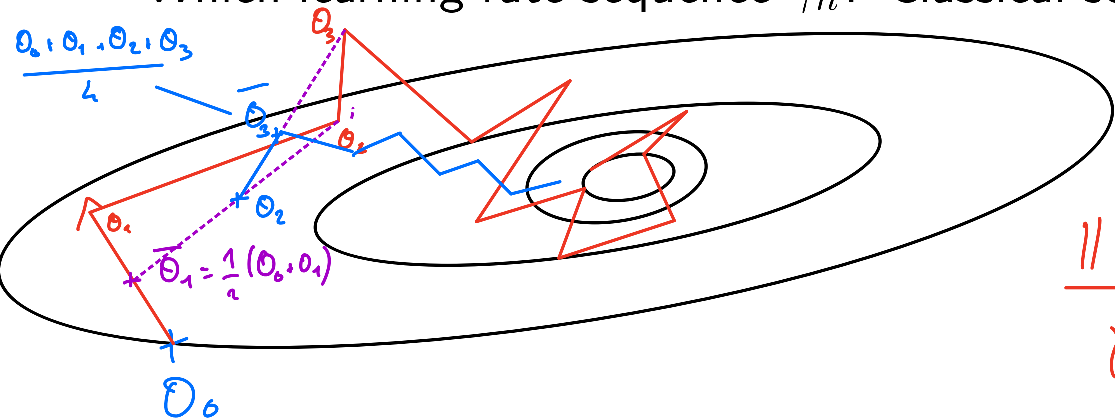
Convex stochastic approximation

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

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

$$\boxed{\theta_n = \theta_{n-1} - \gamma_n f_n'(\theta_{n-1})}$$

  - Polyak-Ruppert averaging: $\bar{\theta}_n = \frac{1}{n}\sum_{k=0}^{n-1}\theta_k$ $\rightarrow$ $\tilde{\theta}_n = \frac{1}{\frac{n(n+1)}{2}}\sum_{0}^{n-1} k\,\theta_n$
  - Which learning rate sequence γ_n? Classical setting: $\boxed{\gamma_n = Cn^{-\alpha}}$



$$\frac{\|\theta_0 - \theta_*\|^2}{\gamma t} + \underline{\underline{\gamma\sigma^2}}$$

Convex stochastic approximation

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

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

- **Desirable practical behavior**
  - Applicable (at least) to classical supervised learning problems
  - Robustness to (potentially unknown) constants (L,B,μ)
  - Adaptivity to difficulty of the problem (e.g., strong convexity)

Stochastic subgradient "descent"/method

- **Assumptions**
  - f_n convex and B-Lipschitz-continuous on $\{\|\theta\|_2 \leqslant D\} = \mathcal{C}$
  - (f_n) i.i.d. functions such that $\mathbb{E} f_n = f$
  - θ_* global optimum of f on $\mathcal{C} = \{\|\theta\|_2 \leqslant D\}$

- **Algorithm**: $\theta_n = \Pi_D\Big(\theta_{n-1} - \dfrac{2D}{B\sqrt{n}} f_n'(\theta_{n-1})\Big)$

Stochastic subgradient "descent"/method

- **Assumptions**
  - f_n convex and B-Lipschitz-continuous on $\{\|\theta\|_2 \leqslant D\}$
  - (f_n) i.i.d. functions such that $\mathbb{E} f_n = f$
  - θ_* global optimum of f on $\mathcal{C} = \{\|\theta\|_2 \leqslant D\}$

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

$\forall t \in [\![1;n]\!]$

$\gamma_t = \frac{2D}{B\sqrt{n}}$

- **Bound**:

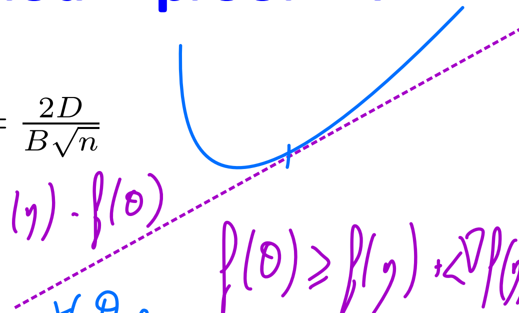
$$\mathbb{E} f\Big(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\Big) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$$

- "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

Stochastic subgradient method - proof - I



- Iteration: $\theta_n = \Pi_D(\theta_{n-1} - \gamma_n f'_n(\theta_{n-1}))$ with $\gamma_n = \frac{2D}{B\sqrt{n}}$

$\langle \nabla f(\eta), \eta - \theta \rangle \geqslant f(\eta) - f(\theta)$

- $\mathcal{F}_n$: information up to time n

$\langle \nabla f(\eta), \eta - \theta^* \rangle \geqslant f(\eta) - f(\theta^*)$ $\quad \forall \theta, \eta \quad$ $f(\theta) \geqslant f(\eta) + \langle \nabla f(\eta), \theta - \eta \rangle$

- $\|f'_n(\theta)\|_2 \leqslant B$ and $\|\theta\|_2 \leqslant D$, unbiased gradients/functions $\mathbb{E}(f_n|\mathcal{F}_{n-1}) = f$

$$\|\theta_n - \theta_*\|_2^2 \leqslant \|\theta_{n-1} - \theta_* - \gamma_n f'_n(\theta_{n-1})\|_2^2 \text{ by contractivity of projections}$$

$$\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f'_n(\theta_{n-1}) \text{ because } \|f'_n(\theta_{n-1})\|_2$$

$\mathbb{E}\left[f'_n(\theta_{n-1}) \mid \mathcal{F}_{n-1} \right] = f'(\theta_{n-1})$

$$\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2 | \mathcal{F}_{n-1}\big] \leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f'(\theta_{n-1})$$

$$\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*)\big] \text{ (subgradient prope}$$

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

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

$\gamma_t = \frac{1}{\sqrt{t}}$ $\forall t \in [\![1;T]\!]$, $\gamma_t = \gamma_0 = \frac{1}{\sqrt{T}}$

Stochastic subgradient method - proof - II

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

$\left(-\frac{1}{2\gamma_u} + \frac{1}{2\gamma_{u+1}}\right)$ $\mathbb{E}\|\theta_u - \theta_*\|^2$

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

$c\gamma + \frac{d}{\gamma} \geq 2\sqrt{cd}$

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

$\forall k \in [\![1;n]\!]$

$= \frac{B^2\gamma_n}{2} + \frac{4D^2}{2\gamma_n}$

$\gamma_n = \frac{2D}{B\sqrt{n}}$

$2ab \leq a^2 + b^2$

- 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 method
Extension to online learning

- Assume different and arbitrary functions $f_n : \mathbb{R}^d \to \mathbb{R}$
  - Observations of $f_n'(\theta_{n-1}) + \varepsilon_n$
  - with $\mathbb{E}(\varepsilon_n | \mathcal{F}_{n-1}) = 0$ and $\| f_n'(\theta_{n-1}) + \varepsilon_n \| \leqslant B$ almost surely

- **Performance criterion**: (normalized) regret

$$\frac{1}{n}\sum_{i=1}^{n} f_i(\theta_{i-1}) - \inf_{\|\theta\|_2 \leqslant D} \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$$

  - Warning: often not normalized
  - May not be non-negative (typically is)

Stochastic subgradient method - online learning - I

- Iteration: $\theta_n = \Pi_D(\theta_{n-1} - \gamma_n(f_n'(\theta_{n-1}) + \varepsilon_n))$ with $\gamma_n = \frac{2D}{B\sqrt{n}}$
- $\mathcal{F}_n$: information up to time n - θ an arbitrary point such that $\|\theta\| \leqslant D$
- $\|f_n'(\theta_{n-1}) + \varepsilon_n\|_2 \leqslant B$ and $\|\theta\|_2 \leqslant D$, unbiased gradients $\mathbb{E}(\varepsilon_n|\mathcal{F}_{n-1}) = 0$

$$\begin{aligned}\|\theta_n - \theta\|_2^2 &\leqslant \|\theta_{n-1} - \theta - \gamma_n(f_n'(\theta_{n-1}) + \varepsilon_n)\|_2^2 \text{ by contractivity of projections}\\ &\leqslant \|\theta_{n-1} - \theta\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta)^\top(f_n'(\theta_{n-1}) + \varepsilon_n) \text{ because } \|f_n'(\theta_{n-1}) +\end{aligned}$$

$$\begin{aligned}\mathbb{E}\big[\|\theta_n - \theta\|_2^2|\mathcal{F}_{n-1}\big] &\leqslant \|\theta_{n-1} - \theta\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta)^\top f_n'(\theta_{n-1})\\ &\leqslant \|\theta_{n-1} - \theta\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f_n(\theta_{n-1}) - f_n(\theta)\big] \text{ (subgradient proper}\\ \mathbb{E}\|\theta_n - \theta\|_2^2 &\leqslant \mathbb{E}\|\theta_{n-1} - \theta\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[\mathbb{E}f_n(\theta_{n-1}) - f_n(\theta)\big]\end{aligned}$$

- leading to $\mathbb{E}f_n(\theta_{n-1}) - f_n(\theta) \leqslant \dfrac{B^2\gamma_n}{2} + \dfrac{1}{2\gamma_n}\big[\mathbb{E}\|\theta_{n-1} - \theta\|_2^2 - \mathbb{E}\|\theta_n - \theta\|_2^2\big]$

Stochastic subgradient method - online learning - II

- Starting from $\mathbb{E} f_n(\theta_{n-1}) - f_n(\theta) \leqslant \frac{B^2\gamma_n}{2} + \frac{1}{2\gamma_n}\big[\mathbb{E}\|\theta_{n-1} - \theta\|_2^2 - \mathbb{E}\|\theta_n - \theta\|_2^2\big]$

$$\sum_{u=1}^n \big[\mathbb{E} f_u(\theta_{u-1}) - f_u(\theta)\big] \leqslant \sum_{u=1}^n \frac{B^2\gamma_u}{2} + \sum_{u=1}^n \frac{1}{2\gamma_u}\big[\mathbb{E}\|\theta_{u-1} - \theta\|_2^2 - \mathbb{E}\|\theta_u - \theta\|_2^2\big]$$

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

- For any θ such that $\|\theta\| \leqslant D$: $\frac{1}{n}\sum_{k=1}^n \mathbb{E} f_k(\theta_{k-1}) - \frac{1}{n}\sum_{k=1}^n f_k(\theta) \leqslant \frac{2DB}{\sqrt{n}}$

- Online to batch conversion: assuming convexity

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 μ-strongly convex on $\{\|\theta\|_2 \leqslant D\}$
  - θ_* global optimum of f over $\{\|\theta\|_2 \leqslant D\}$

γ_n depends on μ
$\neq$t algo for cvx
vs strgly cvx.

- **Algorithm**: $\theta_n = \Pi_D\Big(\theta_{n-1} - \dfrac{2}{\mu(n+1)} f_n'(\theta_{n-1})\Big)$

- **Bound**:

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

- "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: $\|f_n'(\theta)\|_2 \leqslant B$ and $\|\theta\|_2 \leqslant D$ and μ-strong convexity of f

$$\begin{aligned}
\|\theta_n - \theta_*\|_2^2 &\leqslant \|\theta_{n-1} - \theta_* - \gamma_n f_n'(\theta_{t-1})\|_2^2 \text{ by contractivity of projections} \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{t-1}) \text{ because } \|f_n'(\theta_{t-1})\|_2 \\
\mathbb{E}(\cdot|\mathcal{F}_{n-1}) &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*) + \frac{\mu}{2}\|\theta_{n-1} - \theta_*\|_2^2\big]
\end{aligned}$$

(property of subgradients and strong convexity)

- leading to

$$f(\theta) \geqslant f(\eta) + \nabla f(\eta)^\top(\theta - \eta) + \frac{\mu}{2}\|\theta - \eta\|^2$$

$$\Longrightarrow \nabla f(\eta)(\eta - \theta_*) \geqslant f(\eta) - f(\theta_*) + \frac{\mu}{2}\|\theta - \theta_*\|^2$$

$$\begin{aligned}
\mathbb{E}f(\theta_{n-1}) - f(\theta_*) &\leqslant \frac{B^2\gamma_n}{2} + \frac{1}{2}\Big[\frac{1}{\gamma_n} - \mu\Big]\|\theta_{n-1} - \theta_*\|_2^2 - \frac{1}{2\gamma_n}\|\theta_n - \theta_*\|_2^2 \\
&\leqslant \frac{B^2}{\mu(n+1)} + \frac{\mu}{2}\Big[\frac{n-1}{2}\Big]\|\theta_{n-1} - \theta_*\|_2^2 - \frac{\mu(n+1)}{4}\|\theta_n - \theta_*\|_2^2
\end{aligned}$$

Stochastic subgradient - strong convexity - proof - II

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

$$\sum_{u=1}^{n} u\left[\mathbb{E} f(\theta_{u-1}) - f(\theta_*)\right] \leqslant \sum_{u=1}^{n} \frac{B^2 u}{\mu(u+1)} + \frac{1}{4}\sum_{u=1}^{n}\left[u(u-1)\mathbb{E}\|\theta_{u-1} - \theta_*\|_2^2 - u(u+1)\mathbb{E}\|\theta_u\right.$$

$$\leqslant \frac{B^2 n}{\mu} + \frac{1}{4}\left[0 - n(n+1)\mathbb{E}\|\theta_n - \theta_*\|_2^2\right] \leqslant \frac{B^2 n}{\mu}$$

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

- 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 $\mathbb{E} f_n = f$
  - θ_* global optimum of $g = f + \frac{\mu}{2} \| \cdot \|_2^2$
  - No compactness assumption - no projections

- **Algorithm**:

$$\theta_n = \theta_{n-1} - \frac{2}{\mu(n+1)} g_n'(\theta_{n-1}) = \theta_{n-1} - \frac{2}{\mu(n+1)} \big[f_n'(\theta_{n-1}) + \mu \theta_{n-1} \big]$$

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

- Minimax convergence rate

Strong convexity - proof with $\log n$ factor - I

- Iteration: $\theta_n = \Pi_D(\theta_{n-1} - \gamma_n f_n'(\theta_{t-1}))$ with $\gamma_n = \frac{1}{\mu n}$

- Assumption: $\|f_n'(\theta)\|_2 \leqslant B$ and $\|\theta\|_2 \leqslant D$ and μ-strong convexity of f

$$
\begin{aligned}
\|\theta_n - \theta_*\|_2^2 &\leqslant \|\theta_{n-1} - \theta_* - \gamma_n f_n'(\theta_{t-1})\|_2^2 \text{ by contractivity of projections} \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{t-1}) \text{ because } \|f_n'(\theta_{t-1})\|_2 \\
\mathbb{E}(\cdot|\mathcal{F}_{n-1}) &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*) + \frac{\mu}{2}\|\theta_{n-1} - \theta_*\|_2^2\big]
\end{aligned}
$$

(property of subgradients and strong convexity)

- leading to

$$
\begin{aligned}
\mathbb{E}f(\theta_{n-1}) - f(\theta_*) &\leqslant \frac{B^2\gamma_n}{2} + \frac{1}{2}\Big[\frac{1}{\gamma_n} - \mu\Big]\|\theta_{n-1} - \theta_*\|_2^2 - \frac{1}{2\gamma_n}\|\theta_n - \theta_*\|_2^2 \\
&\leqslant \frac{B^2}{2\mu n} + \frac{\mu}{2}\big[n-1\big]\|\theta_{n-1} - \theta_*\|_2^2 - \frac{n\mu}{2}\|\theta_n - \theta_*\|_2^2
\end{aligned}
$$

Strong convexity - proof with $\log n$ factor - II

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

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

$$\frac{\sum 1}{n^2} \text{ vs } \frac{\sum 1/k}{n} \qquad \leqslant \frac{B^2 \log n}{2\mu} + \frac{1}{2}\big[0 - n\mathbb{E}\|\theta_n - \theta_*\|_2^2\big] \leqslant \frac{B^2 \log n}{2\mu}$$

- Using convexity: $\boxed{\mathbb{E} f\Big(\dfrac{1}{n}\displaystyle\sum_{u=1}^n \theta_{u-1}\Big) - f(\theta_*) \leqslant \dfrac{B^2}{2\mu}\dfrac{\log n}{n}}$

- Why could this be useful?

Stochastic subgradient descent - strong convexity
Online learning

- Need $\log n$ term for uniform averaging. For all θ:

$$\frac{1}{n}\sum_{i=1}^{n} f_i(\theta_{i-1}) - \frac{1}{n}\sum_{i=1}^{n} f_i(\theta) \leqslant \frac{B^2}{2\mu}\frac{\log n}{n}$$

- Optimal. See Hazan and Kale (2014).

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**: $\mathbb{E}f\Big(\frac{1}{n}\sum_{k=0}^{n-1}\theta_k\Big) - f(\theta_*) \leqslant \frac{2DB}{\sqrt{n}}$
  - Obtained with simple conditioning arguments

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

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

- See also Bach (2013) for logistic regression

Stochastic subgradient method - high probability - 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
- $\|f_n'(\theta)\|_2 \leqslant B$ and $\|\theta\|_2 \leqslant D$, unbiased gradients/functions $\mathbb{E}(f_n|\mathcal{F}_{n-1}) = f$

$$\begin{aligned}\|\theta_n - \theta_*\|_2^2 &\leqslant \|\theta_{n-1} - \theta_* - \gamma_n f_n'(\theta_{n-1})\|_2^2 \text{ by contractivity of projections} \\ &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{n-1}) \text{ because } \|f_n'(\theta_{n-1})\|_2\end{aligned}$$

$$\begin{aligned}\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2|\mathcal{F}_{n-1}\big] &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f'(\theta_{n-1}) \\ &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*)\big] \text{ (subgradient prope}\end{aligned}$$

- Without expectations and with $Z_n = -2\gamma_n(\theta_{n-1} - \theta_*)^\top [f_n'(\theta_{n-1}) - f'(\theta_{n-1})]$

$$\|\theta_n - \theta_*\|_2^2 \leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*)\big] + Z_n$$

$\mathbb{E}(Z_n | \mathcal{F}_{n-1}) = 0$

Stochastic subgradient method - high probability - II

- Without expectations and with $Z_n = -2\gamma_n(\theta_{n-1} - \theta_*)^\top [f_n'(\theta_{n-1}) - f'(\theta_{n-1})]$

$$
\begin{aligned}
\|\theta_n - \theta_*\|_2^2 &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 + B^2\gamma_n^2 - 2\gamma_n\big[f(\theta_{n-1}) - f(\theta_*)\big] + Z_n \\
f(\theta_{n-1}) - f(\theta_*) &\leqslant \frac{1}{2\gamma_n}\big[\|\theta_{n-1} - \theta_*\|_2^2 - \|\theta_n - \theta_*\|_2^2\big] + \frac{B^2\gamma_n}{2} + \frac{Z_n}{2\gamma_n}
\end{aligned}
$$

$$
\begin{aligned}
\sum_{u=1}^n \big[f(\theta_{u-1}) - f(\theta_*)\big] &\leqslant \sum_{u=1}^n \frac{B^2\gamma_u}{2} + \sum_{u=1}^n \frac{1}{2\gamma_u}\big[\|\theta_{u-1} - \theta_*\|_2^2 - \|\theta_u - \theta_*\|_2^2\big] + \sum_{u=1}^n \frac{Z_u}{2\gamma_u} \\
&\leqslant \sum_{u=1}^n \frac{B^2\gamma_u}{2} + \frac{4D^2}{2\gamma_n} + \sum_{u=1}^n \frac{Z_u}{2\gamma_u} \leqslant \frac{2DB}{\sqrt{n}} + \sum_{u=1}^n \frac{Z_u}{2\gamma_u} \text{ with } \gamma_n = \frac{2D}{B\sqrt{n}}
\end{aligned}
$$

- Need to study $\displaystyle\sum_{u=1}^n \frac{Z_u}{2\gamma_u}$ with $\mathbb{E}(Z_n|\mathcal{F}_{n-1}) = 0$ and $|Z_n| \leqslant 8\gamma_n DB$

Stochastic subgradient method - high probability - III

- Need to study $\displaystyle\sum_{u=1}^{n}\frac{Z_u}{2\gamma_u}$ with $\mathbb{E}(\frac{Z_n}{2\gamma_n}|\mathcal{F}_{n-1}) = 0$ and $\dfrac{|Z_n|}{2\gamma_n} \leqslant 4DB$

- Azuma-Hoeffding inequality for bounded martingale increments:

$$\mathbb{P}\Big(\sum_{u=1}^{n}\frac{Z_u}{2\gamma_u} \geqslant t\sqrt{n}\cdot 4DB\Big) \leqslant \exp\Big(-\frac{t^2}{2}\Big)$$

- Moments with Burkholder-Rosenthal-Pinelis inequality (Pinelis, 1994)

Beyond stochastic gradient method

$$\Omega(\theta) = 1\!\!1_{\mathcal{C}}(\theta) = \begin{cases} 0 & \text{if } \theta \in \mathcal{C} \\ +\infty & \text{otherwise} \end{cases}$$

- **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

$$\theta_n = \min_{\theta \in \mathbb{R}^d} \underbrace{\big\| \theta - \theta_{n-1} + \gamma_n f_n'(\theta_n) \big\|_2^2 + C\Omega(\theta)}$$

$$= \min_{\theta \in \mathcal{C}} \| \theta - \theta_{n-1} - \gamma f_n' \|^2$$

$$= \Pi_{\mathcal{C}} (\theta_{n-1} - \gamma f_n')$$

  - 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)

Mirror descent

- Projected (stochastic) gradient descent adapted to Euclidean geometry
  - bound: $$\frac{\overbrace{\max_{\theta,\theta'\in\Theta}\|\theta-\theta'\|_2}^{2D} \cdot \overbrace{\max_{\theta\in\Theta}\|f'(\theta)\|_2}^{B}}{\sqrt{n}}$$

$\|f'(\theta)\|_2 \leqslant \sqrt{d}\, \|f'(\theta)\|_\infty$

- What about other norms?
  - Example: natural bound on $\max_{\theta\in\Theta}\|f'(\theta)\|_\infty$ leads to $\sqrt{d}$ factor
  - Avoidable with mirror descent, which leads to factor $\sqrt{\log d}$
  - Nemirovski et al. (2009); Lan et al. (2012)

Mirror descent

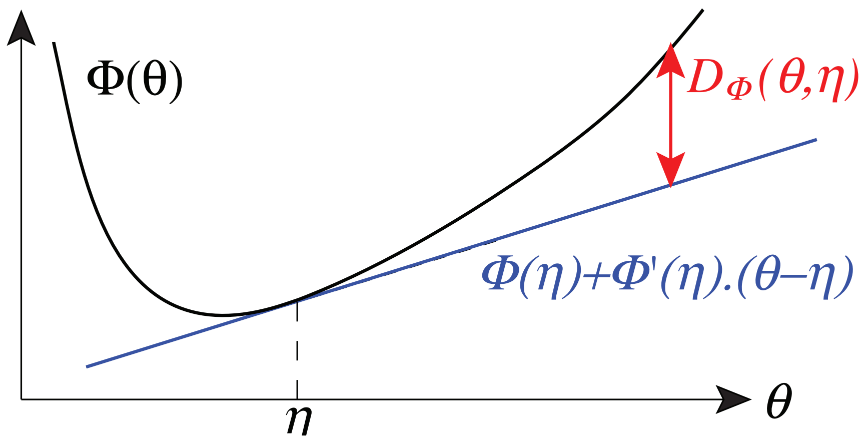
- Projected (stochastic) gradient descent adapted to Euclidean geometry
  - bound: $\dfrac{\max_{\theta,\theta'\in\Theta}\|\theta-\theta'\|_2 \cdot \max_{\theta\in\Theta}\|f'(\theta)\|_2}{\sqrt{n}}$
- What about other norms?
  - Example: natural bound on $\max_{\theta\in\Theta}\|f'(\theta)\|_\infty$ leads to $\sqrt{d}$ factor
  - Avoidable with mirror descent, which leads to factor $\sqrt{\log d}$
  - Nemirovski et al. (2009); Lan et al. (2012)
- From Hilbert to Banach spaces
  - Gradient $f'(\theta)$ defined through $f(\theta+d\theta)-f(\theta)=\langle f'(\theta),d\theta\rangle$ for a certain dot-product
  - Generally, the differential is an element of the dual space

Mirror descent set-up

- Function f defined on domain $\mathcal{C}$
- Arbitrary norm $\|\cdot\|$ with dual norm $\|s\|_* = \sup_{\|\theta\|\leqslant 1} \theta^\top s$
- B-Lipschitz-continuous function w.r.t. $\|\cdot\|$: $\|f'(\theta)\|_* \leqslant B$
- Given a strictly-convex function Φ, define the Bregman divergence

$$D_\Phi(\theta,\eta) = \Phi(\theta) - \Phi(\eta) - \Phi'(\eta)^\top(\theta - \eta)$$ > 0 if $\theta \neq \eta$

non symetric



Mirror map

- Strongly-convex function $\Phi : \mathcal{C}_\Phi \to \mathbb{R}$ such that

(a) the gradient Φ' takes all possible values in $\mathbb{R}^d$, leading to a bijection from $\mathcal{C}_\Phi$ to $\mathbb{R}^d$

(b) the gradient Φ' diverges on the boundary of $\mathcal{C}_\Phi$

(c) $\mathcal{C}_\Phi$ contains the closure of the domain $\mathcal{C}$ of the optimization problem

- Bregman projection on $\mathcal{C}$ uniquely defined on $\mathcal{C}_\Phi$:

$$
\begin{aligned}
\Pi_{\mathcal{C}}^{\Phi}(\theta) &= \arg \min_{\eta \in \mathcal{C}_\Phi \cap \mathcal{C}} D_\Phi(\eta, \theta) \\
&= \arg \min_{\eta \in \mathcal{C}_\Phi \cap \mathcal{C}} \Phi(\eta) - \Phi(\theta) - \Phi'(\theta)^\top (\eta - \theta) \\
&= \arg \min_{\eta \in \mathcal{C}_\Phi \cap \mathcal{C}} \Phi(\eta) - \Phi'(\theta)^\top \eta
\end{aligned}
$$

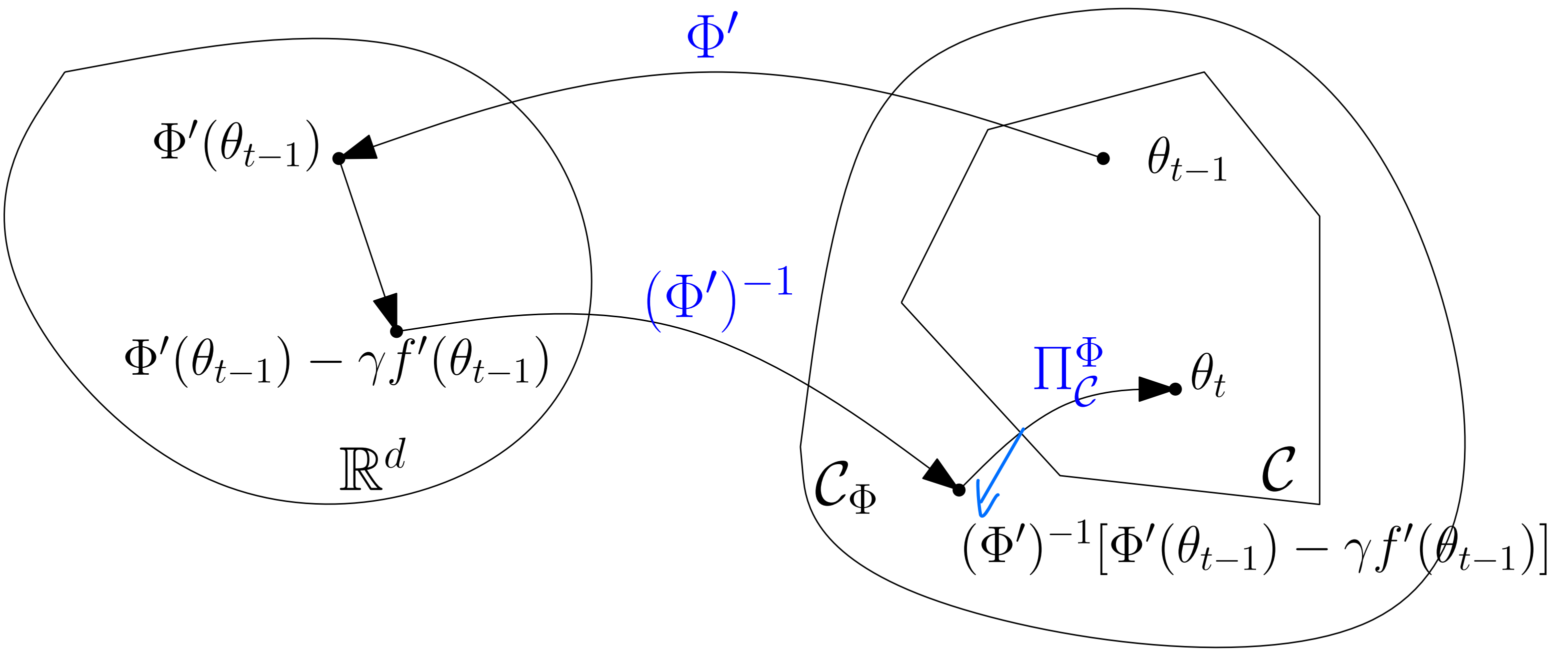
$\forall \eta \in -\ ;\ \langle \Phi'(\eta) - \Phi'(\theta), \Pi_c(\theta) - \eta \rangle$

- Example of squared Euclidean norm and entropy

Mirror descent

- **Iteration**:

$$\theta_t \quad = \quad \Pi_{\mathcal{C}}^{\Phi}\big(\Phi'^{-1}\big[\Phi'(\theta_{t-1}) - \gamma f'(\theta_{t-1})\big]\big)$$



Mirror descent

$\| f'(\theta) \|_*$

- **Iteration**:

$$\theta_t = \Pi_{\mathcal{C}}^{\Phi}\big(\Phi'^{-1}\big[\Phi'(\theta_{t-1}) - \gamma f'(\theta_{t-1})\big]\big)$$

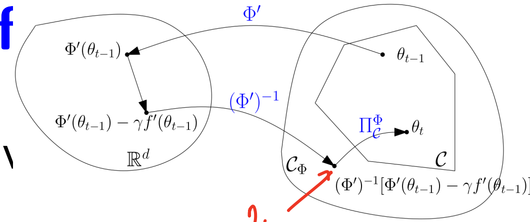
- **Convergence**: assume (a) $D^2 = \sup_{\theta\in\mathcal{C}} \Phi(\theta) - \inf_{\theta\in\mathcal{C}} \Phi(\theta)$, (b) Φ is α-strongly convex with respect to $\|\cdot\|$ and (c) f is B-Lipschitz-continuous wr.t. $\|\cdot\|$. Then with $\gamma = \frac{D}{B}\sqrt{\frac{2\alpha}{t}}$:

$$f\Big(\frac{1}{t}\sum_{u=1}^{t}\theta_u\Big) - \inf_{\theta\in\mathcal{C}} f(\theta) \leqslant DB\sqrt{\frac{2}{\alpha t}}$$

  – See detailed proof in Bubeck (2015, p. 299)
  – "Same" as subgradient method + allows stochastic gradients

$D_\phi(\theta,\eta) = \phi(\eta) - \phi(\theta) - \langle \phi'(\eta), \theta-\eta \rangle$

Mirror descent (proof



- Define $\Phi'(\eta_t) = \Phi'(\theta_{t-1}) - \gamma f'(\theta_{t-1})$. We hav

cvxty

$$
\begin{aligned}
f(\theta_{t-1}) - f(\theta) &\leqslant f'(\theta_{t-1})^\top(\theta_{t-1}-\theta) = \frac{1}{\gamma}(\Phi'(\theta_{t-1}) - \Phi'(\eta_t))^\top(\theta_{t-1}-\theta) \\
&= \frac{1}{\gamma}\big[D_\Phi(\theta,\theta_{t-1}) + D_\Phi(\theta_{t-1},\eta_t) - D_\Phi(\theta,\eta_t)\big]
\end{aligned}
$$

$\langle \phi'(\theta_{t-1}), \theta-\theta_{t-1}\rangle$ $\langle \phi'(\eta_t), \theta_{t-1}-\cancel{\eta_t}\rangle$ $-\langle \phi'(\eta_t), \theta-\cancel{\eta_t}\rangle$

def of Π_C

- By optimality of θ_t: $(\Phi'(\theta_t) - \Phi'(\eta_t))^\top(\theta_t - \theta) \leqslant 0$ which is equivalent to: $D_\Phi(\theta,\eta_t) \geqslant D_\Phi(\theta,\theta_t) + D_\Phi(\theta_t,\eta_t)$. Thus

$$
\begin{aligned}
D_\Phi(\theta_{t-1},\eta_t) - D_\Phi(\theta_t,\eta_t) &= \Phi(\theta_{t-1}) - \Phi(\theta_t) - \Phi'(\eta_t)^\top(\theta_{t-1}-\theta_t) \\
&\leqslant (\Phi'(\theta_{t-1}) - \Phi'(\eta_t))^\top(\theta_{t-1}-\theta_t) - \frac{\alpha}{2}\|\theta_{t-1}-\theta_t\|^2 \\
&= \gamma f'(\theta_{t-1})^\top(\theta_{t-1}-\theta_t) - \frac{\alpha}{2}\|\theta_{t-1}-\theta_t\|^2 \\
&\leqslant \gamma B\|\theta_{t-1}-\theta_t\| - \frac{\alpha}{2}\|\theta_{t-1}-\theta_t\|^2 \leqslant \frac{(\gamma B)^2}{2\alpha}
\end{aligned}
$$

α strg cvxty ϕ

$a^\top b \leq \|a\|_* \|b\|$

$\alpha x - \beta x^2$ $\leq$

- Thus $\sum_{u=1}^t \big[f(\theta_{t-1}) - f(\theta)\big] \leqslant \frac{D_\Phi(\theta,\theta_0)}{\gamma} + \gamma\frac{B^2 t}{2\alpha}$

telescope

$\Phi' = Id$! :)

Mirror descent examples

- **Euclidean**: $\Phi = \frac{1}{2}\|\cdot\|_2^2$ with $\|\cdot\| = \|\cdot\|_2$ and $\mathcal{C}_\Phi = \mathbb{R}^d$
  - Regular gradient descent

$\theta_i \log \theta_i - \cancel{\eta_i \log \eta_i} - (\log \eta_i + 1)(\theta_i - \cancel{\eta_i}) = \theta_i \log \frac{\theta_i}{\eta_i} + \Sigma \theta_i - \Sigma \eta_i$ $\quad 0$

- **Simplex**: $\Phi(\theta) = \sum_{i=1}^d \theta_i \log \theta_i$ with $\|\cdot\| = \|\cdot\|_1$ and $\mathcal{C}_\Phi = \{\theta \in \mathbb{R}_+^d, \sum_{i=1}^d \theta_i = 1\}$

$\Phi(\theta) - \Phi(\eta) - \Phi'(\eta)^\top(\theta - \eta) =$

  - Bregman divergence $=$ Kullback-Leibler divergence
  - Iteration (multiplicative update): $\theta_t \propto \theta_{t-1} \exp(-\gamma f'(\theta_{t-1}))$
  - Constant: $D^2 = \log d$, $\alpha = 1$

- ℓ_p-**ball**: $\Phi(\theta) = \frac{1}{2}\|\theta\|_p^2$, with $\|\cdot\| = \|\cdot\|_p$, $p \in (1, 2]$
  - We have $\alpha = p - 1$
  - Typically used with $p = 1 + \frac{1}{\log d}$ to cover the ℓ_1-geometry
  - See Duchi et al. (2010)

Reminder. **ML framework:** $(x_i, y_i)_{i=1\dots n}$. i.i.d. $\sim \rho$.

$$\min_{\theta \in \mathbb{R}^d} \left\{ R(\theta) := \mathbb{E}_\rho \left[\ell(\theta, (x,y)) \right] \right\}$$

n unbiased estimates of $R(\theta)$, $\nabla R(\theta)$

also if $(x_n, y_n) \perp\!\!\!\perp \theta_{n-1}$

$$\mathbb{E}\left[\nabla \ell(\theta, x_n, y_n) \mid \theta_{n-1}\right] = \nabla R(\theta_{n-1})$$

More general setting: SA : find 0 of a function $h : \mathbb{R}^d \to \mathbb{R}^d$

$\longrightarrow$ Stochastic subgradient descent

Averaging + **link to online learning** : cv of $\frac{1}{n} \sum_{i=1}^{n} f_i(\theta_i) - f_*$

$\geq$

$f(\bar{\theta}_n) - f(\theta_*)$

Non-smooth analysis:

w. or w.o. strg cvxty.

$\gamma_n = \frac{1}{\sqrt{n}} \longrightarrow f(\bar{\theta}_n) - f_* \leq O\left(\frac{1}{\sqrt{n}}\right)$

$\gamma_n \propto \frac{2}{\mu(n+1)}$ $\qquad f(\hat{\theta}_n) - f_*) \leq O\left(\frac{1}{\mu n}\right)$

$$\hat{\theta}_n = \frac{\sum^n k\,\theta_k}{\left(\frac{n(n+1)}{2}\right)}$$

Today's roadmap.

* Minimax rates.

* Analysis of the smooth case.

testing $\theta = \theta_0$ $(\mathbb{P}_{\theta_0})$, $\theta = \theta_1$ $(\mathbb{P}_{\theta_1})$

$$T_1 + T_2 \geq 1 - TV(P_{\theta_0}, P_{\theta_1})$$

$$\mathbb{1}_{\ell(x,\theta_0) > \ell(x,\theta_1)}$$

minimax:

relate opt error / est err)

to

test error.

lower bound

test error

via IT

arguments

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 $k = 0, \dots, n-1$ and outputs θ_n

- **Class of functions**
  - convex B-Lipschitz-continuous (w.r.t. ℓ_2-norm) on a compact convex set $\mathcal{C}$ containing an ℓ_∞-ball

- **Performance measure**
  - for a given algorithm and function $\varepsilon_n(\text{algo}, f) = f(\theta_n) - \inf_{\theta \in \mathcal{C}} f(\theta)$
  - for a given algorithm: $\sup\limits_{\text{functions } f} \varepsilon_n(\text{algo}, f)$

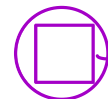
- **Minimax performance**: $\underbrace{\inf\limits_{\text{algo}}}_{\text{best alg.}} \underbrace{\sup\limits_{\text{functions } f} \varepsilon_n(\text{algo}, f)}_{\text{worst case rate of a given alg.}}$

Minimax rates (Agarwal et al., 2012)

- **Convex functions**: domain $\mathcal{C}$ that contains an ℓ_∞-ball of radius D_∞

Minimax rate ''

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



$D' \leq \frac{D}{\sqrt{d}}$

D

  - Consequences for ℓ_2-ball of radius D_2: $BD_2/\sqrt{n}$
  - Upper-bound through stochastic subgradient

$D_\infty = \frac{D_2}{\sqrt{d}}$

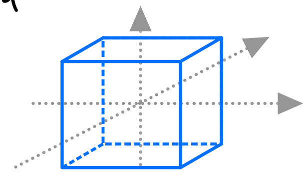
- **μ-strongly-convex functions**:

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

$\hookrightarrow$ also corresponding u.b. for stochastic SubGD.

Minimax rates - sketch of proof

$\{-1,1\}^d$



1. **Create a subclass of functions** indexed by some vertices α^j, $j = 1, \dots, M$ of the hypercube $\{-1,1\}^d$, which are sufficiently far in Hamming metric Δ_H (denote $\mathcal{V}$ this set with $|\mathcal{V}| = M$)

ℓ^d

$$\forall j \neq k, \; \Delta_H(\alpha^i, \alpha^j) \geqslant \frac{d}{4},$$

e.g., a "$\frac{d}{4}$-packing" (possible with M exponential in d - see later)

$\alpha \in \{-1, 1\}^d$; $(\alpha_1 \dots \alpha_d) = (1, -1, \dots, 1)$

$H(\alpha^i, \alpha^j) = \sum_{k=1}^{d} 1\!\!1_{\alpha^i_k \neq \alpha^j_k}$ = nb of coordinates that differ!

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2. **Design functions** so that
   – approximate optimization of the function is equivalent to function identification among the class above
   – stochastic oracle corresponds to a sequence of coin tosses with biases index by α^j, $j = 1, \ldots, M$

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$$\forall j \neq k, \ \Delta_H(\alpha^i, \alpha^j) \geqslant \frac{d}{4},$$
(counting)
e.g., a "$\frac{d}{4}$-packing" (possible with M exponential in d - see later)

2. **Design functions** so that

   – approximate optimization of the function is equivalent to function identification among the class above (simple argument)
   – stochastic oracle corresponds to a sequence of coin tosses with biases index by α^j, $j = 1, \dots, M$ (allows to compute information theoretic quantities).

3. Any such identification procedure (i.e., **a test**) has a lower bound on the probability of error (Fano's ineq)

Packing number for the hyper-cube

Proof

$$\sum_{i=0}^{d/4}\binom{d}{i} = 2^d \sum_{i=0}^{d/4}\binom{d}{i}\left(\frac{1}{2}\right)^i\left(\frac{1}{2}\right)^{d-i} = 2^d \sum_{i=1}^{d/4} \mathbb{P}\left(\mathcal{B}(d, 1/2) = i\right)$$

- **Varshamov-Gilbert's lemma** (Massart, 2003, p. 105): the maximal number of points in the hypercube that are at least $d/4$-apart in Hamming loss is greater than than $\exp(d/8)$.

1. Maximality of family $\mathcal{V} \Rightarrow \bigcup_{\alpha\in\mathcal{V}} \mathcal{B}_H(\alpha, d/4) = \{-1,1\}^d$

$\mathcal{B}(\alpha, 0) = 1$
$\mathcal{B}(\alpha, 1) = d$
$\mathcal{B}(\alpha, 2) = \binom{d}{2}$
$\mathcal{B}(\alpha, k) = \binom{d}{k}$

2. Cardinality: $\sum_{\alpha\in\mathcal{V}} |\mathcal{B}_H(\alpha, d/4)| \geqslant 2^d$

3. Link with deviation of Z distributed as $\mathrm{Binomial}(d, 1/2)$

$$2^{-d}|\mathcal{B}_H(\alpha, d/4)| = \mathbb{P}(Z \leqslant d/4) = \mathbb{P}(Z \geqslant 3d/4)$$

4. Hoeffding inequality: $\mathbb{P}(Z - \frac{d}{2} \geqslant \frac{d}{4}) \leqslant \exp(-\frac{2(d/4)^2}{d}) = \exp(-\frac{d}{8})$

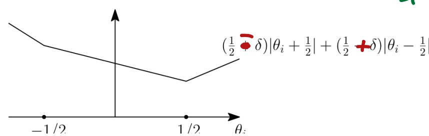
$$|\mathcal{V}| \geqslant \exp\left(\frac{d}{8}\right)$$

Designing a class of functions

- Given $\alpha \in \{-1, 1\}^d$, and a precision parameter $\delta > 0$:

$x \in \mathbb{R}^d$ $\qquad f_i^+(x_i) \qquad f_i^-(x_i)$

$$g_\alpha(x) = \frac{c}{d} \sum_{i=1}^{d} \Big\{ (\underbrace{\frac{1}{2} + \alpha_i \delta}_{3/4}) f_i^+(x) + (\underbrace{\frac{1}{2} - \alpha_i \delta}_{1/4}) f_i^-(x) \Big\}$$



- **Properties**

  – Functions f_i's and constant c to ensure proper regularity and/or strong convexity

- **Oracle**

(a) Pick an index $i \in \{1, \dots, d\}$ at random
(b) Draw $b_i \in \{0, 1\}$ from a Bernoulli with parameter $\frac{1}{2} + \alpha_i \delta$
(c) Consider $\hat{g}_\alpha(x) = c\big[b_i f_i^+ + (1 - b_i) f_i^-\big]$ and its value / gradient

Optimizing is function identification

- **Goal**: if g_α is optimized up to error ε, then this identifies $\alpha \in \mathcal{V}$

- **"Metric" between functions**:

$$\rho(f,g) = \inf_{\theta \in \mathcal{C}} \big(f(\theta) + g(\theta) \big) - \inf_{\theta \in \mathcal{C}} f(\theta) - \inf_{\theta \in \mathcal{C}} g(\theta)$$

  – $\rho(f,g) \geqslant 0$ with equality iff f and g have the same minimizers

- **Lemma**: let $\psi(\delta) = \min_{\alpha \neq \beta \in \mathcal{V}} \rho(g_\alpha, g_\beta)$. For any $\tilde\theta \in \mathcal{C}$, there is at most one function g_α such that $g_\alpha(\tilde\theta) - \inf_{\theta \in \mathcal{C}} g_\alpha(\theta) \leqslant \frac{\psi(\delta)}{3}$ $< \frac{\psi(\delta)}{2}$

α_1, α_2 /

$$g_{\alpha_1}(\tilde\theta) - \inf g_{\alpha_1} < \frac{\psi(\delta)}{2}$$

$$+ \; g_{\alpha_2}(\tilde\theta) - \inf g_{\alpha_2} < \frac{\psi(\delta)}{2}$$

$\psi(\delta)$ $\wedge$ ||

$$\rho(g_{\alpha_1}, g_{\alpha_2}) \leq g_{\alpha_1}(\tilde\theta) + g_{\alpha_2}(\tilde\theta) - \inf 1 - \inf 2 < \psi(\delta)$$

Optimizing is function identification

- **Goal**: if g_α is optimized up to error ε, then this identifies $\alpha \in \mathcal{V}$

Expected opt error $\leqslant \frac{\psi(\delta)}{9}$

$\longrightarrow$ test with prob of error $\leqslant \frac{1}{3}$

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- **Lemma**: let $\psi(\delta) = \min_{\alpha \neq \beta \in \mathcal{V}} \rho(g_\alpha, g_\beta)$. For any $\tilde{\theta} \in \mathcal{C}$, there is at most one function g_α such that $g_\alpha(\tilde{\theta}) - \inf_{\theta \in \mathcal{C}} g_\alpha(\theta) \leqslant \frac{\psi(\delta)}{3}$
  - (a) optimizing an unknown function from the class up to precision $\frac{\psi(\delta)}{3}$ leads to identification of $\alpha \in \mathcal{V}$
  - (b) If the expected minimax error rate is no greater than $\frac{\psi(\delta)}{9}$, there exists a function from the set of random gradient and function values such the probability of error is less than $1/3$

$$\frac{\psi(\delta)}{9} \geqslant \mathbb{E}\Big(g_\alpha(\hat{\theta}) - \inf g_\alpha(\theta)\Big) \geqslant \frac{\psi(\delta)}{3}\, \mathbb{P}\Big(g_\alpha(\hat{\theta}) - \inf g_\alpha(\theta) \geqslant \frac{\psi(\delta)}{3}\Big)$$

Neyman's Pearson Lemma, testing, and lower bounds

Lower bounds on testing.

identifying a_i $\longleftrightarrow$ distinguishing $\mathcal{B}(\frac{1}{2}+\delta)$ vs $\mathcal{B}(\frac{1}{2}-\delta)$

testing pb.

$\rightarrow$ simplest result is $T1 + T2 \geqslant 1 - TV\left(\mathcal{B}(\frac{1}{2}+\delta), \mathcal{B}(\frac{1}{2}-\delta)\right)$

Corollary 11.1 (Fano's inequality for multiple hypothesis testing) *Given M probability distributions dp_j on $\mathcal{D}$, then*

≲ small enough

$$\inf_g \frac{1}{M}\sum_{j=1}^{M}\mathbb{P}_j\big(g(\mathcal{D}) \neq j\big) \geqslant 1 - \frac{1}{M^2\log M}\sum_{j,j'=1}^{M} \overline{D_{\mathrm{KL}}(dp_j \| dp_{j'})} - \frac{\log 2}{\log M}.$$

$\hookrightarrow$ $M \geqslant \exp(d/8)$

Lower bounds on coin tossing (Agarwal et al., 2012, Lemma 3)

- **Lemma**: For $\delta < 1/4$, given α^* uniformly at random in $\mathcal{V}$, if n outcomes of a random single coin (out of the d) are revealed, then any test will have a probability of error greater than

with Fano's ineq

$$1 - \frac{16n\delta^2 + \log 2}{\frac{d}{2}\log(2/\sqrt{e})} \leqslant \text{any test has error} \leqslant \frac{1}{3}$$

  – Proof based on Fano's inequality: If g is a function of X, and Y takes m values, then

$$\mathbb{P}(g(X) \neq Y) \geqslant \frac{H(X|Y) - 1}{\log m} = \frac{H(X)}{\log m} - \frac{I(X,Y) + 1}{\log m}$$

Construction of f_i for convex functions

- $f_i^+(\theta) = |\theta(i) + \frac{1}{2}|$ and $f_i^-(\theta) = |\theta(i) - \frac{1}{2}|$
  - 1-Lipschitz-continuous with respect to the ℓ_2-norm. With $c = B/2$, then g_α is B-Lipschitz.
  - Calling the oracle reveals a coin

- Lower bound on the discrepancy function
  - each g_α is minimized at $\theta_\alpha = \cancel{-}\alpha/2$
  - Fact: $\rho(g_\alpha, g_\beta) = \frac{2c\delta}{d}\Delta_H(\alpha,\beta) \geqslant \frac{c\delta}{2} = \psi(\delta)$

to reach precis° ε in terms of expected $f(\theta) - \inf f(\theta)$

- Set error/precision $\varepsilon = \frac{c\delta}{18}$ so that $\varepsilon < \psi(\delta)/9$

I need at least

- Consequence: $\frac{1}{3} \geqslant 1 - \frac{16n\delta^2 + \log 2}{\frac{d}{2}\log(2/\sqrt{e})}$, that is, $\boxed{n \geqslant \text{cst} \times \frac{L^2 d^2}{\varepsilon^2}}$

$\Longleftrightarrow \quad \varepsilon \geqslant \frac{1}{\sqrt{n}}$.

Construction of f_i for strongly-convex functions

- $f_i^{\pm}(\theta) = \frac{1}{2}\kappa|\theta(i) \pm \frac{1}{2}| + \frac{1-\kappa}{4}(\theta(i) \pm \frac{1}{2})^2$
  - Strongly convex and Lipschitz-continuous

- Same proof technique (more technical details)

- See more details by Agarwal et al. (2012); Raginsky and Rakhlin (2011)

Summary of rates of convergence

- Problem parameters
  - D diameter of the domain
  - B Lipschitz-constant
  - L smoothness constant
  - μ strong convexity constant

* links with online learning.

* non uniform averaging

	convex	strongly convex
nonsmooth	deterministic: $BD/\sqrt{t}$ stochastic: $BD/\sqrt{n}$	deterministic: $B^2/(t\mu)$ 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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**

   - Asymptotic analysis
   - Robbins-Monro algorithm (upper bounds for the last iterate)
   - Polyak-Rupert averaging (________ the averaged it).

5. **Smooth stochastic approximation algorithms**

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

6. **Finite data sets**

   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

"Classical" stochastic approximation

- **General problem of finding zeros of $h : \mathbb{R}^d \to \mathbb{R}^d$**
  - From random observations of values of h at certain points
  - Main example: minimization of $f : \mathbb{R}^d \to \mathbb{R}$, with $h = f'$

- **Classical algorithm (Robbins and Monro, 1951b)**

$$\boxed{\theta_n = \theta_{n-1} - \gamma_n \big[h(\theta_{n-1}) + \varepsilon_n \big]}$$

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- **Goals** (see, e.g., Duflo, 1996)
  - Beyond reducing noise by averaging observations
  - General sufficient conditions for convergence
  - Convergence in quadratic mean vs. convergence almost surely
  - Rates of convergences and choice of step-sizes
  - Asymptotics - no convexity

“Classical” stochastic approximation

- **Intuition from recursive mean estimation**

$\mathbb{E}(x_n) = x$?

  – Starting from $\theta_0 = 0$, getting data $x_n \in \mathbb{R}^d$

$h(\theta) = \theta - \mathbb{E}(x_n)$

$h_n(\theta_{n-1}) = \theta_{n-1} - x_n$

$$\theta_n = \theta_{n-1} - \gamma_n(\theta_{n-1} - x_n)$$

  – If $\gamma_n = 1/n$, then $\theta_n = \frac{1}{n}\sum_{k=1}^n x_k$
  – If $\gamma_n = 2/(n+1)$ then $\theta_n = \frac{2}{n(n+1)}\sum_{k=1}^n k x_k$

$$\theta_{n+1} = \frac{1}{n}\sum x_k - \frac{1}{n+1}\left(\frac{1}{n}\sum x_k\right) + \frac{x_{n+1}}{n+1}$$

$$\left(1 - \frac{1}{n+1}\right)\frac{1}{n} = \frac{n}{n+1}\frac{1}{n} = \frac{1}{n+1}$$

$$= \frac{1}{n+1}\sum_{i=1}^{n+1} x_i$$

“Classical” stochastic approximation

- **Intuition from recursive mean estimation**
  - Starting from $\theta_0 = 0$, getting data $x_n \in \mathbb{R}^d$

$$\theta_n = \theta_{n-1} - \gamma_n(\theta_{n-1} - x_n)$$

  - If $\gamma_n = 1/n$, then $\theta_n = \frac{1}{n}\sum_{k=1}^n x_k$
  - If $\gamma_n = 2/(n+1)$ then $\theta_n = \frac{2}{n(n+1)}\sum_{k=1}^n kx_k$

- In general: $\mathbb{E}x_n = x$ and thus $\theta_n - x = \underbrace{(1-\gamma_n)(\theta_{n-1}-x)}_{\text{deterministic}} + \underbrace{\gamma_n(x_n - x)}_{\text{stochastic}}$

$$\theta_n - x = \underbrace{\prod_{k=1}^n (1-\gamma_k)(\theta_0 - x)}_{\text{deterministic}} + \underbrace{\sum_{i=1}^n \prod_{k=i+1}^n (1-\gamma_k)\gamma_i(x_i - x)}_{\text{stochastic}}$$

"Classical" stochastic approximation

- Expanding the recursion with i.i.d. x_n's and $\sigma^2 = \mathbb{E}\|x_n - x\|^2$:

$\forall i$

$\underline{\mathbb{E}(x_i) = x}$

$$\theta_n - x = \prod_{k=1}^{n}(1-\gamma_k)(\theta_0 - x) + \sum_{i=1}^{n}\gamma_i \prod_{k=i+1}^{n}(1-\gamma_k)(x_i - x)$$

$$\mathbb{E}\|\theta_n - x\|^2 = \prod_{k=1}^{n}(1-\gamma_k)^2\|\theta_0 - x\|^2 + \sum_{i=1}^{n}\gamma_i^2 \prod_{k=i+1}^{n}(1-\gamma_k)^2\sigma^2$$

$\gamma_k = \frac{1}{k}$ $1 - \frac{1}{k} = \frac{k-1}{k}$ $\mathbb{E}(x_i - x)^T(x_j - x) = 0$

$\mathbb{E}\|x_i - x\|^2 = \sigma^2$

$\gamma_k = \frac{1}{n} \quad \forall k \leq n$ $\left(1 - \frac{1}{n}\right)^n \to e^{-1}$

"Classical" stochastic approximation

- Expanding the recursion with i.i.d. x_n's and $\sigma^2 = \mathbb{E}\|x_n - x\|^2$:

$$\theta_n - x = \prod_{k=1}^n (1-\gamma_k)(\theta_0 - x) + \sum_{i=1}^n \gamma_i \prod_{k=i+1}^n (1-\gamma_k)(x_i - x)$$

$$\mathbb{E}\|\theta_n - x\|^2 = \prod_{k=1}^n (1-\gamma_k)^2 \|\theta_0 - x\|^2 + \sum_{i=1}^n \gamma_i^2 \prod_{k=i+1}^n (1-\gamma_k)^2 \sigma^2$$

- Requires study of $\prod_{k=1}^n (1-\gamma_k)$ and $\sum_{i=1}^n \gamma_i^2 \prod_{k=i+1}^n (1-\gamma_k)^2$
  - If $\gamma_n = o(1)$, $\log \prod_{k=1}^n (1-\gamma_k) \sim -\sum_{k=1}^n \gamma_k$ should go to $-\infty$
    Forgetting initial conditions (even arbitrarily far)
  - $\sum_{i=1}^n \gamma_i^2 \prod_{k=i+1}^n (1-\gamma_k)^2 \sim \sum_{i=1}^n \gamma_i^2 \prod_{k=i+1}^n (1-2\gamma_k)$
    Robustness to noise

$\gamma_k = \frac{1}{k^\alpha}$, $0 \leq \alpha \leq 1$

Forgetting of initial conditions

$$\log \prod_{k=1}^{n} (1-\gamma_k) \sim -\sum_{k=1}^{n} \gamma_k$$

- Examples: $\boxed{\gamma_n = C/n^\alpha}$
  - $\alpha = 1$, $\sum_{i=1}^n \frac{1}{i} = \log(n) + \text{ cst } + O(1/n)$
  - $\alpha > 1$, $\sum_{i=1}^n \frac{1}{i^\alpha} = \text{ cst } + O(1/n^{\alpha-1})$
  - $\alpha \in (0,1)$, $\sum_{i=1}^n \frac{1}{i^\alpha} = \text{ cst } \times n^{1-\alpha} + O(1)$
  - Proof using relationship with integrals

- Consequences
  - if $\alpha > 1$, no convergence
  - If $\alpha \in (0,1)$, exponential convergence
  - if $\alpha = 1$, convergence of squared norm in $1/n^{2C}$

Decomposition of the noise term

- Assume (γ_n) is decreasing and less than 1; then for any $m \in \{1, \ldots, n\}$, we may split the following sum as follows:

intuitive proof

cut at m

$$\sum_{k=1}^{n} \prod_{i=k+1}^{n} (1-\gamma_i)\gamma_k^2 = \sum_{k=1}^{m} \prod_{i=k+1}^{n} (1-\gamma_i)\gamma_k^2 + \sum_{k=m+1}^{n} \prod_{i=k+1}^{n} (1-\gamma_i)\gamma_k^2$$

$k \leq m$

$k \geq m$

$\gamma_k \leq \gamma_m$

$$\leqslant \prod_{i=m+1}^{n} (1-\gamma_i) \sum_{k=1}^{m} \gamma_k^2 + \gamma_m \sum_{k=m+1}^{n} \prod_{i=k+1}^{n} (1-\gamma_i)\gamma_k$$

$$\leqslant \underbrace{\exp\Big(-\sum_{i=m+1}^{n} \gamma_i\Big) \sum_{k=1}^{m} \gamma_k^2}_{\text{nearly same as initial cdto.}} + \gamma_m \sum_{k=m+1}^{n} \Big[\prod_{i=k+1}^{n} (1-\gamma_i) - \prod_{i=k}^{n} (1-\gamma_i)\Big]$$

$1 - (1-\gamma_k) = \gamma_k$

$$\leqslant \exp\Big(-\sum_{i=m+1}^{n} \gamma_i\Big) \sum_{k=1}^{m} \gamma_k^2 + \gamma_m \Big[1 - \cancel{\prod_{i=m+1}^{n} (1-\gamma_i)}\Big]$$

telescopic sum.

$$\leqslant \underbrace{\exp\Big(-\sum_{i=m+1}^{n} \gamma_i\Big)}_{\text{diverging as } n \to +\infty} \sum_{k=1}^{n} \gamma_k^2 + \underbrace{\gamma_m}_{\to 0 \text{ as } m \to +\infty}$$

Decomposition of the noise term

$$\sum_{k=1}^{n} \prod_{i=k+1}^{n} (1-\gamma_i)\gamma_k^2 \leqslant \exp\left(-\sum_{i=m+1}^{n}\gamma_i\right)\sum_{k=1}^{n}\gamma_k^2 + \gamma_m$$

- Require γ_n to tend to zero (vanishing decaying step-size)
  - May not need $\sum_n \gamma_n^2 < \infty$ for convergence in quadratic mean
- Examples: $\boxed{\gamma_n = C/n^\alpha}$ and mean estimation, with $m = n/2$
  - No need to consider $\alpha > 1$ ↗ vanishing part
  - $\alpha \in (0,1)$, $\exp(-C'n^{1-\alpha})n^{\max\{1-2\alpha,0\}} + \underline{O(Cn^{-\alpha})}$
  - $\alpha = 1$, convergence of noise term in $O(1/n)$ but forgetting of initial condition in $O(1/n^{2C})$
  - Consequences: need $\alpha \in (0,1]$ and $C \geqslant 1/2$ for $\alpha = 1$

$$\exp\left(-2C\log n\right) \sim \frac{1}{n^C}$$

Robbins-Monro algorithm

$4:05$

- **General problem of finding zeros of** $h:\mathbb{R}^d\to\mathbb{R}^d$
  - From random observations of values of h at certain points
  - Main example: minimization of $f:\mathbb{R}^d\to\mathbb{R}$, with $h=f'$

- **Classical algorithm (Robbins and Monro, 1951b)**

$$\theta_n=\theta_{n-1}-\gamma_n\big[h(\theta_{n-1})+\varepsilon_n\big]$$

- **Goals** (see, e.g., Duflo, 1996)
  - General sufficient conditions for convergence
  - Convergence in quadratic mean vs. convergence almost surely
  - Rates of convergences and choice of step-sizes
  - Asymptotics - no convexity

Different types of convergences

- **Goal**: show that $\theta_n \to \theta_*$ or $d(\theta_n, \Theta_*) \to 0$ or $f(\theta_n) \to f(\theta_*)$
  - Random quantity $\delta_n \in \mathbb{R}$ tending to zero

    $\geqslant 0$

- **Convergence almost-surely**: $\mathbb{P}(\delta_n \to 0) = 1$ if $\forall \varepsilon \ \sum_{n \geqslant 0} P(|\delta_n| \geqslant \varepsilon) < +\infty$

  $\Downarrow$ $\uparrow$ subseq $\uparrow$ Borel C.

- **Convergence in probability**: $\forall \varepsilon > 0, \mathbb{P}(|\delta_n| \geqslant \varepsilon) \to 0$

  dominated $\downarrow$ $\Uparrow$ (Markov)

- **Convergence in mean** $r \geqslant 1$: $\mathbb{E}|\delta_n|^r \to 0$ $(r = 2)$

  L^r

Different types of convergences

- **Goal**: show that $\theta_n \to \theta_*$ or $d(\theta_n, \Theta_*) \to 0$ or $f(\theta_n) \to f(\theta_*)$
  - Random quantity $\delta_n \in \mathbb{R}$ tending to zero

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- **Convergence in probability**: $\forall \varepsilon > 0, \mathbb{P}(|\delta_n| \geqslant \varepsilon) \to 0$

- **Convergence in mean** $r \geqslant 1$: $\mathbb{E}|\delta_n|^r \to 0$

- **Relationship between convergences**
  - Almost surely $\Rightarrow$ in probability
  - In mean $\Rightarrow$ in probability (Markov's inequality)
  - In probability (sufficiently fast) $\Rightarrow$ almost surely (Borel-Cantelli)
  - Almost surely $+$ domination $\Rightarrow$ in mean

Robbins-Monro algorithm
Need for Lyapunov functions (even with no noise)

$$\theta_n = \theta_{n-1} - \gamma_n \big[h(\theta_{n-1}) + \varepsilon_n \big]$$

- The Robbins-Monro algorithm cannot converge all the time...

- **Lyapunov function** $V : \mathbb{R}^d \to \mathbb{R}$ with following properties
  - Non-negative values: $V \geqslant 0$
  - Continuously-differentiable with L-Lipschitz-continuous gradients
  - Control of h: $\forall \theta$, $\|h(\theta)\|^2 \leqslant C(1 + V(\theta))$
  - Gradient condition: $\forall \theta$, $\boxed{h(\theta)^\top V'(\theta) \geqslant \alpha \|V'(\theta)\|^2}$

Robbins-Monro algorithm
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$\hookrightarrow \|\nabla f(\theta)\|^2 \geqslant \alpha \|\nabla f(\theta)\|^2$ $\quad \underline{\alpha = 1}$

- If $h = f'$, then $V(\theta) = f(\theta) - \inf f$ is the default (but not only) choice for Lyapunov function: applies also to non-convex functions
  - Will require often some additional condition $\|V'(\theta)\|^2 \geqslant 2\mu V(\theta)$

strongly cvx

Robbins-Monro algorithm
Martingale noise

$\nabla \ell(\theta_{n-1}, (x_n, y_n))$

$= \nabla f(\theta_{n-1}) + \underbrace{\varepsilon_n(\theta_{n-1})}_{\text{not iid}}$

$\varepsilon_n(\cdot)$ iid

$\varepsilon_n(\theta_{n-1})$ not iid

$$\theta_n = \theta_{n-1} - \gamma_n \big[h(\theta_{n-1}) + \varepsilon_n \big]$$

- **Assumptions about the noise** ε_n
  - Typical assumption: ε_n i.i.d. $\Rightarrow$ not needed
  - "information up to time n": sequence of increasing σ-fields $\mathcal{F}_n$
  - Example from machine learning: $\mathcal{F}_n = \sigma(x_1, y_1, \dots, x_n, y_n)$
  - Assume $\boxed{\mathbb{E}(\varepsilon_n | \mathcal{F}_{n-1}) = 0}$ and $\boxed{\mathbb{E}\big[\|\varepsilon_n\|^2 | \mathcal{F}_{n-1}\big] \leqslant \sigma^2}$ almost surely

- Warning: SGD for machine learning does not correspond to ε_n i.i.d.

- **Key property**: θ_n is $\mathcal{F}_n$-measurable

Robbins-Monro algorithm
Convergence of the Lyapunov function

- Using regularity (and other properties) of V:

smoothness of V

$$V(\theta_n) \leqslant V(\theta_{n-1}) + V'(\theta_{n-1})^\top(\theta_n - \theta_{n-1}) + \frac{L}{2}\|\theta_n - \theta_{n-1}\|^2$$

$\theta_n - \theta_{n-1} = -\gamma(h(\theta_{n-1}) + \varepsilon_n)$

$$= V(\theta_{n-1}) - \gamma_n V'(\theta_{n-1})^\top(h(\theta_{n-1}) + \varepsilon_n) + \frac{L\gamma_n^2}{2}\|h(\theta_{n-1}) + \varepsilon_n\|^2$$

$$\mathbb{E}\big[V(\theta_n)|\mathcal{F}_{n-1}\big] \leqslant V(\theta_{n-1}) - \gamma_n V'(\theta_{n-1})^\top h(\theta_{n-1}) + \frac{L\gamma_n^2}{2}\|h(\theta_{n-1})\|^2 + \frac{L\gamma_n^2}{2}\sigma^2 + 2\times 0$$

$\mathbb{E}[\varepsilon_n \mid \mathcal{F}_{n-1}] = 0$

$$\leqslant V(\theta_{n-1}) - \alpha'\gamma_n\|V'(\theta_{n-1})\|^2 + \frac{LC\gamma_n^2}{2}\big[1 + V(\theta_{n-1})\big] + \frac{L\gamma_n^2}{2}\sigma^2$$

$$= V(\theta_{n-1})\Big[1 + \frac{LC\gamma_n^2}{2}\Big] - \alpha'\gamma_n\|V'(\theta_{n-1})\|^2 + \frac{L\gamma_n^2}{2}(C + \sigma^2)\,.$$

gradient property.

Robbins-Monro algorithm
Convergence of the expected Lyapunov function
with "curvature"

$\left(1 + \square\, \gamma_n^2 - \diamond\, \gamma_n\right)$

$\leqslant \left(1 - \Delta \gamma_n\right)$

- If $\|V'(\theta)\|^2 \geqslant 2\mu V(\theta)$ and $\gamma_n \leqslant \frac{2\alpha'\mu}{LC}$:

$$\mathbb{E}\big[V(\theta_n)|\mathcal{F}_{n-1}\big] \leqslant V(\theta_{n-1})\big[1-\alpha'\mu\gamma_n\big] + M\gamma_n^2$$

$$\boxed{\mathbb{E}V(\theta_n) \leqslant \mathbb{E}V(\theta_{n-1})\big[1-\alpha'\mu\gamma_n\big] + M\gamma_n^2}$$

- Need to study non-negative sequence $\delta_n \leqslant \delta_{n-1}\big[1-\alpha'\mu\gamma_n\big] + M\gamma_n^2$ with $\delta_n = \mathbb{E}V(\theta_n)$

- Sufficient conditions for convergence of the expected Lyapunov function (with curvature)

  – $\sum_n \gamma_n = +\infty$ and $\gamma_n \to 0$
  – Special case of $\gamma_n = C/n^\alpha$

Robbins-Monro algorithm
Convergence of the expected Lyapunov function
with "curvature" - $\gamma_n = C/n^\alpha$

$\to$ good choice? $\gamma_n = \frac{1}{n\mu}$ $(\alpha' = 1)$

$\to$ cvge as $O(\frac{1}{n})$

- Need to study non-negative sequence $\delta_n \leqslant \delta_{n-1}\big[1 - \alpha'\mu\gamma_n\big] + M\gamma_n^2$ with $\delta_n = \mathbb{E}V(\theta_n)$ (NB: forgetting constraint on γ_n - see next class)

$$\delta_n \leqslant \prod_{k=1}^{n}(1 - \alpha'\mu\gamma_k)\delta_0 + M\sum_{i=1}^{n}\gamma_i^2\prod_{k=i+1}^{n}(1 - \alpha'\mu\gamma_k)$$

For $\gamma_n = \frac{C}{n}$

C has to scale as $1/\mu$ for cvge $O(\frac{1}{n})$

- If $\alpha > 1$: no forgetting of initial conditions

- If $\alpha \in (0,1)$: $\delta_0 \exp(-$ cst $\alpha'\mu C \times n^{1-\alpha}) + \gamma_n M$

variance term

- If $\alpha = 1$ and $\gamma_n = C/n$: $\delta_0 n^{-\mu C} + \gamma_n M$

$\boxed{\alpha' = 1}$

$$\prod\left(1 - \alpha'\mu\frac{C}{n}\right) \sim \exp\left(-(\log n)\, C\alpha'\mu\right) = \frac{1}{n^{C\alpha'\mu}}$$

$\frac{1}{n^{C\mu}}$

Robbins-Monro algorithm
Almost-sure convergence

- Using regularity of V:

$$
\begin{aligned}
V(\theta_n) &\leqslant V(\theta_{n-1}) + V'(\theta_{n-1})^\top(\theta_n - \theta_{n-1}) + \frac{L}{2}\|\theta_n - \theta_{n-1}\|^2 \\
&= V(\theta_{n-1}) - \gamma_n V'(\theta_{n-1})^\top(h(\theta_{n-1}) + \varepsilon_n) + \frac{L\gamma_n^2}{2}\|h(\theta_{n-1}) + \varepsilon_n\|^2 \\
\mathbb{E}\big[V(\theta_n)|\mathcal{F}_{n-1}\big] &\leqslant V(\theta_{n-1}) - \gamma_n V'(\theta_{n-1})^\top h(\theta_{n-1}) + \frac{L\gamma_n^2}{2}\|h(\theta_{n-1})\|^2 + \frac{L\gamma_n^2}{2}\sigma^2 \\
&\leqslant V(\theta_{n-1}) - \alpha'\gamma_n\|V'(\theta_{n-1})\|^2 + \frac{LC\gamma_n^2}{2}\big[1 + V(\theta_{n-1})\big] + \frac{L\gamma_n^2}{2}\sigma^2 \\
&= V(\theta_{n-1})\big[1 + \frac{LC\gamma_n^2}{2}\big] - \alpha'\gamma_n\|V'(\theta_{n-1})\|^2 + \frac{L\gamma_n^2}{2}(C + \sigma^2)
\end{aligned}
$$

Same.

$$\mathbb{E}\left[M_n \,|\, \mathcal{F}_{n-1}\right] \leq M_{n-1}$$

Robbins and Siegmund (1985)

χ_n, β_n scales as γ_n^2

- **Assumptions**
  - Measurability: Let V_n, β_n, χ_n, η_n four $\mathcal{F}_n$-adapted real sequences
  - Non-negativity: V_n, β_n, χ_n, η_n non-negative
  - Summability: $\sum_n \beta_n < \infty$ and $\sum_n \chi_n < \infty$
  - Inequality: $\mathbb{E}\big[V_n|\mathcal{F}_{n-1}\big] \leqslant V_{n-1}(1+\beta_{n-1}) + \chi_{n-1} - \eta_{n-1}$

- **Theorem**: (V_n) converges almost surely to a random variable V_∞ and $\sum_n \eta_n$ is finite almost surely

$\Rightarrow \quad \eta_n \xrightarrow{a.s.} 0$

- *Proof*

- Consequence for stochastic approximation (if $\|V'(\theta)\|^2 \geqslant 2\mu V(\theta)$): $V(\theta_n)$ and $\|V'(\theta_n)\|^2$ converges almost surely to zero

$\eta_n \quad \alpha \quad \underline{\|V'(\theta_n)\|^2}$

Robbins and Siegmund (1985) - Proof sketch

- Inequality: $\mathbb{E}\big[V_n|\mathcal{F}_{n-1}\big] \leqslant V_{n-1}(1+\beta_{n-1}) + \chi_{n-1} - \eta_{n-1}$

- Define $\alpha_n = \prod_{k=1}^{n}(1+\beta_k)$ a converging sequence, $V'_n = \alpha_{n-1}^{-1} V_n$, $\chi'_n = \alpha_{n-1}^{-1}\chi_n$ and $\eta'_n = \alpha_{n-1}^{-1}\eta_n$ so that:

$$\mathbb{E}\big[V'_n|\mathcal{F}_{n-1}\big] \leqslant V'_{n-1} + \chi'_{n-1} - \eta'_{n-1}$$

- Define the super-martingale $Y_n = V'_n - \sum_{k=1}^{n-1}(\chi'_k - \eta'_k)$ so that $\mathbb{E}\big[Y_n|\mathcal{F}_{n-1}\big] \leqslant Y_{n-1}$

- Probabilistic proof using Doob convergence theorem (Duflo, 1996)

Robbins-Monro analysis - non random errors

- **Random unbiased errors**: no need for vanishing magnitudes

- **Non-random errors**: need for vanishing magnitudes
  - See Duflo (1996, Theorem 2.III.4)
  - See also Schmidt et al. (2011)

$h(\theta) = \theta - x$

$h'(\theta_*) = \theta_*$,

Robbins-Monro analysis - asymptotic normality (Fabian, 1968)

- Traditional step-size $\gamma = C/n$ (and proof sketch for differential A of h at unique θ_* symmetric) → seems to provide the fastest rate.

$$
\begin{aligned}
\theta_n &= \theta_{n-1} - \gamma_n h(\theta_{n-1}) - \gamma_n \varepsilon_n \\
&\approx \theta_{n-1} - \gamma_n \big[h'(\theta_*)(\theta_{n-1} - \theta_*)\big] - \gamma_n \varepsilon_n + \gamma_n O(\|\theta_n - \theta_*\|^2) \\
&\approx \theta_{n-1} - \gamma_n A(\theta_{n-1} - \theta_*) - \gamma_n \varepsilon_n
\end{aligned}
$$

$\theta_n - \theta_* \approx (I - \gamma A)(\theta_n - \theta_*) - \gamma_n \varepsilon_n$

$$
\theta_n - \theta_* \approx (I - \gamma_n A)\cdots(I - \gamma_1 A)(\theta_0 - \theta_*) - \sum_{k=1}^{n} (I - \gamma_n A)\cdots(I - \gamma_{k+1} A)\gamma_k \varepsilon_k
$$

$$
\theta_n - \theta_* \approx \exp\big[-(\gamma_n + \cdots + \gamma_1)A\big](\theta_0 - \theta_*) - \sum_{k=1}^{n} \exp\big[-(\gamma_n + \cdots + \gamma_{k+1})A\big]\gamma_k \varepsilon_k
$$

same as mean estimate

$$
\approx \underbrace{\exp\big[-CA\log n\big](\theta_0 - \theta_*)}_{\text{deterministic.}} - \underbrace{\sum_{k=1}^{n} \exp\big[-C(\log n - \log k)A\big]\frac{C}{k}\varepsilon_k}_{\text{stochastic}}
$$

- Asymptotic normality by averaging random variables

recall mean estimation ; $\theta_n - x = \underbrace{(1-\gamma_n)(\theta_{n-1} - x)}_{\text{deterministic}} + \underbrace{\gamma_n(x_n - x)}_{\text{stochastic}}$

Robbins-Monro analysis - asymptotic normality (Fabian, 1968)

- Assuming A, $(\theta_0-\theta_*)(\theta_0-\theta_*)^\top$ and $\mathbb{E}(\varepsilon_k\varepsilon_k^\top)=\Sigma$ commute

↳ in practice assume A, $\|\theta_0-\theta_*\|^2 I$, $\tau^2 A$ commute

$$\theta_n-\theta_* \approx \exp\big[-CA\log n\big](\theta_0-\theta_*)-\sum_{k=1}^n \exp\big[-C(\log n-\log k)A\big]\frac{C}{k}\varepsilon_k$$

$$\begin{aligned}
\mathbb{E}(\theta_n-\theta_*)(\theta_n-\theta_*)^\top &\approx \exp\big[-2CA\log n\big](\theta_0-\theta_*)(\theta_0-\theta_*)^\top \\
&\quad + \sum_{k=1}^n \exp\big[-2C(\log n-\log k)A\big]\frac{C^2}{k^2}\mathbb{E}(\varepsilon_k\varepsilon_k^\top) \\
&\approx n^{-2CA}(\theta_0-\theta_*)(\theta_0-\theta_*)^\top + n^{-2CA}\sum_{k=1}^n C^2 k^{2CA-2}\Sigma \\
&\approx n^{-2CA}(\theta_0-\theta_*)(\theta_0-\theta_*)^\top + n^{-2CA}C^2\frac{n^{2CA-1}}{2CA-1}\Sigma
\end{aligned}$$

Robbins-Monro analysis - asymptotic normality (Fabian, 1968)

proof requires $2CA \succcurlyeq I \Rightarrow C \geqslant \frac{1}{\lambda_{min}(A)} = \frac{1}{\mu}$

step size depends on the strong convexity

$$\mathbb{E}(\theta_n - \theta_*)(\theta_n - \theta_*)^\top \approx n^{-2CA}(\theta_0 - \theta_*)(\theta_0 - \theta_*)^\top + \frac{1}{n}C^2 \frac{1}{2CA - 1}\Sigma$$

- Step-size $\gamma = C/n$ (note that this only a sketch of proof)
  - Need $2C\lambda_{\min}(A) \geqslant 1$ for convergence, which implies that the first term depending on initial condition $\theta_* - \theta_0$ is negligible
  - C too small $\Rightarrow$ no convergence - C too large $\Rightarrow$ large variance
- Dependence on the conditioning of the problem

  limit variance scaling as $\left(\frac{1}{\mu^2 n}\right)$

  - If $\lambda_{\min}(A)$ is small, then C is large
  - "Choosing" A proportional to identity for optimal behavior (by premultiplying A by a conditioning matrix that make A close to a constant times identity)

<u>Summary</u> : Smooth SA. * mean example. (proof 1)

* cvgce in mean (Lyapunov fct) (proof 2)

↳ depending on choices for $(\gamma_n)_{n \geq 0}$

* cvgce a.s. (proof n°2)

(proof n°1)

* cvgce (CLT-like) if $h(\theta_n) \simeq \underbrace{h'(\theta_*)}_{A} (\theta_n - \theta_*)$

| step size
| $\lambda_{min}(A)$.

$\longrightarrow$ Best iterate cvges $C \geq \frac{1}{\lambda_{min}(A)}$

$$n \, \mathbb{E}(\theta_n - \theta_*)(\theta_n - \theta_*)^T \simeq \frac{C^2 \, \Sigma}{2CA - I}$$

16h10.

Lecture n° 5. 28.02.22.

- PR averaging smooth fct° asymptotic rate
- Non asymptotic rates
  - → proof / proof n°2 within proof n°1) ; commenting on plots.
  - → Logistic regression — Bach & Moulines 2011, 13
  - → LSR — – 2011, 13
  - → extens° to Hilbert spaces / better rates in f.d. — Dieuleveut & Bach 16
  - → accelerat°, order re Newton

Polyak-Ruppert averaging

for the last iterate

* stepsize scaling as $\left(1/\mu n\right)$

* cvgce rate (asympt) $\left(1/\mu^2\right)$

- **Problems with Robbins-Monro algorithm**
  - Choice of step-sizes in Robbins-Monro algorithm
  - Dependence on the unknown conditioning of the problem

- **Simple but impactful idea** (Polyak and Juditsky, 1992; Ruppert, 1988)
  - Consider the averaged iterate $\boxed{\bar{\theta}_n = \frac{1}{n}\sum_{k=1}^{n} \theta_k}$
  - NB: "Offline" averaging
  - Can be computed recursively as $\bar{\theta}_n = (1 - 1/n)\bar{\theta}_{n-1} + \frac{1}{n}\theta_n$
  - In practice, may start the averaging "after a while"

- **Analysis**
  - Unique optimum θ_*. See details by Polyak and Juditsky (1992)

Cesaro means

- Assume $\theta_n \to \theta_*$, with convergence rate $\|\theta_n - \theta_*\| \leqslant \alpha_n$
- Cesaro's theorem: $\bar{\theta}_n = \frac{1}{n}\sum_{k=1}^{n} \theta_n$ converges to θ_*
- What about convergence rate $\|\bar{\theta}_n - \theta_*\|$?

Cesaro means

$\alpha_0 = 1$

$\alpha_1 = \alpha_2 \cdots = 0$

- Assume $\theta_n \to \theta_*$, with convergence rate $\|\theta_n - \theta_*\| \leqslant \alpha_n$
- Cesaro's theorem: $\bar\theta_n = \frac{1}{n}\sum_{k=1}^n \theta_n$ converges to θ_*

$\bar\theta_n - \theta_* = \frac{1}{n}(\theta_0 - \theta_*$

- What about convergence rate $\|\bar\theta_n - \theta_*\|$?

$$\|\bar\theta_n - \theta_*\| \;\leqslant\; \frac{1}{n}\sum_{k=1}^n \|\theta_k - \theta_*\| \leqslant \frac{1}{n}\sum_{k=1}^n \alpha_k$$

- Will depend on rate α_n
- If $\sum_n \alpha_n < \infty$, the rate becomes $1/n$ independently of α_n

$\hookrightarrow$ $\alpha_n = o\left(\frac{1}{n}\right)$ $\left(\text{often } \alpha_n = O\left(\frac{1}{n^\alpha}\right);\ \alpha > 1\right)$

$\hookrightarrow$ averaging would slow down cvg if cvg was very fast.
(linked to acceleration : see in Ch!)

≠ce between 2 proof techniques:

unbiasedness

bounded variance

Proof n°2 : $\underbrace{\mathbb{E}_{n-1}\left[\|\theta_n-\theta_*\|^2\right]}_{\in\mathbb{R}} \leq \|\theta_{n-1}-\theta_*\|^2 - \underbrace{2\gamma\langle\nabla f(\theta_{n-1}),\theta_{n-1}-\theta_*\rangle}_{\leq f(\theta_{n-1})-f(\theta_*)} + 2\gamma^2\underbrace{\|\varepsilon_n(\theta_{n-1})\|^2}_{\nabla f_n(\theta_{n-1})-\nabla f(\theta_{n-1})}$

in $\mathbb{E}$

$\Longrightarrow 2\gamma\left(f(\theta_{n-1})-f_*\right) \leq \|\theta_{n-1}-\theta_*\|^2 - \|\theta_n-\theta_*\|^2 + 2\gamma^2\sigma^2$

+ jensen + sum these ineq from 1 to n.

$$f\left(\frac{1}{n}\sum\theta_i\right)-f_* \leq \frac{1}{n}\sum_{i=1}^{n} f(\theta_i)-f_* \lesssim \frac{\|\theta_0-\theta_*\|^2}{\gamma n} + \gamma\sigma^2$$

possibly $\ll$

(result for $f(\bar\theta_n)-f_*$)

result for $\mathbb{E}\left[f(\theta_I)-f_*\right]$, $I\sim\mathcal{U}[\![1;n]\!]$.

this technique (picking one iterate along the sequence) is crucial in non cvx)

Polyak-Ruppert averaging - Proof sketch - I

Proof n°1 : we deal with θ_n as a stochastic process

- Recursion: $\theta_n = \theta_{n-1} - \gamma_n\big(h(\theta_{n-1}) + \varepsilon_n\big)$ with $\gamma_n = C/n^\alpha$
  - From before, we know that $\|\theta_n - \theta_*\|^2 = O(n^{-\alpha})$

$$\frac{\sigma^2}{n} = \Big\|\frac{1}{n}\sum \varepsilon_i\Big\|^2 \ll \frac{1}{n}\underbrace{\sum \|\varepsilon_i\|^2}_{\sigma^2}$$

based (always) on linear approx of h around θ_*

$$h(\theta_{n-1}) = \frac{1}{\gamma_n}[\theta_{n-1} - \theta_n] - \varepsilon_n$$

$$\boxed{A(\theta_{n-1} - \theta_*) + O(\|\theta_{n-1} - \theta_*\|^2)} = \frac{1}{\gamma_n}[\theta_{n-1} - \theta_n] - \varepsilon_n \text{ with } A = h'(\theta_*)$$

$$A(\theta_{n-1} - \theta_*) = \frac{1}{\gamma_n}[\theta_{n-1} - \theta_n] - \varepsilon_n + O(n^{-\alpha})$$

using non averaged analysis.

averaging these equalities

$$\frac{1}{n}\sum_{k=1}^{n} A(\theta_{k-1} - \theta_*) = \frac{1}{n}\sum_{k=1}^{n}\frac{1}{\gamma_k}[\theta_{k-1} - \theta_k] - \frac{1}{n}\sum_{k=1}^{n}\varepsilon_k + O(n^{-\alpha})$$

$$\underbrace{\frac{1}{n}\sum_{k=1}^{n} A(\theta_{k-1} - \theta_*)}_{\mathbb{R}^d} = \underbrace{\frac{1}{n}\sum_{k=1}^{n}\frac{1}{\gamma_k}[\theta_{k-1} - \theta_k]}_{} + \underbrace{\text{Normal}(0, \Sigma/n)}_{\left(\text{variance } \frac{1}{n}\right)} + O(n^{-\alpha})$$

if $\gamma_k = \gamma \longrightarrow \dfrac{\theta_0 - \theta_n}{\gamma n}$

Polyak-Ruppert averaging - Proof sketch - II

- **Goal**: Bounding $\frac{1}{n}\sum_{k=1}^{n}\frac{1}{\gamma_k}\big[\theta_{k-1}-\theta_k\big]$ given $\|\theta_n-\theta_*\|^2 = O(n^{-\alpha})$

- Abel's summation formula: We have, summing by parts,

derivating

$$\underbrace{\frac{1}{n}\sum_{k=1}^{n}\frac{1}{\gamma_k}(\theta_{k-1}-\theta_k)}_{A} = \underbrace{\frac{1}{n}\sum_{k=1}^{n-1}(\theta_k-\theta_*)(\gamma_{k+1}^{-1}-\gamma_k^{-1}) - \frac{1}{n}(\theta_n-\theta_*)\gamma_n^{-1}}_{B} + \frac{1}{n}(\theta_0-\theta_*)\gamma_0^{-1} \; ?$$

$\left(\theta_{n-1}-\theta_* - (\theta_k-\theta_*)\right)$

integrating

$$A - B = \sum\left((\theta_n-\theta_k)\gamma_n^{-1} - (\theta_{n-1}-\theta_k)\gamma_{n-1}^{-1}\right)$$

leading to

$(k+1)^{\alpha} - k^{\alpha}$

$$\left\|\frac{1}{n}\sum_{k=1}^{n}\frac{1}{\gamma_k}(\theta_{k-1}-\theta_k)\right\| \leqslant \underbrace{\frac{1}{n}\sum_{k=1}^{n-1}\underbrace{\|\theta_k-\theta_*\|}_{O(k^{-\alpha/2})}\cdot\underbrace{|\gamma_{k+1}^{-1}-\gamma_k^{-1}|}_{(\dots)} + \frac{1}{n}\underbrace{\|\theta_n-\theta_*\|}_{O(n^{-\alpha/2})}\gamma_n^{-1}}_{=} + \underbrace{\frac{1}{n}\|\theta_0-\theta_*\|\gamma_1^{-1}}_{O(1/n)}$$

which is negligible

Abel formula: (a_k) / $A_n = \sum_{k=1}^{n} a_n$ is bounded. $\sum a_k b_k$ is cvging.

$(b_n) \searrow 0$ $\quad$ $\sum_{n\geq 1}\frac{(-1)^n}{n}$ is cvging $(\ln(2))$

IBP: $\int (uv' + v'u) = [uv]$

$$\sum a_k b_k = \sum (A_{k+1}-\cancel{A_k})\cancel{b_k} = [A\,b] - \sum \cancel{A_k}(b_{k+1}-\cancel{b_k})$$

Overall: ctrl of bias term as $O(n^{-1+\alpha/2})$

Polyak-Ruppert averaging - Proof sketch - III

- Recursion: $\theta_n = \theta_{n-1} - \gamma_n\big(h(\theta_{n-1}) + \varepsilon_n\big)$ with $\gamma_n = C/n^\alpha$
  - From before, we know that $\|\theta_n - \theta_*\|^2 = O(n^{-\alpha})$

$$\frac{1}{n}\sum_{k=1}^{n} A(\theta_{k-1} - \theta_*) \quad = \quad \text{Normal}(0, \Sigma/n) + \underbrace{O(n^{-\alpha})}_{\ll \frac{1}{\sqrt{n}} \text{ if } \alpha > 1/2} + \underbrace{O(n^{\cancel{\alpha-1}\, -1+\alpha/2})}_{\ll \frac{1}{\sqrt{n}} \text{ if } \alpha < 1}$$

- **Consequence**: $\bar{\theta}_n - \theta_*$ is asymptotically normal with mean zero and covariance $\frac{1}{n}A^{-1}\Sigma A^{-1}$ $\longrightarrow$ much better than $\frac{1}{n} \times \frac{1}{\lambda_{\min}(A)^2}\Sigma$ / e.g. $A^{-1} = \Sigma$. $\frac{A^{-1}}{n} \ll \frac{I}{n\lambda_{\min}(A)}$
  - Achieves the Cramer-Rao lower bound (see next lecture)
  - Independent of step-size (see next lecture)
  - Where are the initial conditions? (see next lecture)

before PR $\quad \mathbb{E}\left[(\theta_n - \theta_*)(\theta_n - \theta_*)^T\right] \preccurlyeq C^2\Sigma = \frac{1}{\mu^2}\Sigma \;//\; C \propto \frac{1}{\mu}$

Beyond the classical analysis

- **Lack of strong-convexity**
  - Step-size $\gamma_n = 1/n$ not robust to ill-conditioning
- **Robustness of step-sizes** (cvgce $\forall \alpha \in [\frac{1}{2}; 1]$)
- **Explicit forgetting of initial conditions**

Take away: key difference between proofs that rely on UB on $\|\theta_n - \theta_*\|^2$ vs proofs that rely on expanding $\bar{\theta}_n - \theta_*$ as a sum of vectors (including $\frac{1}{n}\sum_{i=1}^{n} \varepsilon_i(\theta_{i-1})$)

expansion relies on a Taylor approx of h.

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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**

   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging just covered

5. **Smooth stochastic approximation algorithms**

   - Non-asymptotic analysis for smooth functions
   - Logistic regression (self concordance).
   - Least-squares regression without decaying step-sizes

6. **Finite data sets**

   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

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: $O((\mu n)^{-1})$ *(weighted)
    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 $\gamma_n \propto n^{-1/2}$

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 $\gamma_n \propto n^{-1/2}$

- **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)

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

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: $O(n^{-1/2})$
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- **Non-asymptotic analysis for smooth problems?**

$f_n(\theta) = \ell(x_n^T\theta, y_n)$

Smoothness/convexity assumptions

$h \leftarrow f'$

∇f

$f_n'(\theta) = \ell'(x_n^T\theta, y_n)\, x_n$ $\quad f_n''(\theta) = \ell''(x_n^T\theta, y_n)(x_n x_n^T)$

- Iteration: $\boxed{\theta_n = \theta_{n-1} - \gamma_n f_n'(\theta_{n-1})}$
  - Polyak-Ruppert averaging: $\bar{\theta}_n = \frac{1}{n}\sum_{k=0}^{n-1}\theta_k$

f_n : e.g. loss$(\cdot,(x_n,y_n))$

- **Smoothness of f_n**: For each $n \geqslant 1$, the function f_n is a.s. convex, differentiable with L-Lipschitz-continuous gradient f_n':

SC :
  - Smooth loss and bounded data (a.s.)

a.s. UB on Lipschitz constant L

↳ can be relaxed. (Hardt, Ma, Needle '16) UB on $\nabla^2 f_n$:

- **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 $\frac{\mu}{2}\|\theta\|^2$

"we will use strg cvx after taking expectations"

require
1) Smoothness on f_n (a.s.) 2) strg cvxty on f.

Summary of new results (Bach and Moulines, 2011)

- Stochastic gradient descent with learning rate $\gamma_n = Cn^{-\alpha}$
- **Strongly convex smooth objective functions**
  - Old: $O(n^{-1}\mu^{-1})$ rate achieved without averaging for $\alpha = 1$
  - New: $O(n^{-1}\mu^{-1})$ rate achieved with averaging for $\alpha \in [1/2, 1]$
  - Non-asymptotic analysis with explicit constants
  - Forgetting of initial conditions $\left(\|\theta_0 - \theta_*\|^2\right)$
  - Robustness to the choice of C

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

- Stochastic gradient descent with learning rate $\gamma_n = Cn^{-\alpha}$

based on (proof n°1)

- **Strongly convex smooth objective functions**
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  - Robustness to the choice of C

* is slightly sub optimal

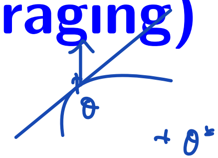
- **Convergence rates** for $\mathbb{E}\|\theta_n - \theta_*\|^2$ and $\mathbb{E}\|\bar\theta_n - \theta_*\|^2$
  - no averaging: $O\Big(\frac{\sigma^2\gamma_n}{\mu}\Big) + O(e^{-\mu n\gamma_n})\|\theta_0 - \theta_*\|^2$
  - averaging: $\frac{\operatorname{tr} H(\theta_*)^{-1}}{n} + \mu^{-1}O(n^{-2\alpha} + n^{-2+\alpha}) + O\Big(\frac{\|\theta_0 - \theta_*\|^2}{\mu^2 n^2}\Big)$

$\hookrightarrow$ proof n°1 (:)) : * requires a ctrl of $\|\theta_n - \theta_*\|^2$

$\|\nabla f(\theta) - \nabla f(\eta)\|^2 \leqslant L^2 \|\theta - \eta\|^2$ // $\|\nabla f(\theta) - \nabla f(\eta)\|^2 \leqslant L \langle \theta - \eta, \nabla f(\theta) - \nabla f(\eta) \rangle$ cocoercivity

Classical proof sketch (no averaging) - I

$\Rightarrow \langle \theta - \theta_*, \nabla f(\theta) \rangle \geqslant 0$



proof n°2

(what was missing in BM 11)

co_co

strg cvxty

$$
\begin{aligned}
\|\theta_n - \theta_*\|_2^2 &= \|\theta_{n-1} - \gamma_n f_n'(\theta_{n-1}) - \theta_*\|_2^2 \\
&= \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{n-1}) + \gamma_n^2 \|f_n'(\theta_{n-1})\|_2^2 \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{n-1}) \\
&\qquad + 2\gamma_n^2 \|f_n'(\theta_*)\|_2^2 + 2\gamma_n^2 \|f_n'(\theta_{n-1}) - f_n'(\theta_*)\|_2^2 \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f_n'(\theta_{n-1}) \\
&\qquad + 2\gamma_n^2 \|f_n'(\theta_*)\|_2^2 + 2\gamma_n^2 L [f_n'(\theta_{n-1}) - f_n'(\theta_*)]^\top (\theta_{n-1} - \theta_*) \\
\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2 | \mathcal{F}_{n-1}\big] &\leqslant \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(\theta_{n-1} - \theta_*)^\top f'(\theta_{n-1}) \\
&\qquad + 2\gamma_n^2 \mathbb{E}\|f_n'(\theta_*)\|_2^2 + 2\gamma_n^2 L [f'(\theta_{n-1}) - 0]^\top (\theta_{n-1} - \theta_*) \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(1 - \gamma_n L)(\theta_{n-1} - \theta_*)^\top f'(\theta_{n-1}) + 2\gamma_n^2 \sigma^2 \\
&\leqslant \|\theta_{n-1} - \theta_*\|_2^2 - 2\gamma_n(1 - \gamma_n L)\frac{1}{2}\mu \|\theta_{n-1} - \theta_*\|_2^2 + 2\gamma_n^2 \sigma^2 \\
&= \big[1 - \mu\gamma_n(1 - \gamma_n L)\big] \|\theta_{n-1} - \theta_*\|_2^2 + 2\gamma_n^2 \sigma^2 \\
\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2\big] &\leqslant \big[1 - \mu\gamma_n(1 - \gamma_n L)\big] \mathbb{E}\big[\|\theta_{n-1} - \theta_*\|_2^2\big] + 2\gamma_n^2 \sigma^2
\end{aligned}
$$

$a_n \lesssim (1 - \mu\gamma_n)\, a_{n-1} + \gamma_n^2 \sigma^2$

Classical proof sketch (no averaging) - II

- **Main bound**

$$\begin{aligned}\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2\big] &\leqslant \big[1 - \mu\gamma_n(1 - \gamma_n L)\big]\mathbb{E}\big[\|\theta_{n-1} - \theta_*\|_2^2\big] + 2\gamma_n^2\sigma^2 \\ &\leqslant \big[1 - \mu\gamma_n/2\big]\mathbb{E}\big[\|\theta_{n-1} - \theta_*\|_2^2\big] + 2\gamma_n^2\sigma^2 \text{ if } \gamma_n L \leqslant 1/2\end{aligned}$$

- **Classical results from stochastic approximation** (Kushner and Yin, 2003): $\mathbb{E}\big[\|\theta_n - \theta_*\|_2^2\big]$ is smaller than

$$\leqslant \prod_{i=1}^{n}\big[1 - \mu\gamma_i/2\big]\mathbb{E}\big[\|\theta_0 - \theta_*\|_2^2\big] + \sum_{k=1}^{n}\prod_{i=k+1}^{n}\big[1 - \mu\gamma_i/2\big]2\gamma_k^2\sigma^2$$

$$\leqslant \exp\Big[-\frac{\mu}{2}\sum_{i=1}^{n}\gamma_i\Big]\mathbb{E}\big[\|\theta_0 - \theta_*\|_2^2\big] + \sum_{k=1}^{n}\prod_{i=k+1}^{n}\big[1 - \mu\gamma_i/2\big]2\gamma_k^2\sigma^2$$

if $\gamma \equiv \text{cst}$

$a_n \leqslant (1-\gamma\mu)\, a_{n-1} + \gamma^2\sigma^2$

$a_n \leqslant (1-\gamma\mu)^n a_0 + \gamma^{\cancel{2}}\sigma^2 \overbrace{\sum (1-\gamma\mu)^k}^{1/(\cancel{\gamma}\mu)}$ $\quad \dfrac{\cancel{\gamma}\sigma^2}{\mu}$

Decomposition of the noise term

- Assume (γ_n) is decreasing and less than $1/\mu$; then for any $m \in \{1, \dots, n\}$, we may split the following sum as follows:

$$
\begin{aligned}
\sum_{k=1}^{n} \prod_{i=k+1}^{n} (1-\mu\gamma_i)\gamma_k^2 &= \sum_{k=1}^{m} \prod_{i=k+1}^{n} (1-\mu\gamma_i)\gamma_k^2 + \sum_{k=m+1}^{n} \prod_{i=k+1}^{n} (1-\mu\gamma_i)\gamma_k^2 \\
&\leqslant \prod_{i=m+1}^{n} (1-\mu\gamma_i) \sum_{k=1}^{m} \gamma_k^2 + \gamma_m \sum_{k=m+1}^{n} \prod_{i=k+1}^{n} (1-\mu\gamma_i)\gamma_k \\
&\leqslant \exp\left(-\mu \sum_{i=m+1}^{n} \gamma_i\right) \sum_{k=1}^{m} \gamma_k^2 + \frac{\gamma_m}{\mu} \sum_{k=m+1}^{n} \left[\prod_{i=k+1}^{n} (1-\mu\gamma_i) - \prod_{i=k}^{n} (1-\mu \right. \\
&\leqslant \exp\left(-\mu \sum_{i=m+1}^{n} \gamma_i\right) \sum_{k=1}^{m} \gamma_k^2 + \frac{\gamma_m}{\mu} \left[1 - \prod_{i=m+1}^{n} (1-\mu\gamma_i) \right] \\
&\leqslant \exp\left(-\mu \sum_{i=m+1}^{n} \gamma_i\right) \sum_{k=1}^{n} \gamma_k^2 + \frac{\gamma_m}{\mu}, \text{ with e.g. } m = n/2
\end{aligned}
$$

Decomposition of the noise term

$$\left(\sum_{k=1}^{n} \prod_{i=k+1}^{n} (1-\mu\gamma_i)\gamma_k^2 \leqslant \exp\left(-\mu \sum_{i=m+1}^{n} \gamma_i\right) \sum_{k=1}^{n} \gamma_k^2 + \frac{\gamma_m}{\mu}\right) \times \sigma^2$$

If $\gamma = \text{cst}$: $\quad (1-\gamma\mu)^n \quad + \quad \frac{\gamma \sigma^2}{\mu}$

- Require γ_n to tend to zero (vanishing decaying step-size)
  - May not need $\sum_n \gamma_n^2 < \infty$ for convergence in quadratic mean

- Examples: $\boxed{\gamma_n = C/n^\alpha}$
  - $\alpha = 1$, $\sum_{i=1}^{n} \frac{1}{i} = \log(n) + \text{ cst } + O(1/n)$
  - $\alpha > 1$, $\sum_{i=1}^{n} \frac{1}{i^\alpha} = \text{ cst } + O(1/n^{\alpha-1})$
  - $\alpha \in (0,1)$, $\sum_{i=1}^{n} \frac{1}{i^\alpha} = \text{ cst} \times n^{1-\alpha} + O(1)$
  - Proof using relationship with integrals
  - Consequences: need $\alpha \in (0,1)$

to ctrl $\|\theta_n - \theta_*\|^2$

Proof sketch (averaging)

proof n° 1 (:)) within it, use the result on $\|\theta_n - \theta_*\|^2$ non asympt

- From Polyak and Juditsky (1992):

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

move terms around

$$\Leftrightarrow \quad f_n'(\theta_{n-1}) = \frac{1}{\gamma_n}(\theta_{n-1} - \theta_n)$$

expansion around θ_*

$$\Leftrightarrow \quad f_n'(\theta_*) + f_n''(\theta_*)(\theta_{n-1} - \theta_*) = \frac{1}{\gamma_n}(\theta_{n-1} - \theta_n) + O(\|\theta_{n-1} - \theta_*\|^2)$$

$$\Leftrightarrow \quad f_n'(\theta_*) + \underbrace{f''}_{\approx}(\theta_*)(\theta_{n-1} - \theta_*) = \frac{1}{\gamma_n}(\theta_{n-1} - \theta_n) + O(\|\theta_{n-1} - \theta_*\|^2)$$
$$+ O(\|\theta_{n-1} - \theta_*\|)\varepsilon_n$$

$$\Leftrightarrow \quad \theta_{n-1} - \theta_* \overset{(*)}{=} -f''(\theta_*)^{-1}\underbrace{f_n'(\theta_*)}_{\varepsilon_n(\theta_*)} + \frac{1}{\gamma_n} f''(\theta_*)^{-1}(\theta_{n-1} - \theta_n) \longrightarrow f''(\theta_*)(\theta_n - \theta_*)$$

$$+ O(\|\theta_{n-1} - \theta_*\|^2) + O(\|\theta_{n-1} - \theta_*\|)\varepsilon_n$$

same as before

make an assp° on $f^{(3)} \leq M$.

- Averaging to cancel the term $\frac{1}{\gamma_n} f''(\theta_*)^{-1}(\theta_{n-1} - \theta_n)$

$$\frac{\theta_n - \theta_0}{n} = -f''(\theta_*)\frac{\sum \varepsilon_n(\theta_*)}{n} + \frac{1}{\gamma} f''(\theta_*)(\bar\theta_n - \theta_*)$$

Robustness to wrong constants for $\gamma_n = Cn^{-\alpha}$

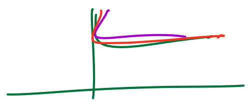
- $f(\theta) = \frac{1}{2}|\theta|^2$ with i.i.d. Gaussian noise ($d = 1$)
- Left: $\alpha = 1/2$

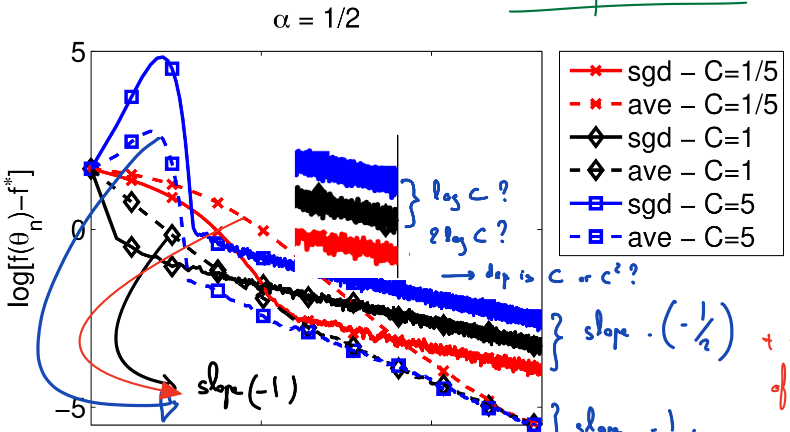
$\frac{C}{\sqrt{n}}$

intuit: for averaging → no impact

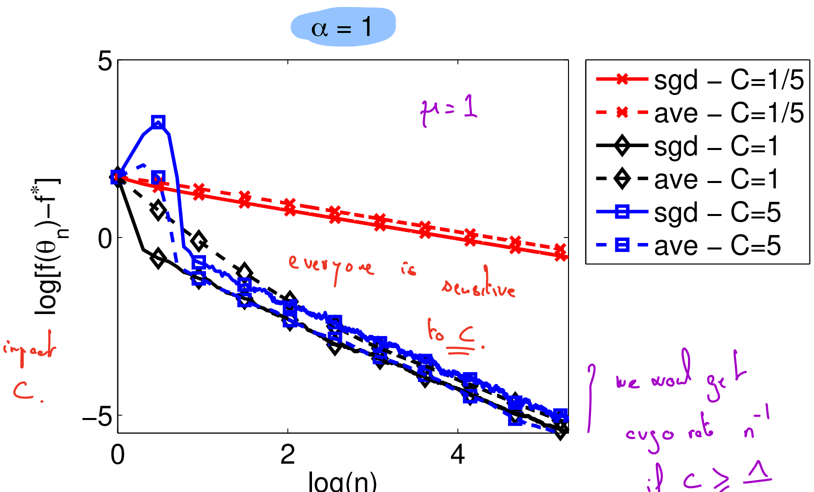
w/o. → impact.

- Right: $\alpha = 1$





} log c ?
} 2 log c ?
→ dep is c or c² ?
slope (-1)
} slope. (-1/2)
+ impact of C.
} slope -1.
↳ no impact of C asympt



μ = 1

everyone is sensitive to C.

} we would get cvg rate n^{-1} if $C \geq \frac{1}{\mu}$

Remark :

- See also `http://leon.bottou.org/projects/sgd`

$f(\tilde\theta_n) - f_* \leq \frac{1}{n^\alpha}$.

$\log\left(f(\tilde\theta_n) - f_*\right) \leq -\alpha \log n$

$\log\left(f(\theta_n) - f_*\right) \leq -\kappa n$.

* to visualize : $f(\tilde\theta_n) - f_* \leq e^{-\kappa n}$

→ log.lin plot → line with slope $-\kappa$.

* to viz. $f(\tilde\theta_n) - f_* \leq \frac{1}{\mu n}$

→ log-log plot

Summary of new results (Bach and Moulines, 2011)

- Stochastic gradient descent with learning rate $\gamma_n = Cn^{-\alpha}$
- **Strongly convex smooth objective functions**
  - Old: $O(\mu^{-1}n^{-1})$ rate achieved without averaging for $\alpha = 1$
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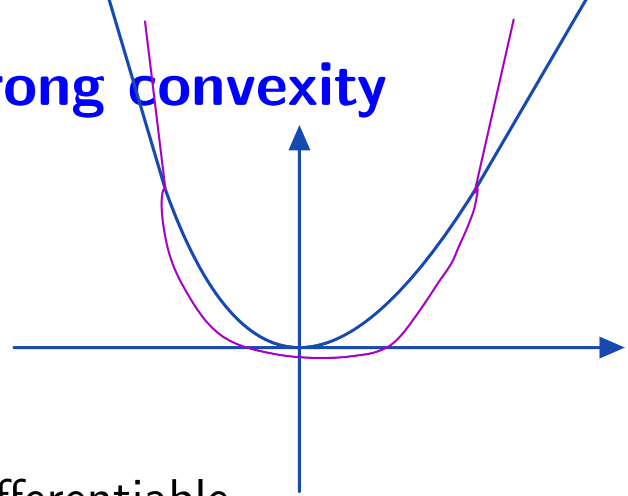
- **Non-strongly convex smooth objective functions**
  - Old: $O(n^{-1/2})$ rate achieved with averaging for $\alpha = 1/2$
  - New: $O(\max\{n^{1/2-3\alpha/2}, n^{-\alpha/2}, n^{\alpha-1}\})$ rate achieved without averaging for $\alpha \in [1/3, 1]$

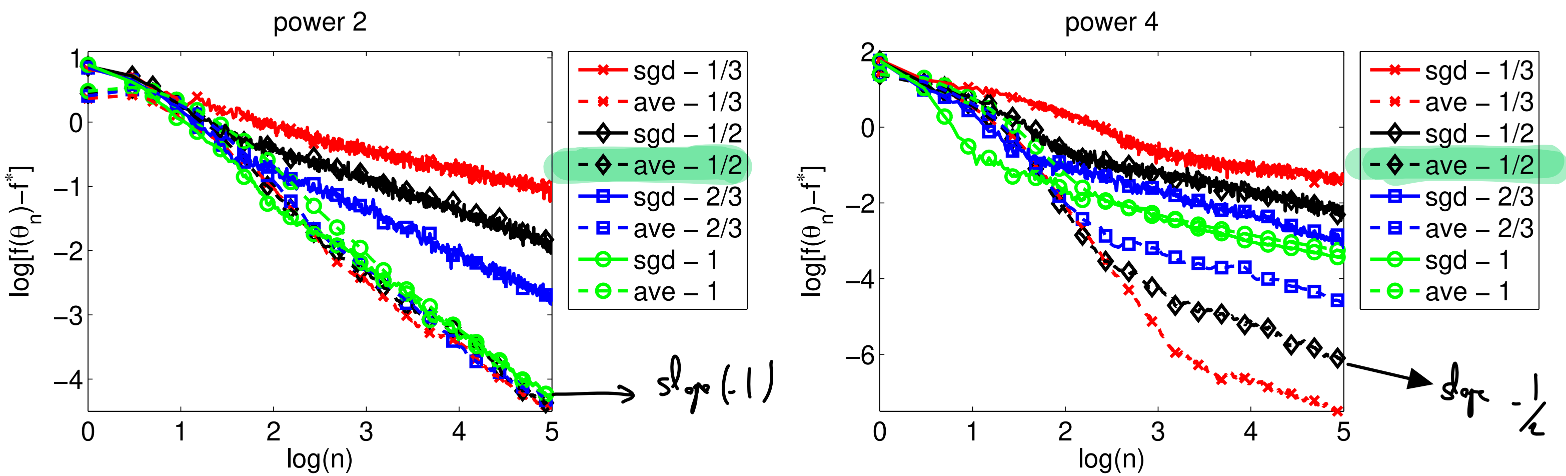
same alg. performs better w. strg cvxty.

- **Take-home message**
  - $\boxed{\text{Use } \alpha = 1/2 \text{ with averaging to be adaptive to strong convexity}}$

Robustness to lack of strong convexity



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



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Existing work

- **Known global minimax rates of convergence for non-smooth problems** (Nemirovsky and Yudin, 1983; Agarwal et al., 2012)
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- **Asymptotic analysis of averaging** (Polyak and Juditsky, 1992; Ruppert, 1988)
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- **A single adaptive algorithm for smooth problems with convergence rate $O(\min\{1/\mu n, 1/\sqrt{n}\})$ in all situations?**

Adaptive algorithm for logistic regression

- **Logistic regression**: $(\Phi(x_n), y_n) \in \mathbb{R}^d \times \{-1, 1\}$
  - Single data point: $f_n(\theta) = \log(1 + \exp(-y_n \theta^\top \Phi(x_n)))$
  - Generalization error: $f(\theta) = \mathbb{E} f_n(\theta)$

$\frac{1}{n\mu} \to$ global strg cvxty cst

$\to \frac{1}{n\mu_{loc}}$ μ_{loc} : local strg cvxty cst.

$\mu_{loc} = \lambda_{min}(f''(\theta_*))$

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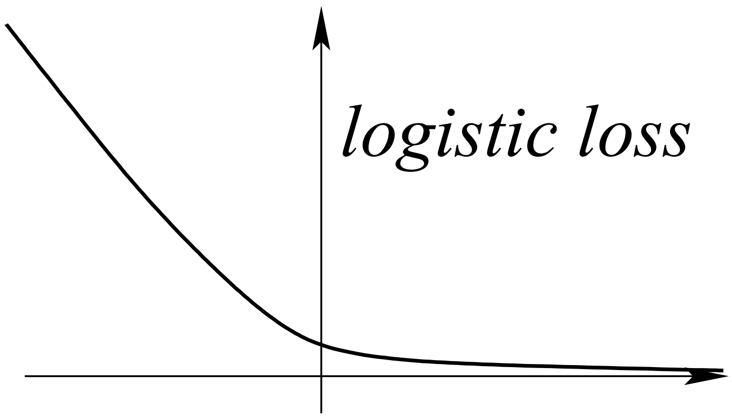
- **Cannot be strongly convex** $\Rightarrow$ local strong convexity
  - unless restricted to $|\theta^\top \Phi(x_n)| \leqslant M$ (with constants e^M - *proof*)
  - $\mu =$ lowest eigenvalue of the Hessian at the optimum $f''(\theta_*)$



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  - μ = lowest eigenvalue of the Hessian at the optimum $f''(\theta_*)$
    loc

- n **steps of averaged SGD with constant step-size** $1/(2R^2\sqrt{n})$
  - with R = radius of data (Bach, 2013):

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

adaptivity.

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

Self-concordance - I

- Usual definition for convex $\varphi : \mathbb{R} \to \mathbb{R}$: $|\varphi'''(t)| \leqslant 2\varphi''(t)^{3/2}$
  - 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)
  - $\varphi(t) = \log(1 + e^{-t})$, $\varphi'(t) = (1 + e^{t})^{-1}$, etc...

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- **Important properties**
  - Allows global Taylor expansions
  - Relates expansions of derivatives of different orders

Global Taylor expansions

- **Lemma**: If $\forall t \in \mathbb{R}$, $|g'''(t)| \leqslant S g''(t)$, for $S \geqslant 0$. Then, $\forall t \geqslant 0$:

$$\frac{g''(0)}{S^2}(e^{-St} + St - 1) \leqslant g(t) - g(0) - g'(0)t \leqslant \frac{g''(0)}{S^2}(e^{St} - St - 1)$$

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- **Proof**: Let us first assume that $g''(t)$ is strictly positive for all $t \in \mathbb{R}$. We have, for all $t \geqslant 0$: $-S \leqslant \frac{d \log g''(t)}{dt} \leqslant S$. Then, by integrating once between 0 and t, taking exponentials, and then integrating twice:

$$-St \leqslant \log g''(t) - \log g''(0) \leqslant St,$$

$$g''(0)e^{-St} \leqslant g''(t) \leqslant g''(0)e^{St}, \quad (1)$$
$$g''(0)S^{-1}(1 - e^{-St}) \leqslant g'(t) - g'(0) \leqslant g''(0)S^{-1}(e^{St} - 1),$$
$$g(t) \geqslant g(0) + g'(0)t + g''(0)S^{-2}(e^{-St} + St - 1), \quad (2)$$
$$g(t) \leqslant g(0) + g'(0)t + g''(0)S^{-2}(e^{St} - St - 1), \quad (3)$$

which leads to the desired result (simple reasoning for strict positivity of g'')

Relating Taylor expansions of different orders

- **Lemma**: If $h : t \mapsto f\big[\theta_1 + t(\theta_2 - \theta_1)\big]$ satisfies: $\forall t \in \mathbb{R}$, $|h'''(t)| \leqslant R\|\theta_1 - \theta_2\| h''(t)$. We have, for all $\theta_1, \theta_2 \in \mathbb{R}^d$:

$$\underbrace{\Big\| f'(\theta_1) - \underbrace{f'(\theta_2) - f''(\theta_2)(\theta_2 - \theta_1)}_{\text{linear approx of } f' \text{ around } \theta_2.} \Big\|}_{\text{what we need to use prop n°1}} \leqslant R\big[f(\theta_1) - f(\theta_2) - \langle f'(\theta_2), \theta_2 - \theta_1 \rangle\big]$$

Relating Taylor expansions of different orders

- **Lemma**: If $h : t \mapsto f\big[\theta_1 + t(\theta_2 - \theta_1)\big]$ satisfies: $\forall t \in \mathbb{R}$, $|h'''(t)| \leqslant R\|\theta_1 - \theta_2\| h''(t)$. We have, for all $\theta_1, \theta_2 \in \mathbb{R}^d$:
$$\big\|f'(\theta_1) - f'(\theta_2) - f''(\theta_2)(\theta_2 - \theta_1)\big\| \leqslant R\big[f(\theta_1) - f(\theta_2) - \langle f'(\theta_2), \theta_2 - \theta_1\rangle\big]$$

- **Proof**: For $\|z\| = 1$, let $\varphi(t) = \big\langle z, f'\big(\theta_2 + t(\theta_1 - \theta_2)\big) - f'(\theta_2) - t f''(\theta_2)(\theta_2 - \theta_1)\big\rangle$ and $\psi(t) = R\big[f(\theta_2 + t(\theta_1 - \theta_2)) - f(\theta_2) - t\langle f'(\theta_2), \theta_2 - \theta_1\rangle\big]$. Then $\varphi(0) = \psi(0) = 0$, and:

$$\begin{aligned}
\varphi'(t) &= \big\langle z, f''\big(\theta_2 + t(\theta_1 - \theta_2)\big) - f''(\theta_2), \theta_1 - \theta_2\big\rangle \\
\varphi''(t) &= f'''\big(\theta_2 + t(\theta_1 - \theta_2)\big)[z, \theta_1 - \theta_2, \theta_1 - \theta_2] \\
&\leqslant R\|z\|_2 f''\big(\theta_2 + t(\theta_1 - \theta_2)\big)[\theta_1 - \theta_2, \theta_1 - \theta_2], \text{ using App. A of Bach (2010)} \\
&= R\big\langle \theta_2 - \theta_1, f''\big(\theta_2 + t(\theta_1 - \theta_2)\big)(\theta_1 - \theta_2)\big\rangle \\
\psi'(t) &= R\big\langle f'\big(\theta_2 + t(\theta_1 - \theta_2)\big) - f'(\theta_2), \theta_1 - \theta_2\big\rangle \\
\psi''(t) &= R\big\langle \theta_2 - \theta_1, f''\big(\theta_2 + t(\theta_1 - \theta_2)\big)(\theta_1 - \theta_2)\big\rangle,
\end{aligned}$$

Thus $\varphi'(0) = \psi'(0) = 0$ and $\varphi''(t) \leqslant \psi''(t)$, leading to $\varphi(1) \leqslant \psi(1)$ by integrating twice, which leads to the desired result by maximizing with respect to z.

Adaptive algorithm for logistic regression

Proof sketch

"weak proof & result"

- Step 1: use existing result $f(\bar\theta_n) - f(\theta_*) + \frac{R^2}{\sqrt{n}}\|\theta_0 - \theta_*\|_2^2 = O(1/\sqrt{n})$

- Step 2a: $f_n'(\theta_{n-1}) = \frac{1}{\gamma}(\theta_{n-1} - \theta_n) \Rightarrow \frac{1}{n}\sum_{k=1}^n f_k'(\theta_{k-1}) = \frac{1}{n\gamma}(\theta_0 - \theta_n)$

- Step 2b: $\frac{1}{n}\sum_{k=1}^n f'(\theta_{k-1}) = \frac{1}{n}\sum_{k=1}^n \underbrace{\big[f'(\theta_{k-1}) - f_k'(\theta_{k-1})\big]}_{\varepsilon_k(\theta_{k-1})} + \underbrace{\frac{1}{\gamma n}(\theta_0 - \theta_*) + \frac{1}{\gamma n}(\theta_* - \theta_n)}_{\frac{1}{\gamma n}(\theta_0 - \theta_n)} = O(1/\sqrt{n})$

- Step 3: $\Big\| f'\Big(\frac{1}{n}\sum_{k=1}^n \theta_{k-1}\Big) - \frac{1}{n}\sum_{k=1}^n f'(\theta_{k-1})\Big\|_2$
$= O\big(f(\bar\theta_n) - f(\theta_*)\big) = O(1/\sqrt{n})$ using self-concordance

- Step 4a: if f μ-strongly convex, $f(\bar\theta_n) - f(\theta_*) \leqslant \frac{1}{2\mu}\big\|f'(\bar\theta_n)\big\|_2^2$

- Step 4b: if f self-concordant, "locally true" with $\mu = \lambda_{\min}(f''(\theta_*))$

proof n° 1 :

$$\theta_n = \theta_{n-1} - \gamma\left(f'(\theta_{n-1}) + \varepsilon_n\right)$$

$$\Leftrightarrow \quad f'(\theta_{n-1}) = \frac{\theta_{n-1} - \theta_n}{\gamma} + \varepsilon_n$$

$$\Rightarrow \quad \frac{1}{n}\sum_{i=1}^{n} f'(\theta_{i-1}) = \frac{\theta_0 - \theta_n}{n\gamma} + \frac{\sum_{i=1}^{n} \varepsilon_i}{n}$$

easiest quantity to control

$$f'(\theta_n) \simeq f''(\theta_*)(\theta_n - \theta_*) + O\left(\|\theta_n - \theta_*\|^2\right)$$

(1)

$$\frac{1}{n}\sum f'(\theta_n) \simeq f''(\theta_*)(\theta_n - \theta_*)$$

Instead.

$$\frac{1}{n}\sum_{i=1}^{n} f'(\theta_i) - f'\left(\frac{1}{n}\sum_{i=1}^{n}\theta_i\right)$$

use self concordance to control and not

Adaptive algorithm for logistic regression

- **Logistic regression**: $(\Phi(x_n), y_n) \in \mathbb{R}^d \times \{-1, 1\}$
  - Single data point: $f_n(\theta) = \log(1 + \exp(-y_n \theta^\top \Phi(x_n)))$
  - Generalization error: $f(\theta) = \mathbb{E} f_n(\theta)$

- **Cannot be strongly convex** $\Rightarrow$ local strong convexity
  - unless restricted to $|\theta^\top \Phi(x_n)| \leqslant M$ (and with constants e^M)
  - $\mu =$ lowest eigenvalue of the Hessian at the optimum $f''(\theta_*)$

- n **steps of averaged SGD with constant step-size** $1/(2R^2\sqrt{n})$
  - with $R =$ radius of data (Bach, 2013):

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

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

Adaptive algorithm for logistic regression

- **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):

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

  - **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 $\mathbb{E}\big[\Phi(x_n) \otimes \Phi(x_n)\big] = H \succcurlyeq \mu \cdot \mathrm{Id}$

Smooth

up to now: ideal algo is $\gamma_n \propto \frac{1}{\sqrt{n}}$.

* adaptive to strg cvxty vs cvxty

* adapts to local strg cvxty for logistic reg.

note $\frac{1}{n\mu}$ for μ s.c., $\frac{1}{\sqrt{n}}$ for cvx, $\frac{1}{n\,\mu_{loc}}$ for logistic reg.

For LSR: rate $\frac{1}{n}$ w.o. dep. on μ !!

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 = strg cvxty cst !
  - Main result: $\boxed{\mathbb{E}f(\bar\theta_{n-1}) - f(\theta_*) \leqslant \underbrace{\frac{4\sigma^2 d}{n}}_{\text{noise term}} + \underbrace{\frac{4R^2\|\theta_0-\theta_*\|^2}{n}}_{\text{initial cdtn term.}}}$

- **Matches statistical lower bound** (Tsybakov, 2003)
  - Non-asymptotic robust version of Györfi and Walk (1996)

Intuit°: from asymptotic analysis, we had $\mathcal{N}\left(0, \frac{\Sigma}{n}\right) + \cancel{O(n^{-\alpha})} + O\left(n^{-1+\alpha/2}\right)$

$\alpha = 0$ seems good!

was coming from linear approx of f' (or h) $\Rightarrow 0$ for quad

Least-squares - Proof technique - I

$H = \mathbb{E}\left[x_n x_n^\top\right]$

- LMS recursion:

$$\theta_n - \theta_* = \left[I - \gamma \overset{x_n}{\Phi(x_n)} \otimes \overset{x_n^\top}{\Phi(x_n)}\right](\theta_{n-1} - \theta_*) + \gamma\, \varepsilon_n \Phi(x_n)$$

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

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

easy to analyse.

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

$$\theta_n - \theta_* = \underbrace{\left[I - \gamma H\right]^n (\theta_0 - \theta_*)}_{\text{bias term.}} + \underbrace{\gamma \sum_{k=1}^{n} \left[I - \gamma H\right]^{n-k} \varepsilon_k \Phi(x_k)}_{\text{variance term}}$$

- Infinite expansion of Aguech, Moulines, and Priouret (2000) in powers of γ

Least-squares - Proof technique - II

- Explicit expansion of $\bar{\theta}_n$:

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

$$\bar{\theta}_n - \theta_* = \frac{1}{n+1} \sum_{i=0}^{n} \big[I - \gamma H\big]^i (\theta_0 - \theta_*) + \frac{\gamma}{n+1} \sum_{i=0}^{n} \sum_{k=1}^{i} \big[I - \gamma H\big]^{i-k} \varepsilon_k \Phi($$

$$\approx \frac{1}{n} (\gamma H)^{-1} \big[I - (I - \gamma H)^n\big] (\theta_0 - \theta_*) + \frac{\gamma}{n} \sum_{k=0}^{n} (\gamma H)^{-1} \varepsilon_k \Phi(x_k)$$

  - Need to bound $\big(\mathbb{E}\|H^{1/2}(\bar{\theta}_n - \theta_*)\|^2\big)^{1/2}$
  - Using Minkowski inequality

$$\sum_{i=1}^{n} a^i = \frac{1 - a^n}{1 - a}$$

Least-squares - Proof technique - III

- Explicit expansion of $\bar\theta_n$:

$$\bar\theta_n - \theta_* \approx \frac{1}{n}(\gamma H)^{-1}\big[I-(I-\gamma H)^n\big](\theta_0-\theta_*) + \frac{\gamma}{n}\sum_{k=0}^{n}(\gamma H)^{-1}\varepsilon_k\Phi(x_k)$$

- **Bias - I**: $(\gamma H)^{-1}\big[I-(I-\gamma H)^n\big] \preccurlyeq (\gamma H)^{-1}$ leading to

$$\big(\mathbb{E}\|H^{1/2}(\bar\theta_n-\theta_*)\|^2\big)^{1/2} \leqslant \frac{1}{\gamma n}\|H^{-1/2}(\theta_0-\theta_*)\|$$

- **Bias - II**: $(\gamma H)^{-1}\big[I-(I-\gamma H)^n\big] \preccurlyeq \sqrt{n}(\gamma H)^{-1/2}$ leading to

$$\big(\mathbb{E}\|H^{1/2}(\bar\theta_n-\theta_*)\|^2\big)^{1/2} \leqslant \frac{1}{\sqrt{\gamma n}}\|(\theta_0-\theta_*)\|$$

- **Variance** (next slide)

Least-squares - Proof technique - III

- Explicit expansion of $\bar\theta_n$:

$$\bar\theta_n - \theta_* \approx \frac{1}{n}(\gamma H)^{-1}\big[I - (I-\gamma H)^n\big](\theta_0 - \theta_*) + \underbrace{\frac{\gamma}{n}\sum_{k=0}^{n}(\gamma H)^{-1}\varepsilon_k \Phi(x_k)}$$

- **Variance** (~~next slide~~)

$$\underbrace{\mathbb{E}\|H^{1/2}(\bar\theta_n - \theta_*)\|^2}_{\text{"}} = \frac{1}{n^2}\sum_{k=0}^{n}\mathbb{E}\varepsilon_k^2 \underbrace{\langle \Phi(x_k), H^{-1}\Phi(x_k)\rangle}$$

$\mathbb{E}\big(f(\bar\theta_n) - f(\theta_*)\big)$ $\quad = \frac{1}{n}\sigma^2 d$

$\mathbb{E}\langle \phi(x), H^{-1}\phi(x)\rangle$

$= \operatorname{tr}\mathbb{E}\langle \quad \rangle$

$= \mathbb{E}\operatorname{tr}\big(H^{-1}\phi(x)\phi(x)^\top\big)$

$= \operatorname{tr}(\mathrm{Id}) = d$

Least-squares - Proof technique - IV

- Expansion of Aguech, Moulines, and Priouret (2000) in powers of γ
  - LMS recursion:

$$\theta_n - \theta_* = \big[I - \gamma \Phi(x_n) \otimes \Phi(x_n)\big](\theta_{n-1} - \theta_*) + \overbrace{\gamma\, \varepsilon_n \Phi(x_n)}^{O(\gamma)} \qquad \text{type 1}$$

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

$$\eta_n - \theta_* = \big[I - \gamma H\big](\eta_{n-1} - \theta_*) + \gamma\, \varepsilon_n \Phi(x_n) \qquad \text{type 2}$$

- Expansion of the difference:

$$\theta_n - \eta_n = \big[I - \gamma \Phi(x_n) \otimes \Phi(x_n)\big](\theta_{n-1} - \eta_{n-1}) + \gamma \underbrace{\big[H - \Phi(x_n) \otimes \Phi(x_n)\big](\eta_{n-1} - \theta_*)}_{O(\gamma^2)\ \ldots}$$

is of type 1

we call the "type 2" of $(\theta_n - \eta_n)$, and the difference is again type 1, etc

Least-squares - Proof technique - IV

- Expansion of Aguech, Moulines, and Priouret (2000) in powers of γ
  - LMS recursion:

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

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

$$\eta_n - \theta_* = \big[I - \gamma H\big](\eta_{n-1} - \theta_*) + \gamma\, \varepsilon_n \Phi(x_n)$$

- Expansion of the difference:

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

  - New noise process
  - May continue the expansion infinitely many times

Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta\rangle\big)^2$

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

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

γ is cst

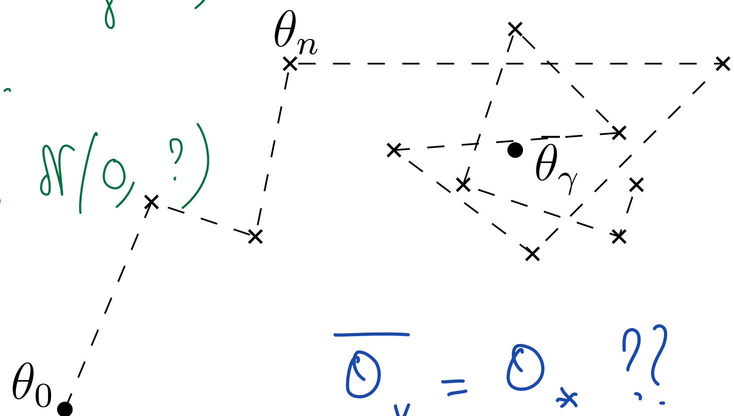
(x_n, y_n) iid seq

$(x_n, y_n) \mid \theta_{n-1} \overset{(d)}{=} (x_n, y_n)$.

$\frac{1}{n}\sum_{i=1}^{n} \theta_i \longrightarrow \mathbb{E}_{\pi_\gamma}(\theta) = \bar\theta_\gamma$

probably CLT for MC.

$\sqrt{n}\left(\bar\theta_n - \bar\theta_\gamma\right) \rightsquigarrow \mathcal{N}(0, ?)$



$\bar\theta_\gamma = \theta_*$??

$\bar{\theta}_n \to \bar{\theta}_\gamma$ on

$\bar{\theta}_\gamma = \theta_*$??

π_γ is the limit distrib.

also stat. distrib.

$\theta_0 \sim \pi_\gamma$

$\theta_1 \sim \pi_\gamma$

$$\theta_1 = \theta_0 - \gamma\left(f'(\theta_0) + \cancel{\varepsilon_1(\theta_0)}\right)$$

$$\mathbb{E}_{\pi_\gamma}(\theta) = \mathbb{E}_{\pi_\gamma}(\theta) - \mathbb{E}_{\pi_\gamma}\left(f'(\theta_0)\right) + 0$$

$\theta_1 \overset{(d)}{=} \theta_0 \sim \pi_\gamma$

$$\Longrightarrow \mathbb{E}_{\pi_\gamma}\left(f'(\theta)\right) = 0 \quad \forall f$$

if f is quad

$f'(\theta) = f''(\theta_*)(\theta - \theta_*)$

$$f''(\theta_*)(\underbrace{\mathbb{E}_{\pi_\gamma}(\theta)}_{\bar{\theta}_\gamma} - \theta_*) = 0$$

$\Longrightarrow \bar{\theta}_\gamma = \theta_*$

(if $f''(\theta_*)$ is inv)

Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta\rangle\big)^2$

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

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

Richardson

approx

$+ \bar{\theta}_{2\gamma}$

$+ \bar{\theta}_\gamma$

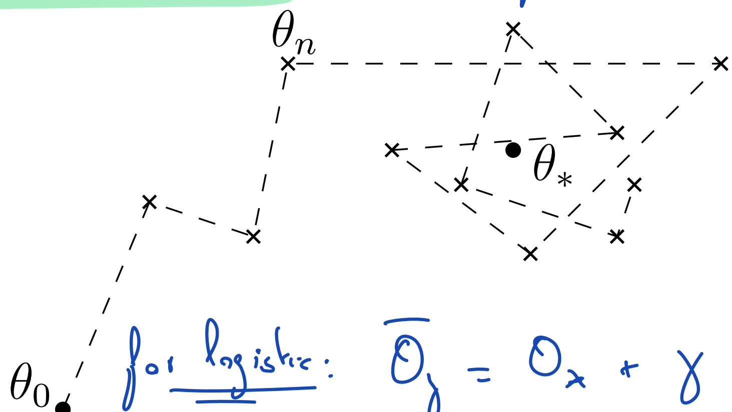
-1

θ_*

AD & Durmus & FB

- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**

(see proof on the previous slide).



for logistic: $\bar{\theta}_\gamma = \theta_* + \gamma \vec{D} + O(\gamma^2)$

$\gamma \to 0$

Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta \rangle\big)^2$

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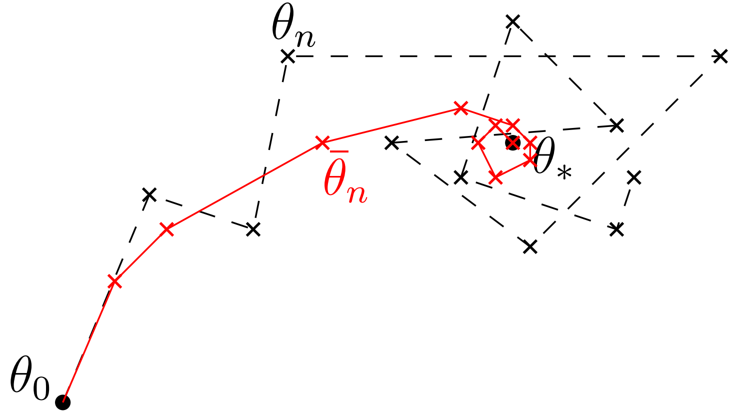
- **For least-squares, $\bar{\theta}_\gamma = \theta_*$**



Markov chain interpretation of constant step sizes

- LMS recursion for $f_n(\theta) = \frac{1}{2}\big(y_n - \langle \Phi(x_n), \theta\rangle\big)^2$

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

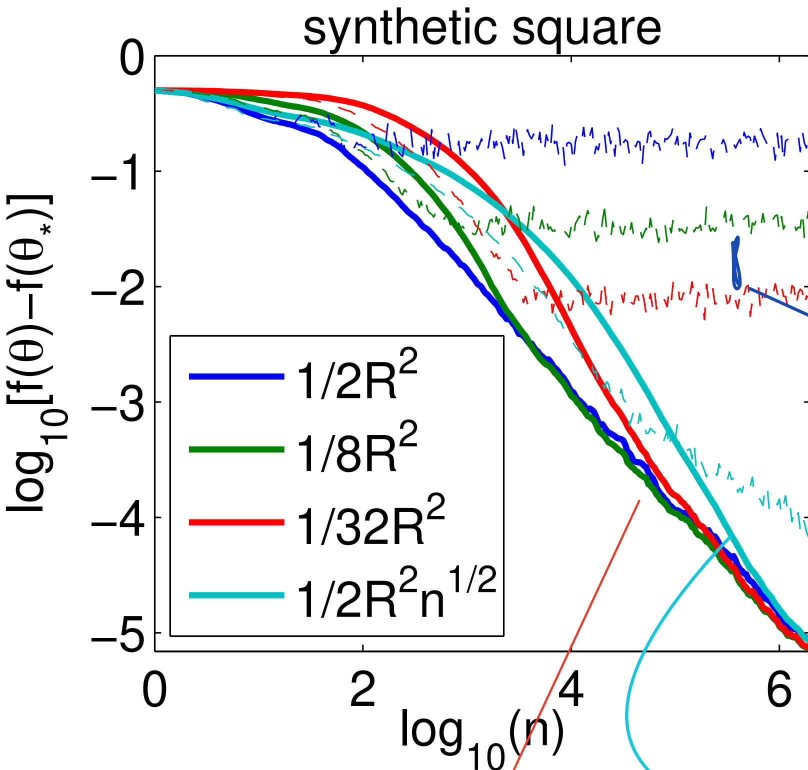
- **For least-squares,** $\bar{\theta}_\gamma = \theta_*$
  - θ_n does not converge to θ_* but oscillates around it
  - oscillations of order $\sqrt{\gamma}$

- **Ergodic theorem:**
  - Averaged iterates converge to $\bar{\theta}_\gamma = \theta_*$ at rate $O(1/n)$

without dependence on μ !!

Simulations - synthetic examples

- Gaussian distributions - $d = 20$



with CSS.

θ_n does not cvge.

$(\log c)$ ~~$2\log c$~~

slope (-1)!

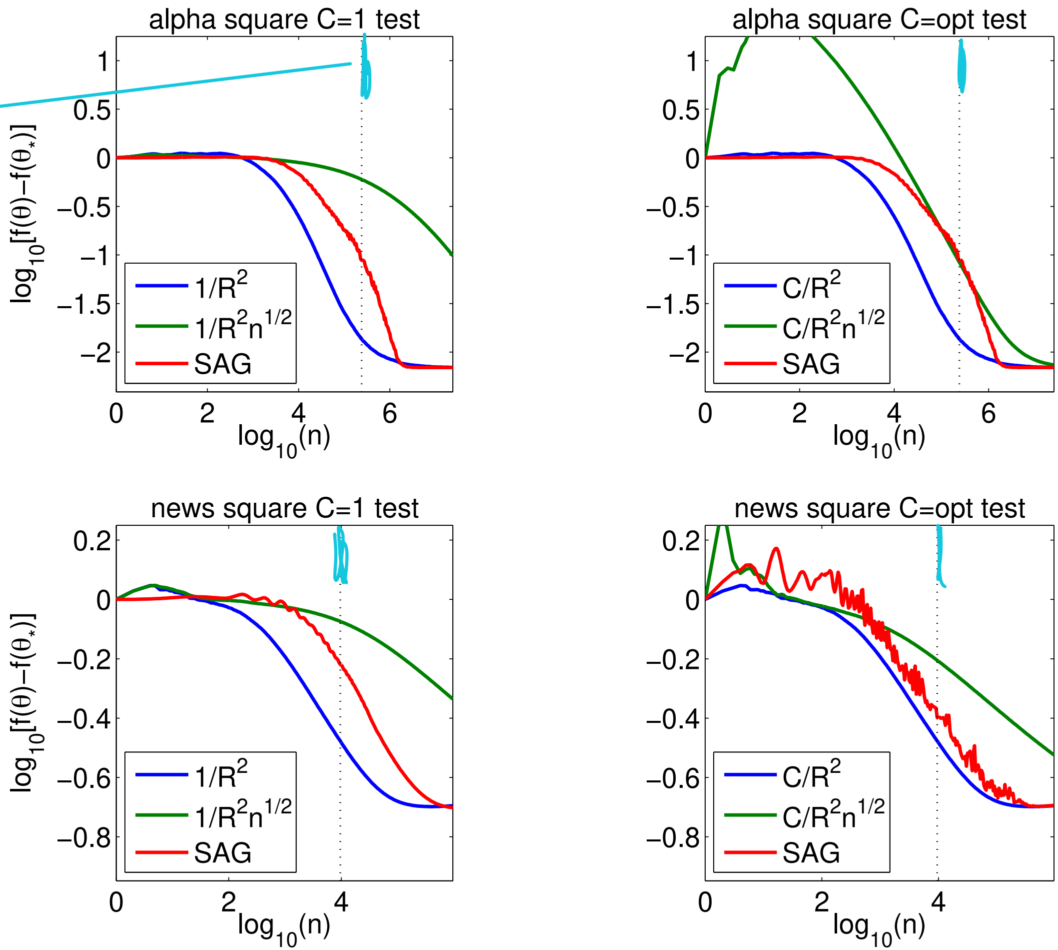
$1/n$

$\frac{1}{\mu n}$

Simulations - benchmarks

- *alpha* $(d = 500,\ n = 500\ 000)$, *news* $(d = 1\ 300\ 000,\ n = 20\ 000)$

results for the first pass on the data



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

One pass SGD gives you

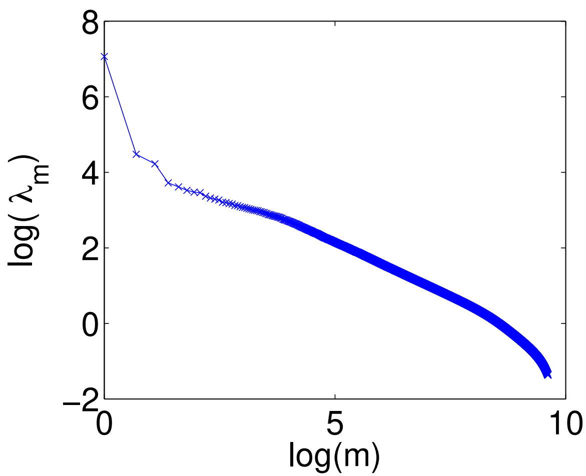
$$\mathbb{E}\left(f(\bar{\theta}_n) - f_* \right) \leq \frac{\sigma^2 d}{n} + \frac{\|\theta_0 - \theta_*\|^2}{\gamma n}$$

minimax bound is $\dfrac{\sigma^2 d}{n}$ (w.o. on θ_* and H).

$\Rightarrow$ using SGD for one pass is nearly optimal!

Finer assumptions (Dieuleveut and Bach, 2014)

- **Covariance eigenvalues**
  - Pessimistic assumption: all eigenvalues λ_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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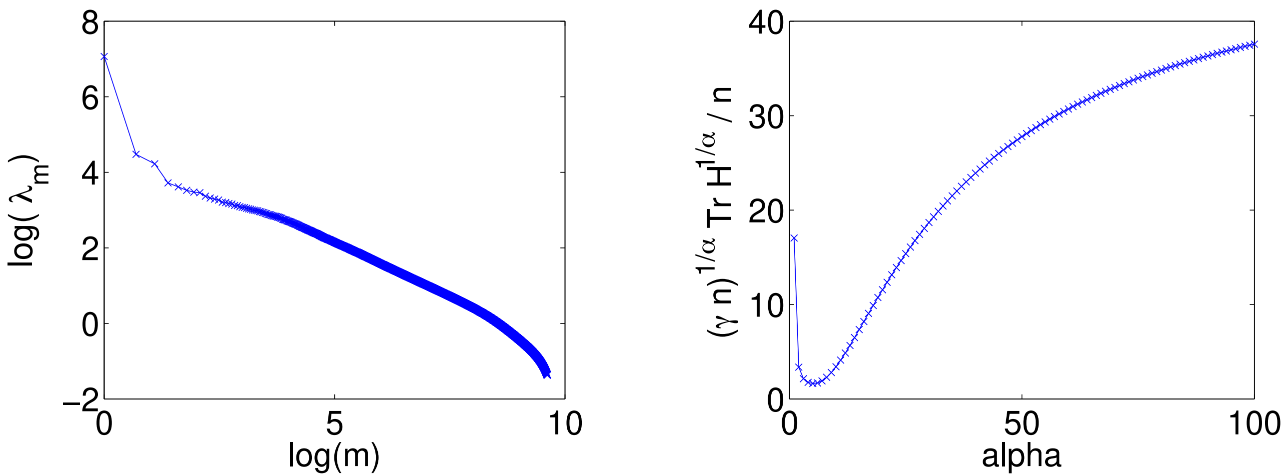
  - New result: replace $\frac{\sigma^2 d}{n}$ by $\frac{\sigma^2 (\gamma n)^{1/\alpha} \operatorname{tr} H^{1/\alpha}}{n}$



Finer assumptions (Dieuleveut and Bach, 2014)

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  - New result: replace $\dfrac{\sigma^2 d}{n}$ by $\dfrac{\sigma^2 (\gamma n)^{1/\alpha} \operatorname{tr} H^{1/\alpha}}{n}$

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

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

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

  - Previous results: $\alpha = +\infty$ and $r = 1/2$
  - Valid for all α 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**: $\Phi(x), \theta \in \mathcal{H}$

Hilbert space

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

$(d = \infty)$

- **If $\theta_0 = 0$, θ_n is a linear combination of $\Phi(x_1), \dots, \Phi(x_n)$**

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

RKHS ; decay rate of eigenvalues, $\left(\frac{d}{n}\right)$

regularity of the optimal pred.

Sobolev space.

From least-squares to non-parametric estimation - I

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

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

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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 $k(x, x') = \sum_j \varphi_j^2 \cos\big[2j\pi(x - x')\big]$
  - Optimal prediction function θ_* has norm $\|\theta_*\|^2 = \sum_j |\mathcal{F}(\theta_*)_j|^2 \varphi_j^{-2}$
  - Depending on smoothness, may or may not be finite

From least-squares to non-parametric estimation - II

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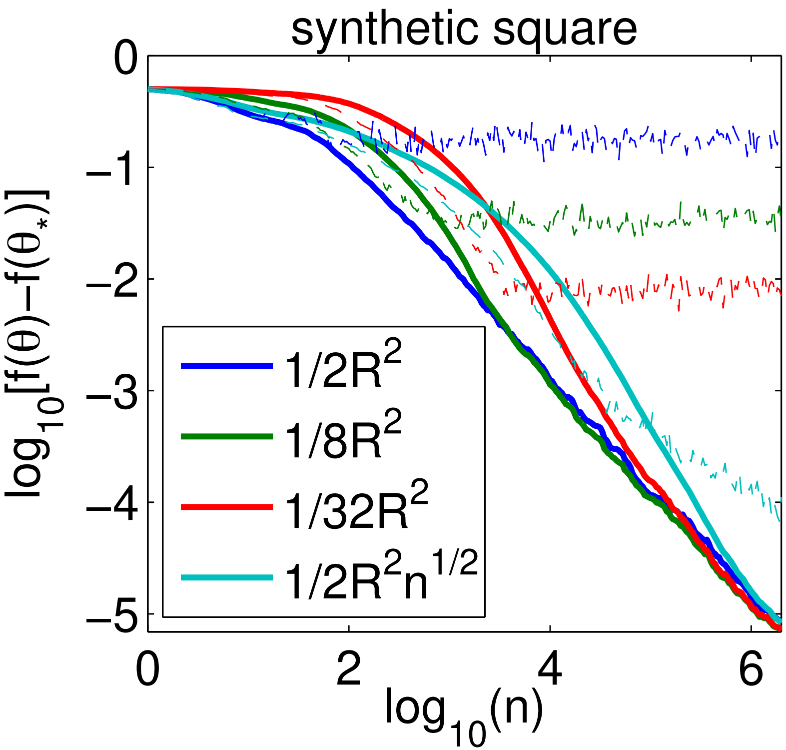
- Adapted norm $\|H^{1/2-r}\theta_*\|^2 = \sum_j |\mathcal{F}(\theta_*)_j|^2 \varphi_j^{-4r}$ may be finite

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

- **Same effect than ℓ_2-regularization with weight λ equal to** $\dfrac{1}{\gamma n}$

Simulations - synthetic examples

- Gaussian distributions - $d = 20$



- **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)

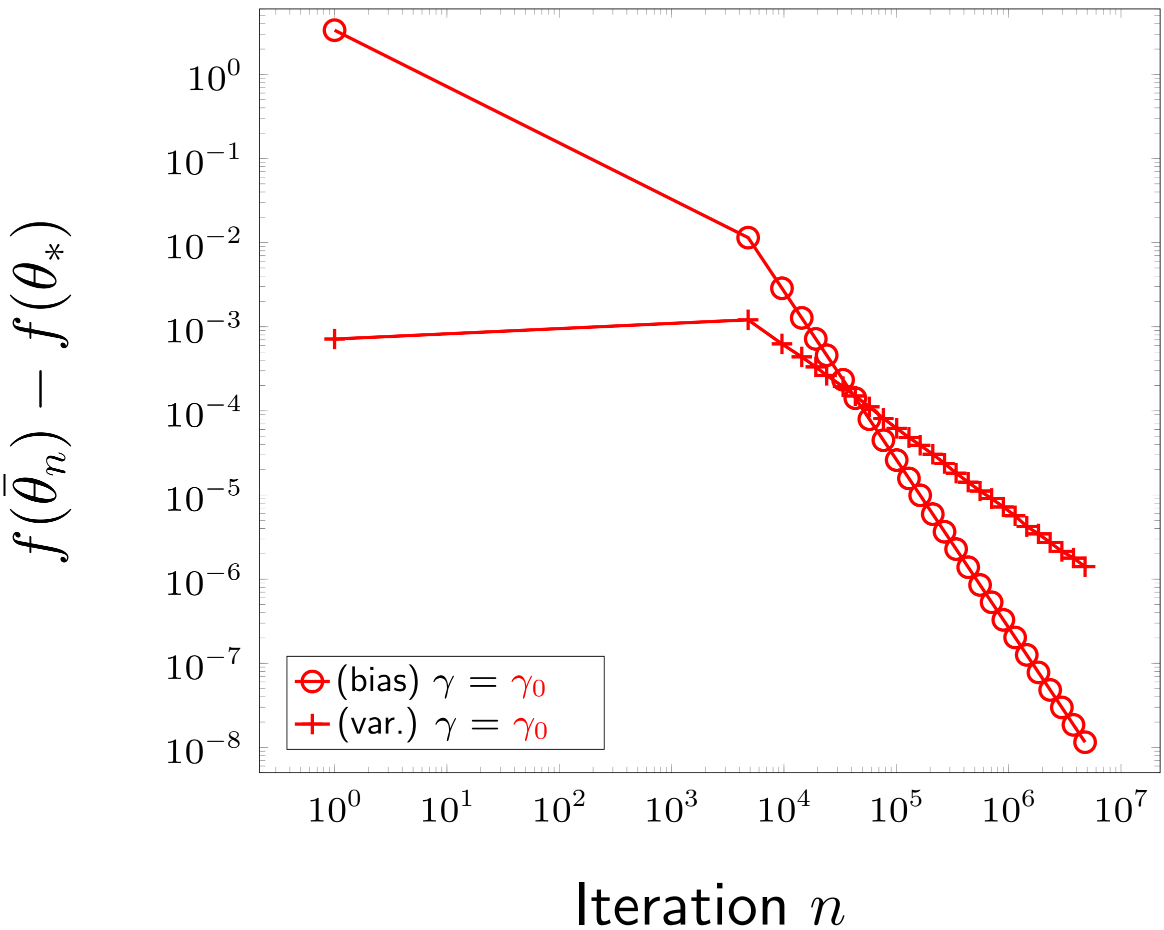
$$f(\bar{\theta}_n) - f(\theta_*) \sim \frac{1}{n} \mathbb{E}\Big[\varepsilon^2 \, \Phi(x)^\top H^{-1} \Phi(x)\Big]$$

  – NB: if noise ε 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 $d = 25$)



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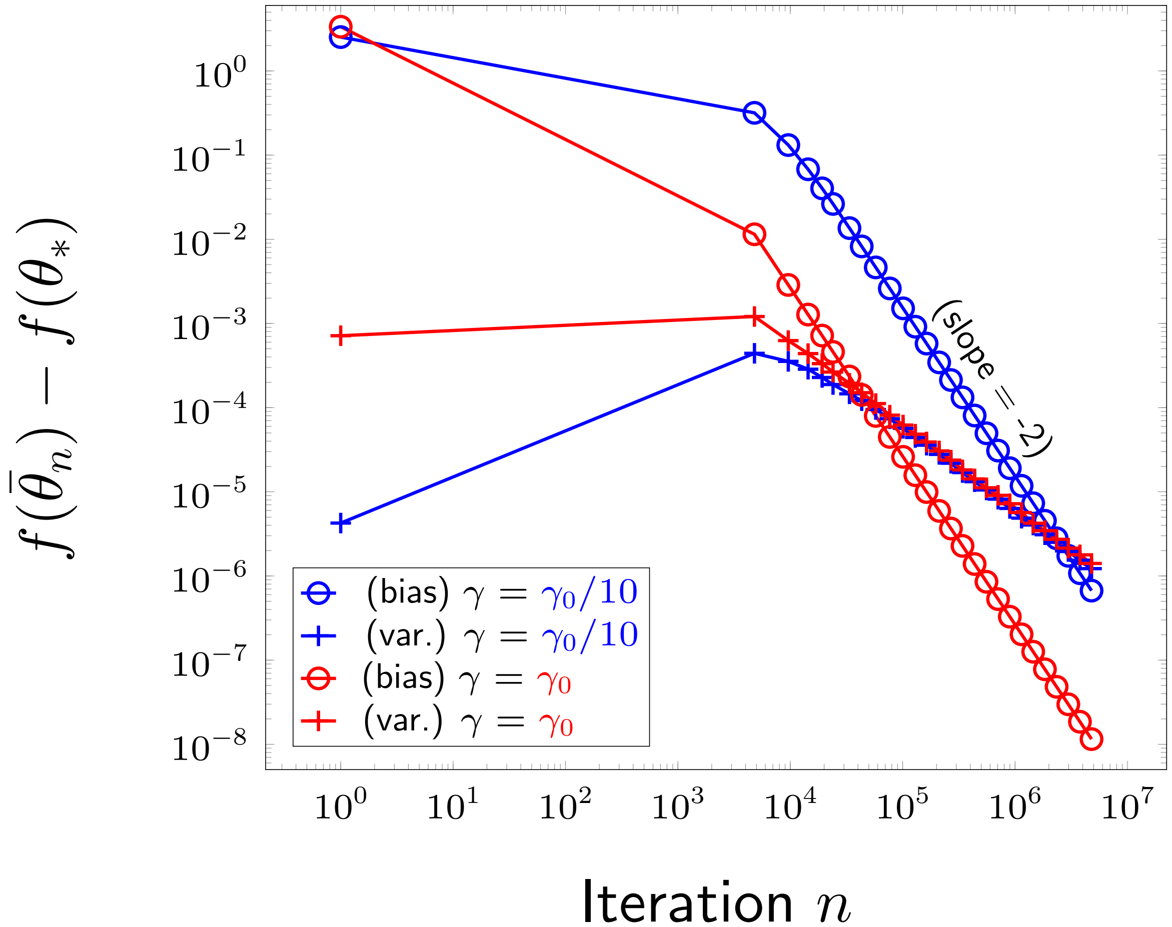

Optimal sampling (Défossez and Bach, 2015)

- **Sampling from a different distribution with importance weights**

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

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

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

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- **Optimal for variance**: $\displaystyle \frac{dq(x)}{dp(x)} \propto \sqrt{\Phi(x)^\top H^{-1} \Phi(x)}$
  – Same density as active learning (Kanamori and Shimodaira, 2003)
  – Limited gains: different between first and second moments
  – Caveat: need to know H

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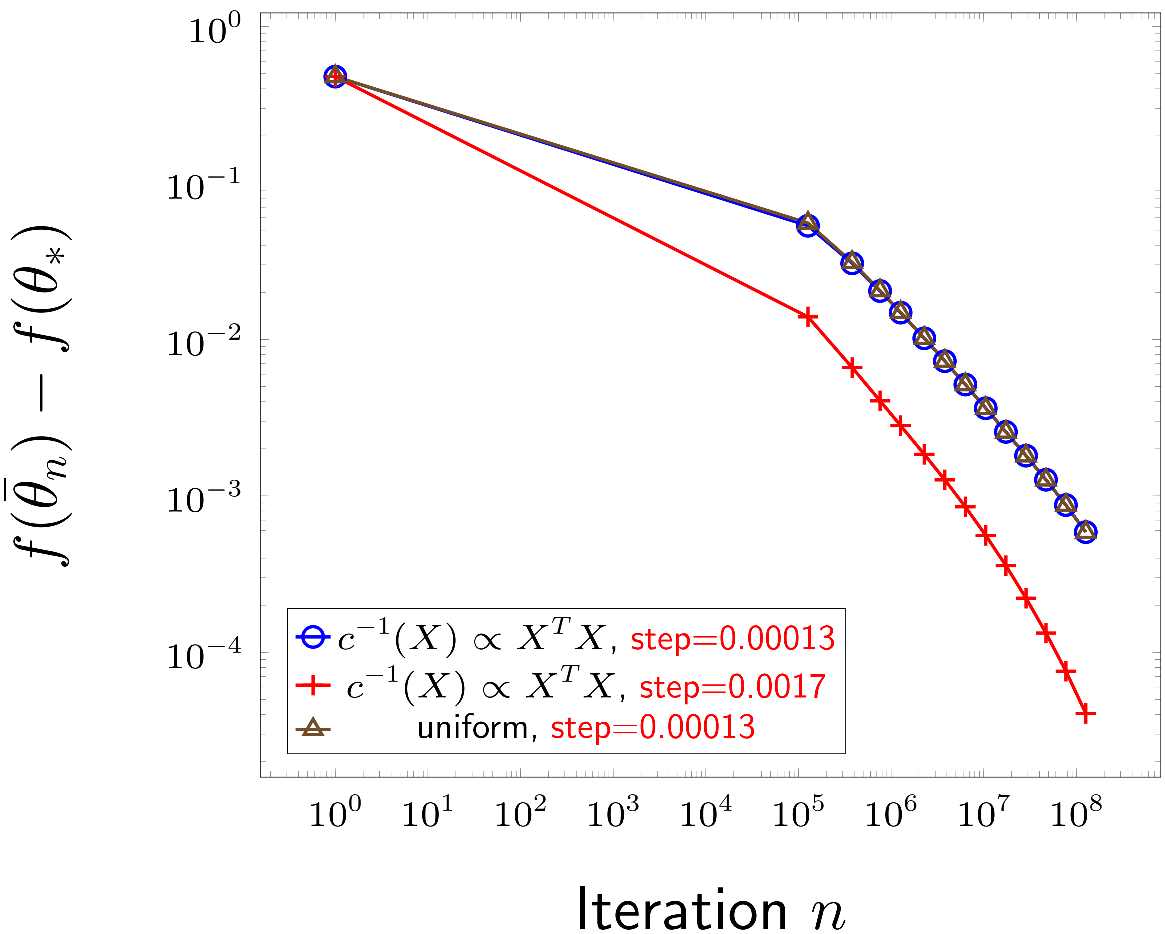
- **Optimal for bias**: $\dfrac{dq(x)}{dp(x)} \propto \|\Phi(x)\|^2$

  – 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 ($d = 4932$)



Achieving optimal bias and variance terms

- **Current results with averaged SGD**
  - **Variance** (starting from optimal θ_*) $= \dfrac{\sigma^2 d}{n}$
  - **Bias** (no noise) $= \min\left\{\dfrac{R^2\|\theta_0 - \theta_*\|^2}{n}, \dfrac{R^4\langle\theta_0 - \theta_*, H^{-1}(\theta_0 - \theta_*)\rangle}{n^2}\right\}$

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

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Accelerated gradient descent (Nesterov, 1983)	$\dfrac{R^2\|\theta_0-\theta_*\|^2}{n^2}$	$\sigma^2 d$

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

Achieving optimal bias and variance terms

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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 π_γ such that $\int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$
  - When f' is not linear, $f'(\int \theta\pi_\gamma(\mathrm{d}\theta)) \neq \int f'(\theta)\pi_\gamma(\mathrm{d}\theta) = 0$

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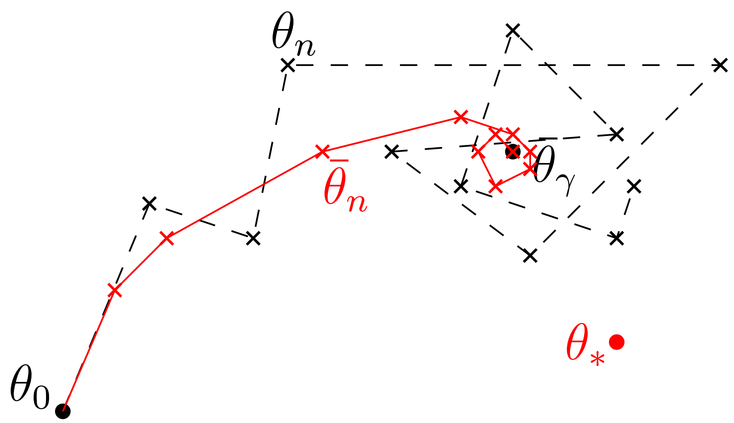
- θ_n **oscillates around the wrong value** $\bar{\theta}_\gamma \neq \theta_*$



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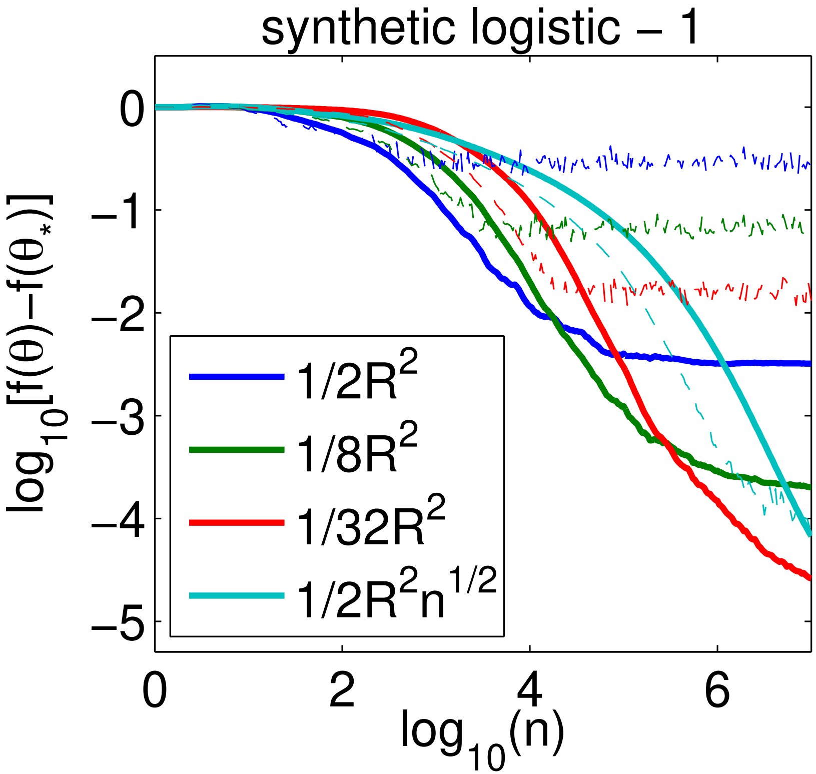
- **θ_n oscillates around the wrong value $\bar\theta_\gamma \neq \theta_*$**
  - moreover, $\|\theta_* - \theta_n\| = O_p(\sqrt{\gamma})$
  - Linear convergence up to the noise level for strongly-convex problems (Nedic and Bertsekas, 2000)

- **Ergodic theorem**
  - averaged iterates converge to $\bar\theta_\gamma \neq \theta_*$ at rate $O(1/n)$
  - moreover, $\|\theta_* - \bar\theta_\gamma\| = O(\gamma)$ (Bach, 2013)

Simulations - synthetic examples

- Gaussian distributions - $d = 20$



Restoring convergence through online Newton steps

- **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 γ_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

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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

Restoring convergence through online Newton steps

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

$$
\begin{aligned}
g(\theta) &= f(\tilde{\theta}) + \langle f'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, f''(\tilde{\theta})(\theta - \tilde{\theta})\rangle \\
&= f(\tilde{\theta}) + \langle \mathbb{E} f_n'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, \mathbb{E} f_n''(\tilde{\theta})(\theta - \tilde{\theta})\rangle \\
&= \mathbb{E}\Big[f(\tilde{\theta}) + \langle f_n'(\tilde{\theta}), \theta - \tilde{\theta}\rangle + \tfrac{1}{2}\langle \theta - \tilde{\theta}, f_n''(\tilde{\theta})(\theta - \tilde{\theta})\rangle\Big]
\end{aligned}
$$

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\end{aligned}
$$

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

$$
\theta_n = \theta_{n-1} - \gamma\big[f_n'(\tilde{\theta}) + f_n''(\tilde{\theta})(\theta_{n-1} - \tilde{\theta})\big]
$$

  - $f_n''(\tilde{\theta}) = \ell''(y_n, \langle \tilde{\theta}, \Phi(x_n)\rangle)\Phi(x_n) \otimes \Phi(x_n)$ 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

Logistic regression - Proof technique

- Using generalized self-concordance of $\varphi : u \mapsto \log(1+e^{-u})$:

$$|\varphi'''(u)| \leqslant \varphi''(u)$$

  – NB: difference with regular self-concordance: $|\varphi'''(u)| \leqslant 2\varphi''(u)^{3/2}$

- Using novel high-probability convergence results for regular averaged stochastic gradient descent

- Requires assumption on the kurtosis in every direction, i.e.,

$$\mathbb{E}\langle \Phi(x_n), \eta\rangle^4 \leqslant \kappa \big[\mathbb{E}\langle \Phi(x_n), \eta\rangle^2\big]^2$$

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

Online Newton algorithm
Current proof (Flammarion et al., 2014)

- Recursion

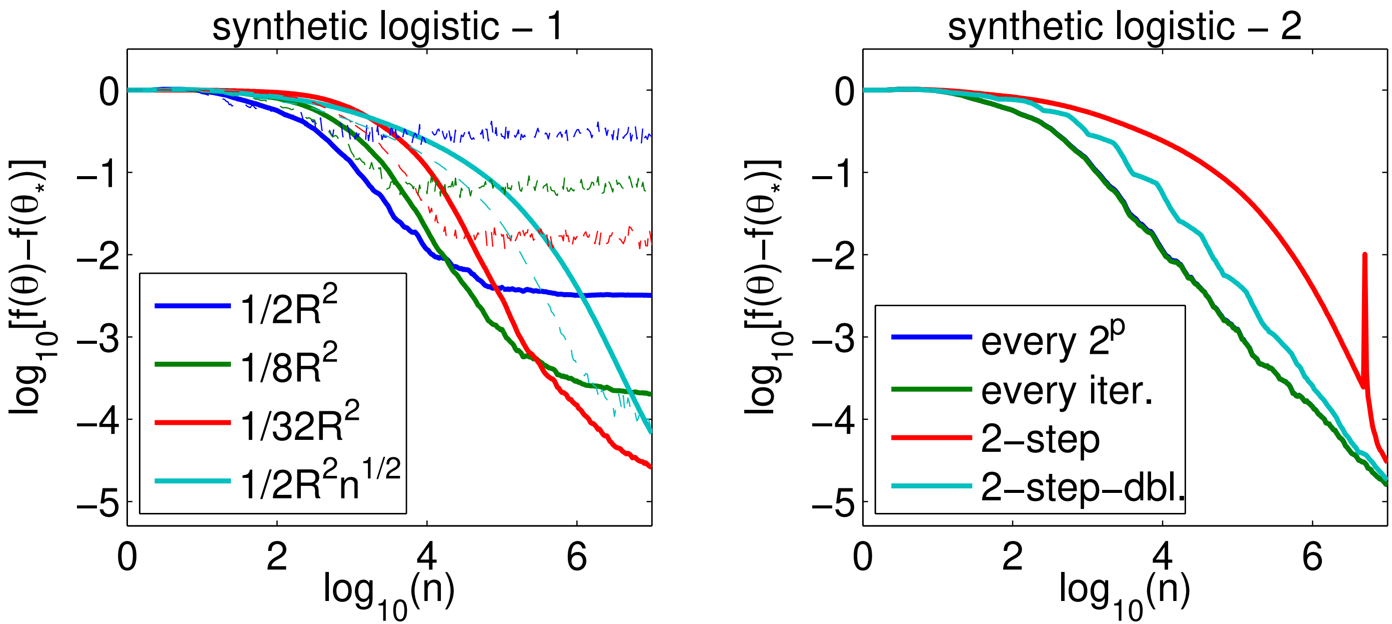
$$\begin{cases} \theta_n &=& \theta_{n-1} - \gamma\big[f_n'(\bar\theta_{n-1}) + f_n''(\bar\theta_{n-1})(\theta_{n-1} - \bar\theta_{n-1})\big] \\ \bar\theta_n &=& \bar\theta_{n-1} + \frac{1}{n}(\theta_n - \bar\theta_{n-1}) \end{cases}$$

- Instance of two-time-scale stochastic approximation (Borkar, 1997)
  - Given $\bar\theta$, $\theta_n = \theta_{n-1} - \gamma\big[f_n'(\bar\theta) + f_n''(\bar\theta)(\theta_{n-1} - \bar\theta)\big]$ defines a homogeneous Markov chain (fast dynamics)
  - $\bar\theta_n$ is updated at rate $1/n$ (slow dynamics)

- **Difficulty**: preserving robustness to ill-conditioning

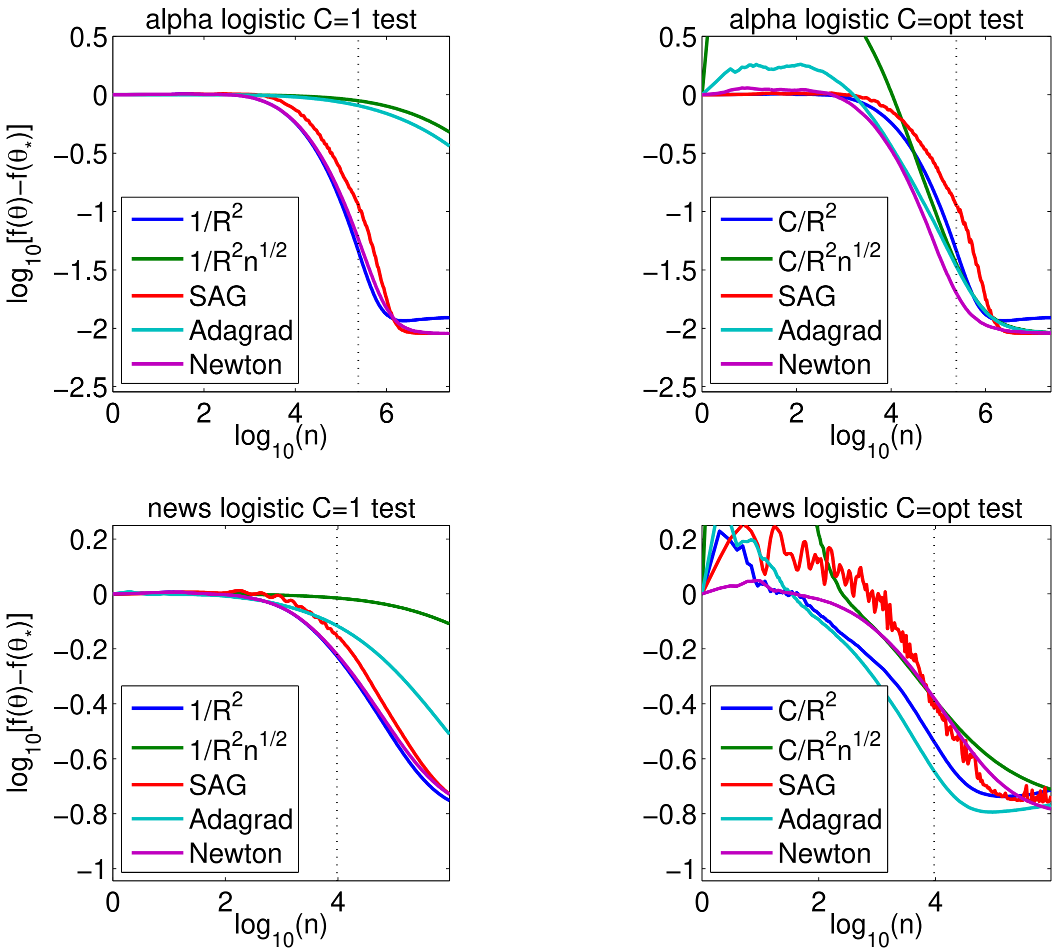
Simulations - synthetic examples

- Gaussian distributions - $d = 20$



Simulations - benchmarks

- *alpha* $(d = 500,\ n = 500\ 000)$, *news* $(d = 1\ 300\ 000,\ n = 20\ 000)$



Why is $\frac{\sigma^2 d}{n}$ optimal for least-squares?

- Reduction to an hypothesis testing problem
  - Application of Varshamov-Gilbert's lemma

- **Best possible prediction independently of computation**
  - To be contrasted with lower bounds based on specific models of computation

- See `http://www-math.mit.edu/~rigollet/PDFs/RigNotes15.pdf`

Summary of rates of convergence

- Problem parameters
  - D diameter of the domain
  - B Lipschitz-constant
  - L smoothness constant
  - μ strong convexity constant

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

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

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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**
   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging
5. **Smooth stochastic approximation algorithms**
   - Non-asymptotic analysis for smooth functions
   - Logistic regression
   - Least-squares regression without decaying step-sizes
6. **Finite data sets**
   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

Going beyond a single pass over the data

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

Going beyond a single pass over the data

- **Stochastic approximation**
  - Assumes infinite data stream
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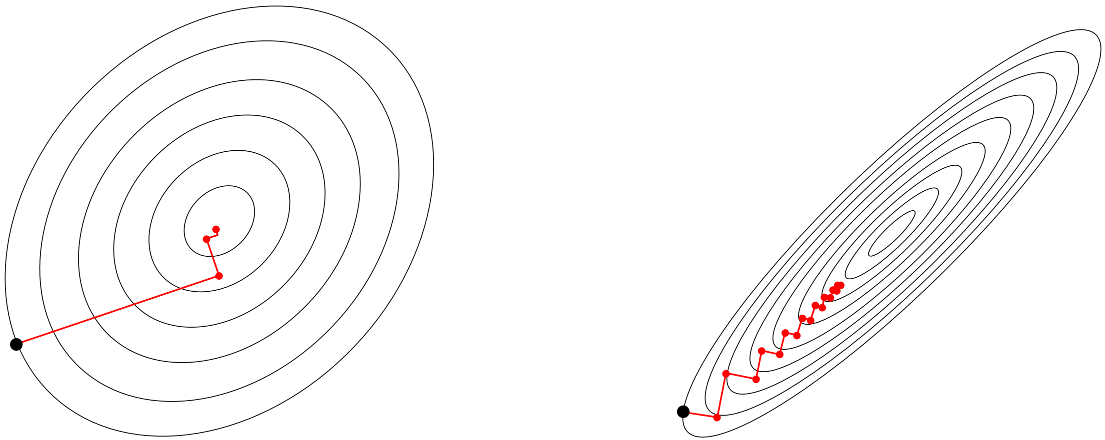
  - Directly minimizes testing cost $\mathbb{E}_{(x,y)}\, \ell(y, \theta^\top \Phi(x))$
- **Machine learning practice**
  - Finite data set $(x_1, y_1, \dots, x_n, y_n)$
  - Multiple passes
  - Minimizes training cost $\frac{1}{n}\sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
  - Need to regularize (e.g., by the ℓ_2-norm) to avoid overfitting
- **Goal**: minimize $g(\theta) = \dfrac{1}{n}\displaystyle\sum_{i=1}^n f_i(\theta)$

Iterative methods for minimizing smooth functions

- **Assumption**: g convex and L-smooth on $\mathbb{R}^d$
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$



(small $\kappa = L/\mu$) (large $\kappa = L/\mu$)

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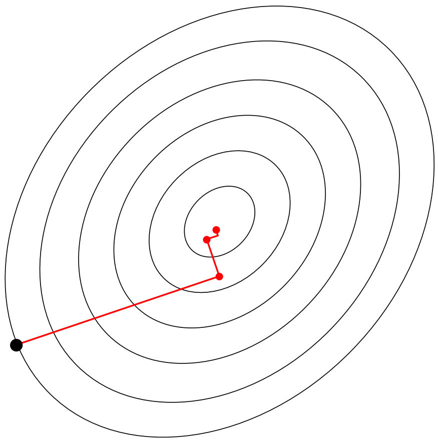

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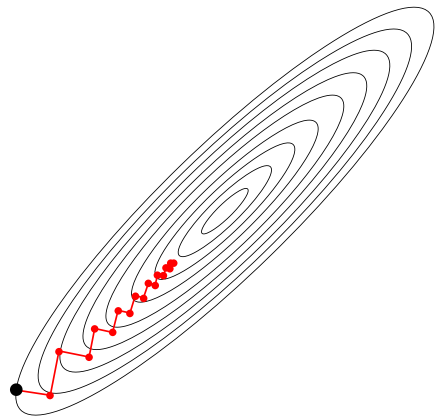

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Iterative methods for minimizing smooth functions

- **Assumption**: g convex and L-smooth on $\mathbb{R}^d$
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$
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Stochastic gradient descent (SGD) for finite sums

$$\min_{\theta \in \mathbb{R}^d} g(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)$$

- **Iteration**: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
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- **Convergence rate** if each f_i is convex L-smooth and g μ-strongly-convex:

$$\mathbb{E} g(\bar{\theta}_t) - g(\theta_*) \leqslant \begin{cases} O(1/\sqrt{t}) & \text{if } \gamma_t = 1/(L\sqrt{t}) \\ O(L/(\mu t)) = O(\kappa/t) & \text{if } \gamma_t = 1/(\mu t) \end{cases}$$

  - No adaptivity to strong-convexity in general
  - Adaptivity with self-concordance assumption (Bach, 2013)
  - Running-time complexity: $O(d \cdot \kappa/\varepsilon)$

Stochastic vs. deterministic methods

- Minimizing $g(\theta) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} f_i(\theta)$ with $f_i(\theta) = \ell\big(y_i, h(x_i,\theta)\big) + \lambda\Omega(\theta)$

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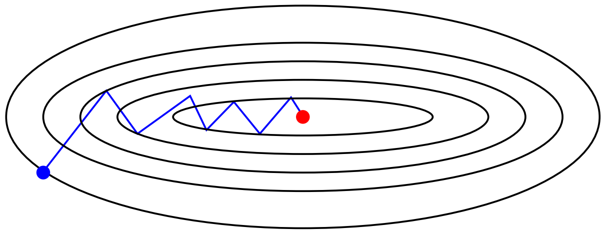

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  - Sampling with replacement: $i(t)$ random element of $\{1,\dots,n\}$
  - Convergence rate in $O(\kappa/t)$
  - Iteration complexity is independent of n

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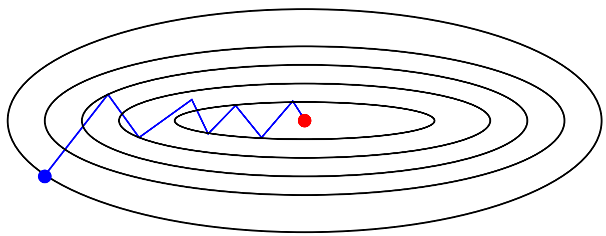

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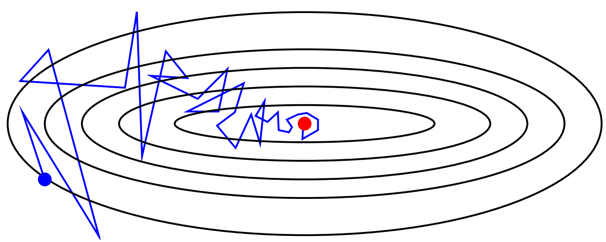

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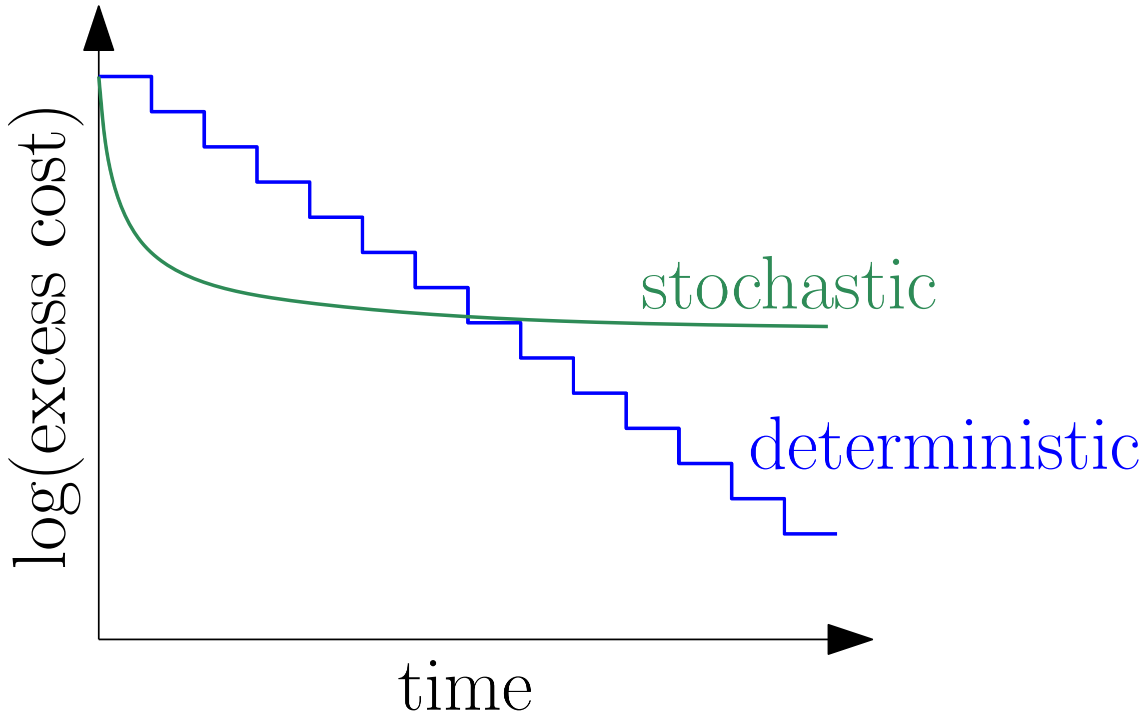

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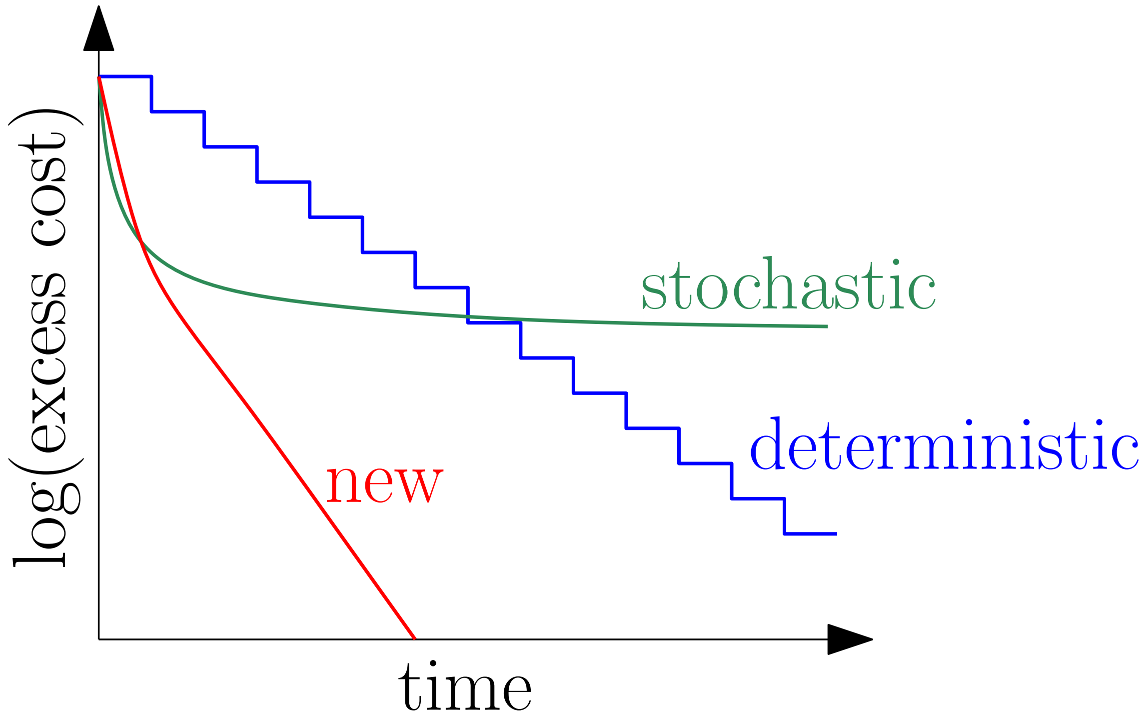

Accelerating gradient methods - Related work

- **Generic acceleration** (Nesterov, 1983, 2004)

$$\theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t(\theta_t - \theta_{t-1})$$

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- **Constant step-size stochastic gradient**
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- **Stochastic version of accelerated batch gradient methods**
  - Tseng (1998); Ghadimi and Lan (2010); Xiao (2010)
  - Can improve constants, but still have sublinear $O(1/t)$ rate

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

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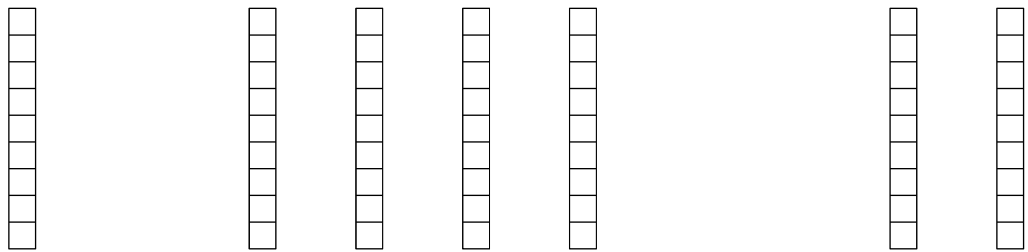

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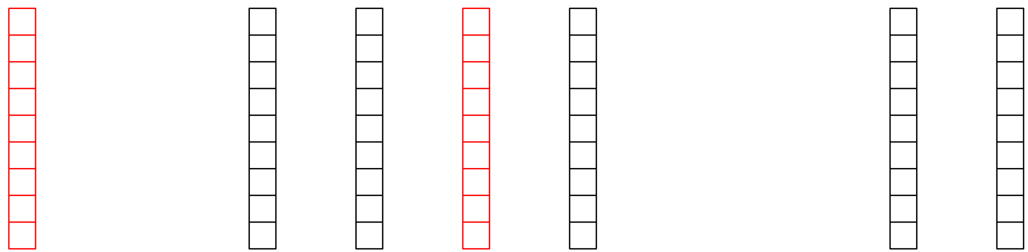

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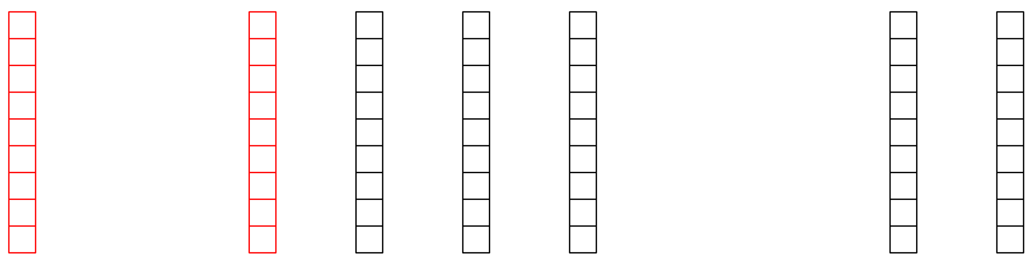

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- Stochastic version of incremental average gradient (Blatt et al., 2008)
- **Extra memory requirement**: n gradients in $\mathbb{R}^d$ in general
- **Linear supervised machine learning**: only n real numbers
  - If $f_i(\theta) = \ell(y_i, \Phi(x_i)^\top \theta)$, then $f_i'(\theta) = \ell'(y_i, \Phi(x_i)^\top \theta)\, \Phi(x_i)$

Stochastic average gradient - Convergence analysis

- **Assumptions**
  - Each f_i is L-smooth, $i = 1, \dots, n$ - *link with* R^2
  - $g = \frac{1}{n} \sum_{i=1}^n f_i$ is μ-strongly convex
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- **Strongly convex case** (Le Roux et al., 2012, 2013)

$$\mathbb{E}\big[g(\theta_t) - g(\theta_*)\big] \leqslant \text{ cst } \times \bigg(1 - \min\Big\{\frac{1}{8n}, \frac{\mu}{16L}\Big\}\bigg)^t$$

  - Linear (exponential) convergence rate with $O(d)$ iteration cost
  - After one pass, reduction of cost by $\exp\Big(-\min\Big\{\frac{1}{8}, \frac{n\mu}{16L}\Big\}\Big)$
  - NB: in machine learning, may often restrict to $\mu \geqslant L/n$
    $\Rightarrow$ constant error reduction after each effective pass

Convergence analysis - Proof sketch

- **Main step**: find “good” Lyapunov function $J(\theta_t, y_1^t, \dots, y_n^t)$
  - such that $\mathbb{E}\big[J(\theta_t, y_1^t, \dots, y_n^t)|\mathcal{F}_{t-1}\big] < J(\theta_{t-1}, y_1^{t-1}, \dots, y_n^{t-1})$
  - 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, μ, L)
  - Check validity with symbolic computations

Running-time comparisons (strongly-convex)

- **Assumptions**: $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$
  - Each f_i convex L-smooth and g μ-strongly convex

Stochastic gradient descent	$d\times \quad \frac{L}{\mu} \quad \times \quad \frac{1}{\varepsilon}$
Gradient descent	$d\times \quad n\frac{L}{\mu} \quad \times \log\frac{1}{\varepsilon}$
Accelerated gradient descent	$d\times \quad n\sqrt{\frac{L}{\mu}} \quad \times \log\frac{1}{\varepsilon}$
SAG	$d\times \quad (n+\frac{L}{\mu}) \quad \times \log\frac{1}{\varepsilon}$

  - NB-1: for (accelerated) gradient descent, $L =$ smoothness constant of g
  - NB-2: with non-uniform sampling, $L =$ average smoothness constants of all f_i's

Running-time comparisons (strongly-convex)

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SAG	$d\times \quad (n+\frac{L}{\mu}) \quad \times \log\frac{1}{\varepsilon}$

- **Beating two lower bounds** (Nemirovsky and Yudin, 1983; Nesterov, 2004): with additional assumptions

(1) stochastic gradient: exponential rate for finite sums
(2) full gradient: better exponential rate using the sum structure

Running-time comparisons (non-strongly-convex)

- **Assumptions**: $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} f_i(\theta)$
  - Each f_i convex L-smooth
  - Ill conditioned problems: g may not be strongly-convex ($\mu = 0$)

Stochastic gradient descent	$d\times$	$1/\varepsilon^2$
Gradient descent	$d\times$	n/ε
Accelerated gradient descent	$d\times$	$n/\sqrt{\varepsilon}$
SAG	$d\times$	$\sqrt{n}/\varepsilon$

- Adaptivity to potentially hidden strong convexity

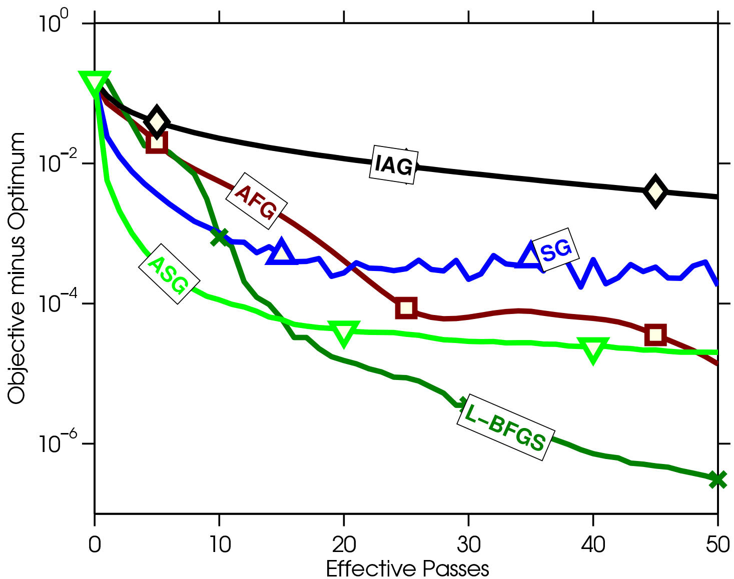
- No need to know the local/global strong-convexity constant

Stochastic average gradient
Implementation details and extensions

- **Sparsity in the features**
  - Just-in-time updates $\Rightarrow$ replace $O(d)$ by number of non zeros
  - See also Leblond, Pedregosa, and Lacoste-Julien (2016)
- **Mini-batches**
  - Reduces the memory requirement $+$ block access to data
- **Line-search**
  - Avoids knowing L in advance
- **Non-uniform sampling**
  - Favors functions with large variations
- See `www.cs.ubc.ca/~schmidtm/Software/SAG.html`

Experimental results (logistic regression)

quantum dataset
$(n = 50\,000,\ d = 78)$



rcv1 dataset
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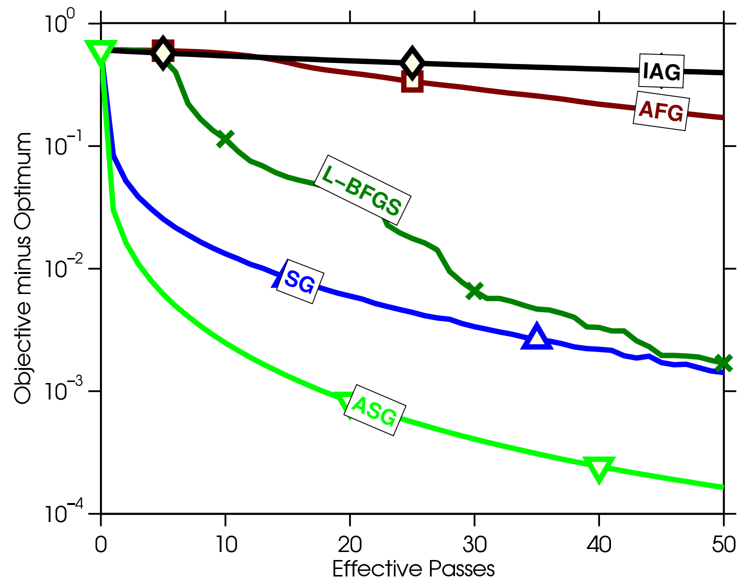

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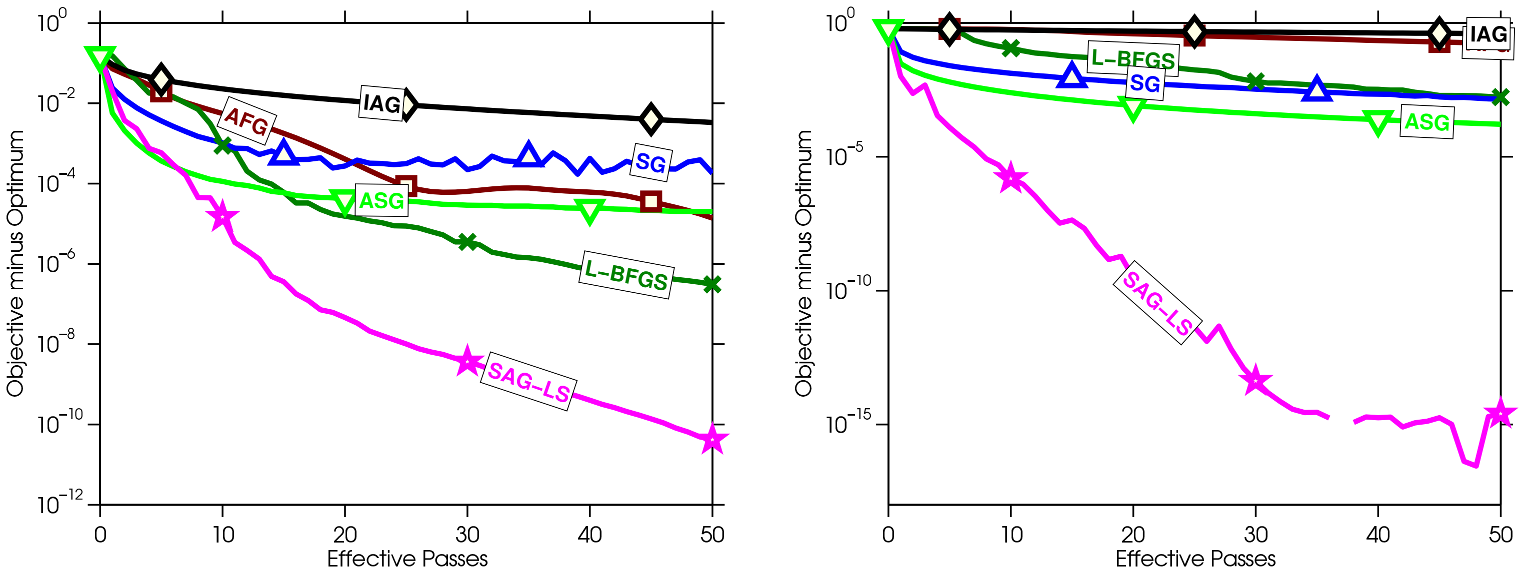
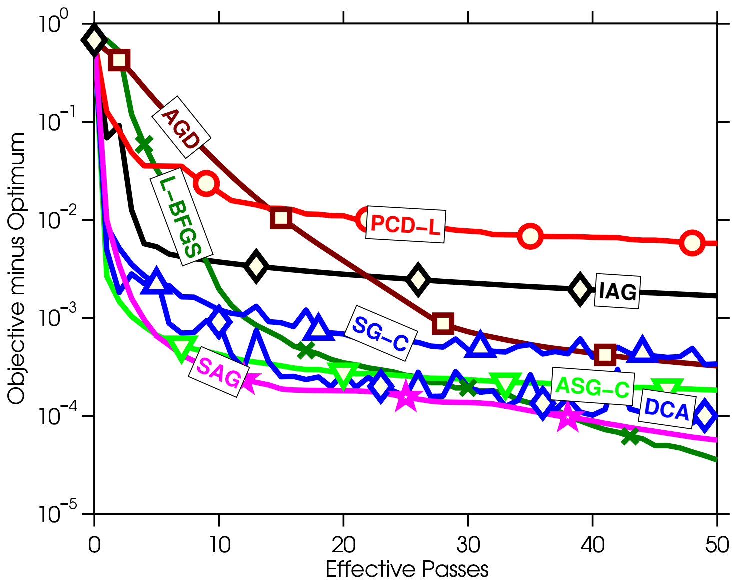
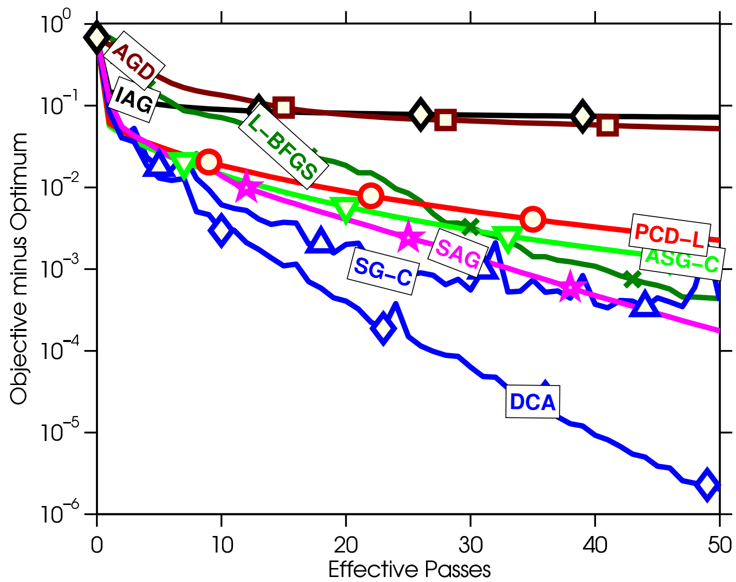


Before non-uniform sampling

`protein` dataset
$(n = 145\ 751,\ d = 74)$



`sido` dataset
$(n = 12\ 678,\ d = 4\ 932)$



After non-uniform sampling

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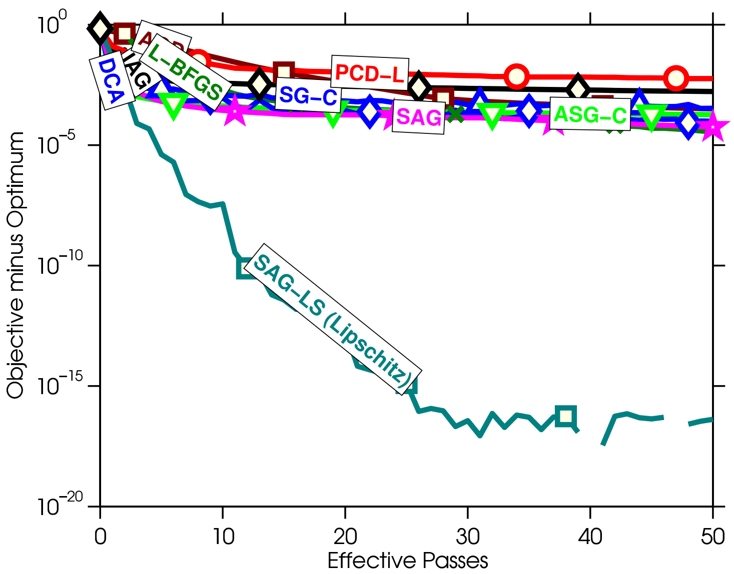

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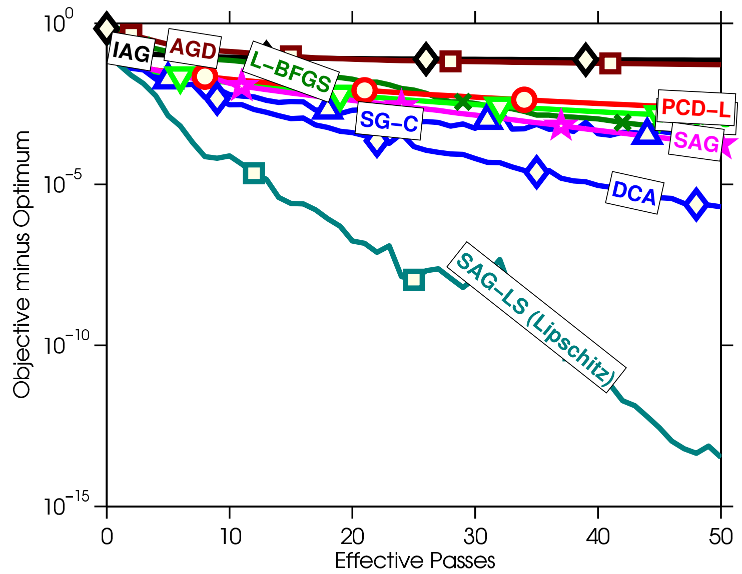

Linearly convergent stochastic gradient algorithms

- **Many related algorithms**
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SDCA (Shalev-Shwartz and Zhang, 2012)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - MISO (Mairal, 2015)
  - Finito (Defazio et al., 2014a)
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  - ...

- **Similar rates of convergence and iterations**

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  - ...

- **Similar rates of convergence and iterations**

- **Different interpretations and proofs / proof lengths**
  - Lazy gradient evaluations
  - Variance reduction

Variance reduction

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

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

  - $\mathbb{E}Z_\alpha = \alpha\mathbb{E}X + (1-\alpha)\mathbb{E}Y$
  - $\mathrm{var}(Z_\alpha) = \alpha^2\big[\,\mathrm{var}(X) + \mathrm{var}(Y) - 2\mathrm{cov}(X,Y)\big]$
  - $\alpha = 1$: no bias, $\alpha < 1$: potential bias (but reduced variance)
  - Useful if Y positively correlated with X

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- **Application to gradient estimation** (Johnson and Zhang, 2013; Zhang, Mahdavi, and Jin, 2013)
  - SVRG: $X = f'_{i(t)}(\theta_{t-1})$, $Y = f'_{i(t)}(\tilde{\theta})$, $\alpha = 1$, with $\tilde{\theta}$ stored
  - $\mathbb{E}Y = \frac{1}{n}\sum_{i=1}^n f'_i(\tilde{\theta})$ full gradient at $\tilde{\theta}$, $X - Y = f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\tilde{\theta})$

Stochastic variance reduced gradient (SVRG) (Johnson and Zhang, 2013; Zhang et al., 2013)

- Initialize $\tilde{\theta} \in \mathbb{R}^d$
- For $i_{\text{epoch}} = 1$ to $\#$ of epochs
  - Compute all gradients $f_i'(\tilde{\theta})$; store $g'(\tilde{\theta}) = \frac{1}{n}\sum_{i=1}^n f_i'(\tilde{\theta})$
  - Initialize $\theta_0 = \tilde{\theta}$
  - For $t = 1$ to length of epochs

$$\theta_t = \theta_{t-1} - \gamma\Big[g'(\tilde{\theta}) + \big(f_{i(t)}'(\theta_{t-1}) - f_{i(t)}'(\tilde{\theta})\big)\Big]$$

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- Output: $\tilde{\theta}$

– No need to store gradients - two gradient evaluations per inner step

– Two parameters: length of epochs + step-size γ

– Same linear convergence rate as SAG, simpler proof

Stochastic variance reduced gradient (SVRG)

- **Algorithm divide into "epochs"**

- At each epoch, starting from $\theta_0 = \tilde{\theta}$, perform the iteration
  - Sample i_t uniformly at random
  - Gradient step: $\theta_t = \theta_{t-1} - \gamma \Big[f'_{i_t}(\theta_{t-1}) - f'_{i_t}(\tilde{\theta}) + g'(\tilde{\theta}) \Big]$

- **Proposition**: If each f_i is R^2-smooth and $g = \frac{1}{n}\sum_{i=1}^n f_i$ is μ-strongly convex, then after $k = 20R^2/\mu$ steps and with $\gamma = 1/10R^2$, then $f(\theta) - f(\theta_*)$ is reduced by 10%

SVRG proof - from Bubeck (2015)

- **Lemma**: $\mathbb{E}\|f_i'(\theta) - f_i'(\theta_*)\|^2 \leqslant 2R^2\big[g(\theta) - g(\theta_*)\big]$
  - Proof: $\mathbb{E}\|f_i'(\theta)-f_i'(\theta_*)\|^2\leqslant 2R^2\mathbb{E}\big[f_i(\theta)-f_i(\theta_*)-f_i'(\theta_*)^\top(\theta-\theta_*)\big]$ by the proof of co-coercivity, which is equal to $2R^2\big[g'(\theta) - g(\theta_*)\big]$

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- From iteration $\theta_t = \theta_{t-1} - \gamma\big[f_{i_t}'(\theta_{t-1}) - f_{i_t}'(\tilde{\theta}) + g'(\tilde{\theta})\big] = \theta_{t-1} - \gamma g_t$

$$
\begin{aligned}
\|\theta_t - \theta_*\|^2 &= \|\theta_{t-1} - \theta_*\|^2 - 2\gamma(\theta_{t-1} - \theta_*)^\top g_t + \gamma^2\|g_t\|^2 \\
\mathbb{E}\big[\|\theta_t - \theta_*\|^2 | \mathcal{F}_{t-1}\big] &\leqslant \|\theta_{t-1} - \theta_*\|^2 - 2\gamma(\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \\
&\quad + 2\gamma^2\|f_{i_t}'(\theta_{t-1}) - f_{i_t}'(\theta_*)\|^2 + 2\gamma^2\|f_{i_t}'(\tilde{\theta}) - f_{i_t}'(\theta_*) - g'(\tilde{\theta})\|^2 \\
&\leqslant \|\theta_{t-1} - \theta_*\|^2 - 2\gamma(\theta_{t-1} - \theta_*)^\top g'(\theta_{t-1}) \\
&\quad + 2\gamma^2 R^2\big[g(\theta_{t-1}) - g(\theta_*) + g(\tilde{\theta}) - g(\theta_*)\big] \\
&\leqslant \|\theta_{t-1} - \theta_*\|^2 - 2\gamma(1 - 2\gamma R^2)[g(\theta_{t-1}) - g(\theta_*)] + 4R^2\gamma^2[g(\tilde{\theta}) - g(
\end{aligned}
$$

- By summing k times, we get:

$$
\mathbb{E}\|\theta_k - \theta_*\|^2 \leqslant \|\theta_0 - \theta_*\|^2 - 2\gamma(1 - 2\gamma R^2)\sum_{t=1}^{k}\mathbb{E}[g(\theta_{t-1}) - g(\theta_*)] + 4kR^2\gamma^2[g(\tilde{\theta}) - g
$$

which leads to the desired result

Interpretation of SAG as variance reduction

- **SAG update**: $\theta_t = \theta_{t-1} - \frac{\gamma}{n}\sum_{i=1}^{n} y_i^t$ 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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- **SAGA update**: $\theta_t = \theta_{t-1} - \gamma\Big[\frac{1}{n}\sum_{i=1}^n y_i^{t-1} + \big(f_{i(t)}'(\theta_{t-1}) - y_{i(t)}^{t-1}\big)\Big]$
  – Defazio, Bach, and Lacoste-Julien (2014b)
  – Unbiased update without epochs

SVRG vs. SAGA

- **SAGA update**: $\theta_t = \theta_{t-1} - \gamma \Big[\frac{1}{n} \sum_{i=1}^n y_i^{t-1} + \big(f'_{i(t)}(\theta_{t-1}) - y_{i(t)}^{t-1} \big) \Big]$

- **SVRG update**: $\theta_t = \theta_{t-1} - \gamma \Big[\frac{1}{n} \sum_{i=1}^n f'_i(\tilde{\theta}) + \big(f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\tilde{\theta}) \big) \Big]$

	SAGA	SVRG
Storage of gradients	**yes**	**no**
Epoch-based	no	yes
Parameters	step-size	step-size & epoch lengths
Gradient evaluations per step	1	at least 2
Adaptivity to strong-convexity	yes	no
Robustness to ill-conditioning	yes	no

– See Babanezhad et al. (2015)

Proximal extensions

- **Composite optimization problems**: $\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) + h(\theta)$
  - f_i smooth and convex
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- **Directly extends to variance-reduced gradient techniques**
  - Same rates of convergence

Acceleration

- **Similar guarantees for finite sums**: SAG, SDCA, SVRG (Xiao and Zhang, 2014), SAGA, MISO (Mairal, 2015)

Gradient descent	$d\times$	$n\frac{L}{\mu}$	$\times \log\frac{1}{\varepsilon}$
Accelerated gradient descent	$d\times$	$n\sqrt{\frac{L}{\mu}}$	$\times \log\frac{1}{\varepsilon}$
SAG(A), SVRG, SDCA, MISO	$d\times$	$(n+\frac{L}{\mu})$	$\times \log\frac{1}{\varepsilon}$

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Accelerated versions	$d\times (n+\sqrt{n\frac{L}{\mu}}) \quad \times \log\frac{1}{\varepsilon}$

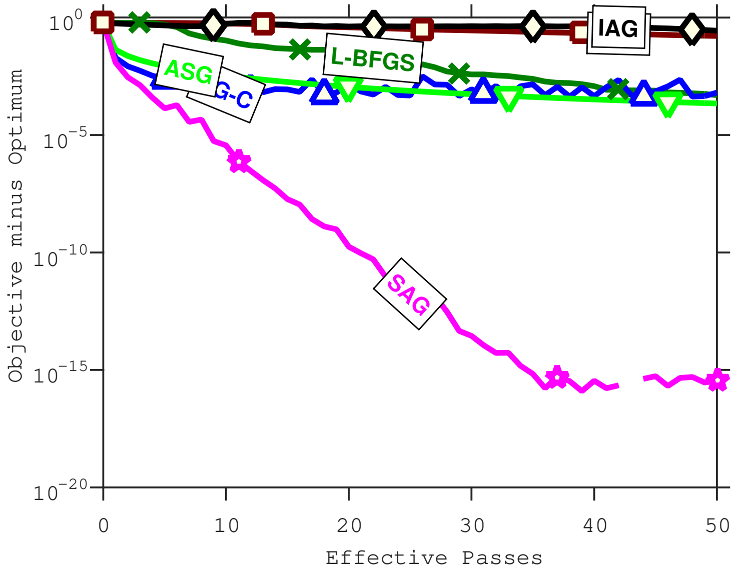
- **Acceleration for special algorithms** (e.g., Shalev-Shwartz and Zhang, 2014; Nitanda, 2014; Lan, 2015)

- **Catalyst** (Lin, Mairal, and Harchaoui, 2015)
  - Widely applicable generic acceleration scheme

From training to testing errors

- `rcv1` dataset ($n = 697\ 641$, $d = 47\ 236$)
  - NB: IAG, SG-C, ASG with optimal step-sizes in hindsight

Training cost



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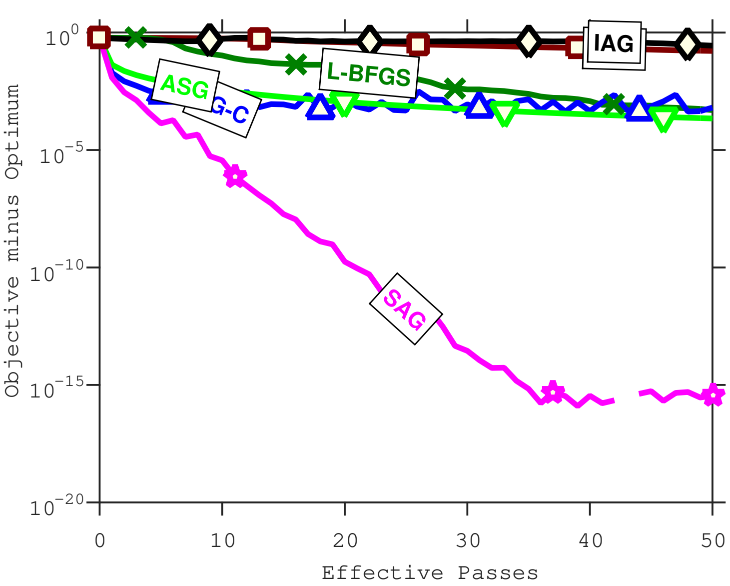

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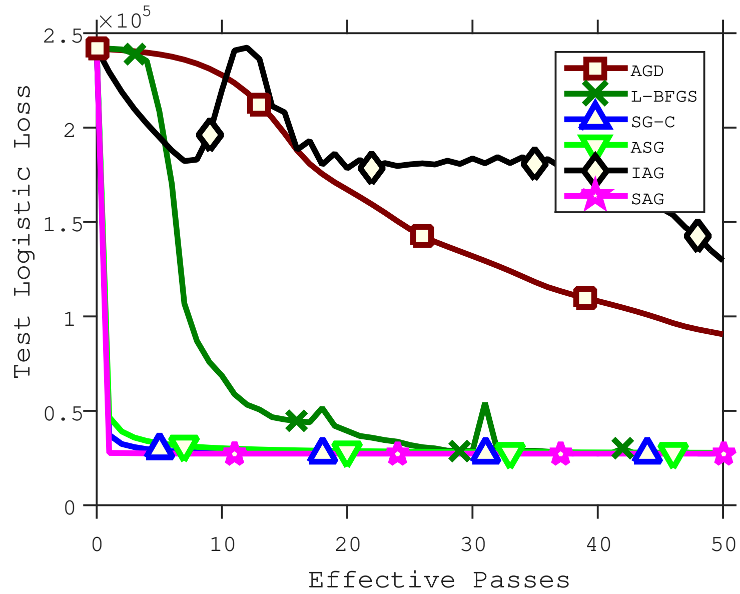

SGD minimizes the testing cost!

- **Goal**: minimize $f(\theta) = \mathbb{E}_{p(x,y)} \ell(y, \theta^\top \Phi(x))$
  - Given n independent samples (x_i, y_i), $i = 1, \dots, n$ from $p(x, y)$
  - Given a single pass of stochastic gradient descent
  - Bounds on the excess testing cost $\mathbb{E} f(\bar{\theta}_n) - \inf_{\theta \in \mathbb{R}^d} f(\theta)$

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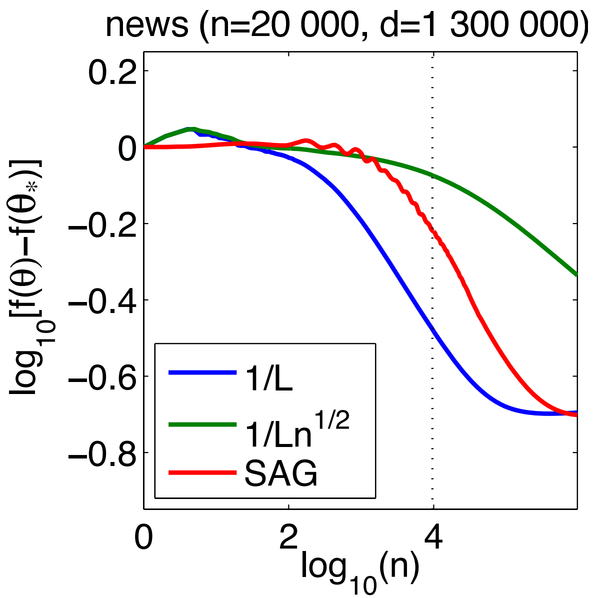
- **Constant-step-size SGD**
  - Linear convergence up to the noise level for strongly-convex problems (Solodov, 1998; Nedic and Bertsekas, 2000)
  - Full convergence and robustness to ill-conditioning?

Robust averaged stochastic gradient (Bach and Moulines, 2013)

- **Constant-step-size SGD is convergent for least-squares**
  - Convergence rate in $O(1/n)$ without any dependence on μ
  - Simple choice of step-size (equal to $1/L$)



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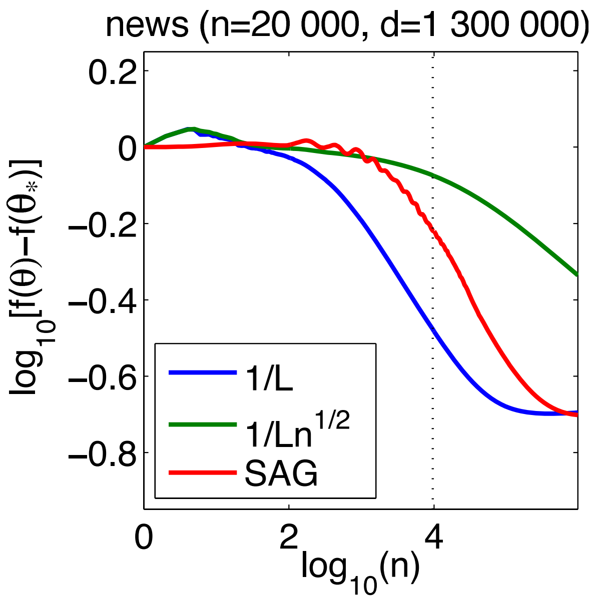

- Convergence in $O(1/n)$ for smooth losses with $O(d)$ online Newton step

Conclusions - variance reduction

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  - Provable and precise rates
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  - Bounds on testing errors for incremental methods (Frostig et al., 2015; Babanezhad et al., 2015)

Fundamentals of constrained optimization

- We consider the following primal optimization problem

$$\boxed{\min_{x \in D} f(x) \quad \text{s.t} \quad \forall i \in \{1,\dots,m\}, h_i(x) = 0 \text{ and } \forall j \in \{1,\dots,r\}, g_j(x) \leqslant 0}$$

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- **Lagrangian**: function $\mathcal{L} : \mathbb{R}^m \times \mathbb{R}^r_+$ defined as

$$\mathcal{L}(x, \lambda, \mu) = f(x) + \lambda^\top h(x) + \mu^\top g(x)$$

  – λ et μ are called Lagrange multipliers or dual variables
  – Primal problem $=$ supremum of Lagrangian with respect to dual variables: for all $x \in D$,

$$\sup_{(\lambda,\mu) \in \mathbb{R}^m \times \mathbb{R}^r_+} \mathcal{L}(x, \lambda, \mu) = \begin{cases} f(x) \text{ si } x \in D^* \\ +\infty \text{ otherwise} \end{cases}$$

Fundamentals of constrained optimization

- **Primal problem** equivalent to $p^* = \inf_{x \in D} \sup_{(\lambda,\mu) \in \mathbb{R}^m \times \mathbb{R}^r_+} \mathcal{L}(x, \lambda, \mu)$

- **Dual function**: $q(\lambda, \mu) = \inf_{x \in D} \mathcal{L}(x, \lambda, \mu) = \inf_{x \in D} f(x) + \lambda^\top h(x) + \mu^\top g(x)$

- **Dual problem**: minimization of q on $\mathbb{R}^m \times \mathbb{R}^r_+$, equivalent to

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- **Weak duality** (no assumption): $\forall (\lambda, \mu) \in \mathbb{R}^m \times \mathbb{R}^r_+$, $\forall x \in D^*$
$$\inf_{x' \in D} \mathcal{L}(x', \lambda, \mu) \leqslant \mathcal{L}(x, \lambda, \mu) \leqslant \sup_{(\lambda',\mu') \in \mathbb{R}^m \times \mathbb{R}^r_+} \mathcal{L}(x, \lambda', \mu')$$
  which implies $q(\lambda, \mu) \leqslant f(x)$ and thus $d^* \leqslant p^*$

Sufficient conditions for strong duality

- **Geometric interpretation** for $\min_{x\in D} f(x)$ s.t $g(x) \leqslant 0$
  - Consider $A = \{(u,t) \in \mathbb{R}^2,\ \exists x \in D, f(x) \leqslant t, g(x) \leqslant u\}$
- **Slater's conditions**
  - D is convex, h_i affine and g_j convex and there is a strictly feasible point, that is $\exists \bar{x} \in D^*$ such that $\forall j$, $g_j(\bar{x}) < 0$
  - then $d^* = p^*$ (strong duality).

Sufficient conditions for strong duality

- **Geometric interpretation** for $\min_{x \in D} f(x)$ s.t $g(x) \leqslant 0$
  - Consider $A = \{(u,t) \in \mathbb{R}^2,\ \exists x \in D, f(x) \leqslant t, g(x) \leqslant u\}$

- **Slater's conditions**
  - D is convex, h_i affine and g_j convex and there is a strictly feasible point, that is $\exists \bar{x} \in D^*$ such that $\forall j$, $g_j(\bar{x}) < 0$
  - then $d^* = p^*$ (strong duality).

- **Karush-Kühn-Tucker (KKT) conditions**: If strong duality holds, then x^* is primal optimal and (λ^*, μ^*) are dual optimal if and only if:
  - *Primal stationarity*: x^* minimizes $x \mapsto \mathcal{L}(x, \lambda^*, \mu^*)$.
  - *Feasibility*: x^* and (λ^*, μ^*) are feasible
  - *Complementary slackness*: $\forall j, \mu_j^* g_j(x^*) = 0$

Strong duality: remarks and examples

- **Remarks**: (a) the dual of the dual is the primal, (b) potentially several dual problems, (c) strong duality does not always hold

- **Linear programming**: $\min_{Ax=b, x \geqslant 0} c^\top x = \max_{A^\top y \leqslant c} b^\top y$

- **Quadratic programming with equality constraint**: $\min_{a^\top x = b} \frac{1}{2} x^\top Q x - q^\top x$

- **Lagrangian relaxation for combinatorial problem - Max Cut**: $\min_{x \in \{-1,1\}^n} x^\top W x$

- **Strong duality for non convex problem**: $\min_{x^\top x \leqslant 1} \frac{1}{2} x^\top Q x - q^\top x$

Dual stochastic coordinate ascent - I

- **General learning formulation**:

$$\begin{aligned}
& \min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n}\sum_{i=1}^{n} \ell_i(\theta^\top \Phi(x_i)) + \frac{\mu}{2}\|\theta\|_2^2 \\
= & \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \quad \frac{1}{n}\sum_{i=1}^{n} \ell_i(u_i) + \frac{\mu}{2}\|\theta\|_2^2 \text{ such that } \forall i, u_i = \theta^\top \Phi(x_i)
\end{aligned}$$

Dual stochastic coordinate ascent - I

- **General learning formulation**:

$$
\begin{aligned}
& \min_{\theta \in \mathbb{R}^d} \ \frac{1}{n} \sum_{i=1}^n \ell_i(\theta^\top \Phi(x_i)) + \frac{\mu}{2} \|\theta\|_2^2 \\
= & \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \ \frac{1}{n} \sum_{i=1}^n \ell_i(u_i) + \frac{\mu}{2} \|\theta\|_2^2 \text{ such that } \forall i, u_i = \theta^\top \Phi(x_i) \\
= & \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \max_{\alpha \in \mathbb{R}^n} \ \frac{1}{n} \sum_{i=1}^n \ell_i(u_i) + \frac{\mu}{2} \|\theta\|_2^2 + \sum_{i=1}^n \alpha_i (u_i - \theta^\top \Phi(x_i)) \\
= & \max_{\alpha \in \mathbb{R}^n} \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \ \frac{1}{n} \sum_{i=1}^n \ell_i(u_i) + \frac{\mu}{2} \|\theta\|_2^2 + \sum_{i=1}^n \alpha_i (u_i - \theta^\top \Phi(x_i)) \\
= & \max_{\alpha \in \mathbb{R}^n} \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \ \frac{1}{n} \sum_{i=1}^n \ell_i(u_i) + \frac{\mu}{2} \|\theta\|_2^2 + \sum_{i=1}^n \alpha_i (u_i - \theta^\top \Phi(x_i))
\end{aligned}
$$

Dual stochastic coordinate ascent - II

- **General learning formulation**:

$$
\begin{aligned}
& \min_{\theta \in \mathbb{R}^d} \ \frac{1}{n}\sum_{i=1}^n \ell_i(\theta^\top \Phi(x_i)) + \frac{\mu}{2}\|\theta\|_2^2 \\
= & \max_{\alpha \in \mathbb{R}^n} \min_{\theta \in \mathbb{R}^d, u \in \mathbb{R}^n} \ \frac{1}{n}\sum_{i=1}^n \ell_i(u_i) + \frac{\mu}{2}\|\theta\|_2^2 + \sum_{i=1}^n \alpha_i (u_i - \theta^\top \Phi(x_i)) \\
= & \max_{\alpha \in \mathbb{R}^n} \ \sum_{i=1}^n \min_{u_i \in \mathbb{R}} \Big\{ \frac{1}{n}\ell_i(u_i) + \alpha_i u_i \Big\} - \frac{1}{2\mu}\Big\| \sum_{i=1}^n \alpha_i \Phi(x_i) \Big\|_2^2 \\
= & \max_{\alpha \in \mathbb{R}^n} \ -\sum_{i=1}^n \psi_i(\alpha_i) - \frac{1}{2\mu}\Big\| \sum_{i=1}^n \alpha_i \Phi(x_i) \Big\|_2^2
\end{aligned}
$$

  – Minimizers obtained as $\theta = \frac{1}{\mu}\sum_{i=1}^n \alpha_i \Phi(x_i)$
  – ψ_i convex (up to affine transform = Fenchel-Legendre dual of ℓ_i)

Dual stochastic coordinate ascent - III

- **General learning formulation**:

$$\min_{\theta\in\mathbb{R}^d} \ \frac{1}{n}\sum_{i=1}^n \ell_i(\theta^\top\Phi(x_i)) + \frac{\mu}{2}\|\theta\|_2^2 = \max_{\alpha\in\mathbb{R}^n} \ -\sum_{i=1}^n \psi_i(\alpha_i) - \frac{1}{2\mu}\Big\|\sum_{i=1}^n \alpha_i\Phi(x_i)\Big\|_2^2$$

- **From primal to dual**
  - ℓ_i smooth $\Leftrightarrow$ ψ_i strongly convex
  - ℓ_i strongly convex $\Leftrightarrow$ ψ_i smooth

- **Applying coordinate descent in the dual**
  - Nesterov (2012); Shalev-Shwartz and Zhang (2012)
  - Linear convergence rate with simple iterations

Dual stochastic coordinate ascent - IV

- **Dual formulation**: $\displaystyle \max_{\alpha \in \mathbb{R}^n} \; -\sum_{i=1}^n \psi_i(\alpha_i) - \frac{1}{2\mu}\Big\| \sum_{i=1}^n \alpha_i \Phi(x_i) \Big\|_2^2$

- **Stochastic coordinate descent**: at iteration t
  - Choose a coordinate i at random
  - Optimzte w.r.t. α_i: $\displaystyle \max_{\alpha_i \in \mathbb{R}} -\psi_i(\alpha_i) - \frac{1}{2\mu}\Big\| \alpha_i \Phi(x_i) + \sum_{j \neq i} \alpha_i \Phi(x_i) \Big\|_2^2$
  - Can be done by a single access to $\Phi(x_i)$ and updating $\sum_{j=1}^n \alpha_j \Phi(x_j)$

- **Convergence proof**
  - See Nesterov (2012); Shalev-Shwartz and Zhang (2012)
  - Similar linear convergence than SAG

Randomized coordinate descent
Proof - I

- **Simplest setting**: minimize $f : \mathbb{R}^n \to \mathbb{R}$ which is L-smooth
  - Local smoothness constants $L_i = \sup_{\alpha \in \mathbb{R}^n} f''_{ii}(\alpha)$
  - $\max_{i \in \{1,\dots,n\}} L_i \leqslant L$ and $L \leqslant \sum_{i=1}^n L_i$
  - NB: in dual problems in machine learning $\max_{i \in \{1,\dots,n\}} L_i \propto R^2$

- **Algorithm**: at iteration t,
  - Choose a coordinate i_t at random with probability p_i
  - Local descent step: $\alpha_t = \alpha_{t-1} - \frac{1}{L_{i_t}} f'(\alpha_{t-1})_{i_t} e_{i_t}$

- **Two choices for p_i**: (a) uniform or (b) proportional to L_i

Randomized coordinate descent

Proof - II

- Iteration $\alpha_t = \alpha_{t-1} - \frac{1}{L_{i_t}} f'(\alpha_{t-1})_{i_t} e_{i_t}$

- From smoothness, $f(\alpha_t) \leqslant f(\alpha_{t-1}) - f'(\alpha_{t-1})^\top(\alpha_t - \alpha_{t-1}) + \frac{L_{i_t}}{2}\|\alpha_t - \alpha_{t-1}\|^2$ leading to $f(\alpha_t) \leqslant f(\alpha_{t-1}) - \frac{1}{2L_{i_t}}|f'(\alpha_{t-1})_{i_t}|^2$

- Taking expectations: $\mathbb{E}[f(\alpha_t)|\mathcal{F}_{t-1}] \leqslant f(\alpha_{t-1}) - \sum_{i=1}^n \frac{p_i}{2L_i}|f'(\alpha_{t-1})_i|^2$

Randomized coordinate descent
Proof - II

- Iteration $\alpha_t = \alpha_{t-1} - \frac{1}{L_{i_t}} f'(\alpha_{t-1})_{i_t} e_{i_t}$

- From smoothness, $f(\alpha_t) \leqslant f(\alpha_{t-1}) - f'(\alpha_{t-1})^\top (\alpha_t - \alpha_{t-1}) + \frac{L_{i_t}}{2} \|\alpha_t - \alpha_{t-1}\|^2$ leading to $f(\alpha_t) \leqslant f(\alpha_{t-1}) - \frac{1}{2L_{i_t}} |f'(\alpha_{t-1})_{i_t}|^2$

- Taking expectations: $\mathbb{E}[f(\alpha_t)|\mathcal{F}_{t-1}] \leqslant f(\alpha_{t-1}) - \sum_{i=1}^n \frac{p_i}{2L_i} |f'(\alpha_{t-1})_i|^2$

- If $p_i = 1/n$ (uniform), $\mathbb{E}[f(\alpha_t)|\mathcal{F}_{t-1}] \leqslant f(\alpha_{t-1}) - \frac{1}{2n \max_i L_i} \|f'(\alpha_{t-1})\|^2$
With strong convexity: $\mathbb{E} f(\alpha_t) \leqslant \mathbb{E} f(\alpha_{t-1}) - \frac{\mu}{n \max_i L_i} \big[\mathbb{E} f(\alpha_{t-1}) - f(\alpha^*)\big]$ leading to a linear convergence rate with factor $1 - \dfrac{\mu}{n \max_i L_i}$

Randomized coordinate descent
Proof - II

- Iteration $\alpha_t = \alpha_{t-1} - \frac{1}{L_{i_t}} f'(\alpha_{t-1})_{i_t} e_{i_t}$

- From smoothness, $f(\alpha_t) \leqslant f(\alpha_{t-1}) - f'(\alpha_{t-1})^\top(\alpha_t - \alpha_{t-1}) + \frac{L_{i_t}}{2}\|\alpha_t - \alpha_{t-1}\|^2$ leading to $f(\alpha_t) \leqslant f(\alpha_{t-1}) - \frac{1}{2L_{i_t}}|f'(\alpha_{t-1})_{i_t}|^2$

- Taking expectations: $\mathbb{E}[f(\alpha_t)|\mathcal{F}_{t-1}] \leqslant f(\alpha_{t-1}) - \sum_{i=1}^n \frac{p_i}{2L_i}|f'(\alpha_{t-1})_i|^2$

- If $p_i = 1/n$ (uniform), $\mathbb{E}[f(\alpha_t)|\mathcal{F}_{t-1}] \leqslant f(\alpha_{t-1}) - \frac{1}{2n\max_i L_i}\|f'(\alpha_{t-1})\|^2$
With strong convexity: $\mathbb{E}f(\alpha_t) \leqslant \mathbb{E}f(\alpha_{t-1}) - \frac{\mu}{n\max_i L_i}\big[\mathbb{E}f(\alpha_{t-1}) - f(\alpha^*)\big]$ leading to a linear convergence rate with factor $1 - \dfrac{\mu}{n\max_i L_i}$

- If $p_i = \frac{L_i}{\sum_{j=1}^n L_j}$, $\mathbb{E}f(\alpha_t) \leqslant f(\alpha_{t-1}) - \frac{1}{2\sum_{j=1}^n L_j}\|f'(\alpha_{t-1})\|^2$
With strong convexity: $\mathbb{E}f(\alpha_t) \leqslant \mathbb{E}f(\alpha_{t-1}) - \frac{\mu}{\sum_{j=1}^n L_j}\big[\mathbb{E}f(\alpha_{t-1}) - f(\alpha^*)\big]$ leading to a linear convergence rate with factor $1 - \dfrac{\mu}{\sum_{j=1}^n L_j}$

Randomized coordinate descent
Discussion

- **Iteration** $\alpha_t = \alpha_{t-1} - \frac{1}{L_{i_t}} f'(\alpha_{t-1})_{i_t} e_{i_t}$
  - If $p_i = 1/n$ (uniform), linear rate $1 - \dfrac{\mu}{n \max_i L_i}$
  - If $p_i = \frac{L_i}{\sum_{j=1}^n L_j}$, linear rate $1 - \dfrac{\mu}{\sum_{j=1}^n L_j}$
- Best-case scenario: f'' is diagonal, and $L = \max_i L_i$
- Worst-case scenario: f'' is constant and $L = \sum_i L_i$

Frank-Wolfe - conditional gradient - I

- **Goal**: minimize smooth convex function $f(\theta)$ on compact set $\mathcal{C}$

- **Standard result**: accelerated projected gradient descent with optimal rate $O(1/t^2)$
  - Requires projection oracle: $\arg\min_{\theta\in\mathcal{C}} \frac{1}{2}\|\theta-\eta\|^2$

- **Only availability of the linear oracle**: $\arg\min_{\theta\in\mathcal{C}} \theta^\top\eta$
  - Many examples (sparsity, low-rank, large polytopes, etc.)
  - Iterative Frank-Wolfe algorithm (see, e.g., Jaggi, 2013, and references therein) *with geometric interpretation*

$$\left\{\begin{array}{l} \bar\theta_t \in \arg\min\limits_{\theta\in\mathcal{C}} \theta^\top f'(\theta_{t-1}) \\ \theta_t = (1-\rho_t)\theta_{t-1} + \rho_t\bar\theta_t \end{array}\right.$$

Frank-Wolfe - conditional gradient - II

- **Convergence rates**: $f(\theta_t) - f(\theta_*) \leqslant \dfrac{2L\mathrm{diam}(\mathcal{C})^2}{t+1}$

Iteration: $\begin{cases} \bar\theta_t \in \arg\min_{\theta\in\mathcal{C}} \theta^\top f'(\theta_{t-1}) \\ \theta_t = (1-\rho_t)\theta_{t-1} + \rho_t\bar\theta_t \end{cases}$

From smoothness: $f(\theta_t) \leqslant f(\theta_{t-1}) + f'(\theta_{t-1})^\top\big[\rho_t(\bar\theta_t - \theta_{t-1})\big] + \dfrac{L}{2}\big\|\rho_t(\bar\theta_t - \theta_{t-1})\big\|^2$

From compactness: $f(\theta_t) \leqslant f(\theta_{t-1}) + f'(\theta_{t-1})^\top\big[\rho_t(\bar\theta_t - \theta_{t-1})\big] + \dfrac{L}{2}\rho_t^2\mathrm{diam}(\mathcal{C})^2$

From convexity, $f(\theta_t) - f(\theta_*) \leqslant f'(\theta_{t-1})^\top(\theta_{t-1} - \theta_*) \leqslant \max_{\theta\in\mathcal{C}} f'(\theta_{t-1})^\top(\theta_{t-1} - \theta)$, which is equal to $f'(\theta_{t-1})^\top(\theta_{t-1} - \bar\theta_t)$

Thus, $f(\theta_t) \leqslant f(\theta_{t-1}) - \rho_t\big[f(\theta_{t-1}) - f(\theta_*)\big] + \dfrac{L}{2}\rho_t^2\mathrm{diam}(\mathcal{C})^2$

With $\rho_t = 2/(t+1)$: $f(\theta_t) \leqslant \frac{2L\mathrm{diam}(\mathcal{C})^2}{t+1}$ *by direct expansion*

Frank-Wolfe - conditional gradient - II

- **Convergence rates**: $f(\theta_t) - f(\theta_*) \leqslant \dfrac{2L\text{diam}(\mathcal{C})^2}{t}$

- **Remarks and extensions**
  - Affine-invariant algorithms
  - Certified duality gaps and dual interpretations (Bach, 2015)
  - Adapted to very large polytopes
  - Line-search extensions: minimize quadratic upper-bound
  - Stochastic extensions (Lacoste-Julien et al., 2013)
  - Away and pairwise steps to avoid oscillations (Lacoste-Julien and Jaggi, 2015)

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)
   - Proximal methods

3. **Non-smooth stochastic approximation**
   - Stochastic (sub)gradient and averaging
   - Non-asymptotic results and lower bounds
   - Strongly convex vs. non-strongly convex

Outline - II

4. **Classical stochastic approximation**
   - Asymptotic analysis
   - Robbins-Monro algorithm
   - Polyak-Rupert averaging

5. **Smooth stochastic approximation algorithms**
   - Non-asymptotic analysis for smooth functions
   - Logistic regression
   - Least-squares regression without decaying step-sizes

6. **Finite data sets**
   - Gradient methods with exponential convergence rates
   - Convex duality
   - (Dual) stochastic coordinate descent - Frank-Wolfe

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 $\Theta = \{\|\theta\|_2 \leqslant D\}$

- **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 $O(n^2 d)$

Stochastic subgradient "descent"/method

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

- **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 $\gamma_n = Cn^{-\alpha}$
- **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: $O\Big(\frac{\sigma^2\gamma_n}{\mu}\Big) + O(e^{-\mu n \gamma_n})\|\theta_0 - \theta_*\|^2$
  - 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: $\boxed{\mathbb{E} f(\bar\theta_{n-1}) - f(\theta_*) \leqslant \frac{4\sigma^2 d}{n} + \frac{4R^2\|\theta_0 - \theta_*\|^2}{n}}$

- **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: $\boxed{\theta_n = \theta_{n-1} - \gamma\big[f_n'(\bar{\theta}_{n-1}) + f_n''(\bar{\theta}_{n-1})(\theta_{n-1} - \bar{\theta}_{n-1})\big]}$
  - 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, $i = 1, \dots, n$
  - Random selection $i(t) \in \{1, \dots, n\}$ with replacement
  - Iteration: $\theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^{n} y_i^t$ 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
  - μ strong convexity constant

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

References

A. Agarwal, P. L. Bartlett, P. Ravikumar, and M. J. Wainwright. Information-theoretic lower bounds on the oracle complexity of stochastic convex optimization. *IEEE Transactions on Information Theory*, 58(5):3235–3249, 2012.

Alekh Agarwal and Leon Bottou. A lower bound for the optimization of finite sums. *arXiv preprint arXiv:1410.0723*, 2014.

R. Aguech, E. Moulines, and P. Priouret. On a perturbation approach for the analysis of stochastic tracking algorithms. *SIAM J. Control and Optimization*, 39(3):872–899, 2000.

Y. Arjevani and O. Shamir. Dimension-free iteration complexity of finite sum optimization problems. In *Advances In Neural Information Processing Systems*, 2016.

R. Babanezhad, M. O. Ahmed, A. Virani, M. W. Schmidt, J. Konecný, and S. Sallinen. Stopwasting my gradients: Practical SVRG. In *Advances in Neural Information Processing Systems*, 2015.

F. Bach. Self-concordant analysis for logistic regression. *Electronic Journal of Statistics*, 4:384–414, 2010. ISSN 1935-7524.

F. Bach. Adaptivity of averaged stochastic gradient descent to local strong convexity for logistic regression. Technical Report 00804431, HAL, 2013.

F. Bach and E. Moulines. Non-asymptotic analysis of stochastic approximation algorithms for machine learning. In *Adv. NIPS*, 2011.

F. Bach and E. Moulines. Non-strongly-convex smooth stochastic approximation with convergence rate $o(1/n)$. Technical Report 00831977, HAL, 2013.

F. Bach, R. Jenatton, J. Mairal, and G. Obozinski. Structured sparsity through convex optimization, 2012a.

Francis Bach. Duality between subgradient and conditional gradient methods. *SIAM Journal on Optimization*, 25(1):115–129, 2015.

Francis Bach, Rodolphe Jenatton, Julien Mairal, and Guillaume Obozinski. Optimization with sparsity-inducing penalties. *Foundations and Trends® in Machine Learning*, 4(1):1–106, 2012b.

P. Balamurugan and F. Bach. Stochastic variance reduction methods for saddle-point problems. Technical Report 01319293, HAL, 2016.

A. Beck and M. Teboulle. A fast iterative shrinkage-thresholding algorithm for linear inverse problems. *SIAM Journal on Imaging Sciences*, 2(1):183–202, 2009.

Albert Benveniste, Michel Métivier, and Pierre Priouret. *Adaptive algorithms and stochastic approximations*. Springer Publishing Company, Incorporated, 2012.

D. P. Bertsekas. *Nonlinear programming*. Athena scientific, 1999.

D. Blatt, A. O. Hero, and H. Gauchman. A convergent incremental gradient method with a constant step size. *SIAM Journal on Optimization*, 18(1):29–51, 2008.

V. S. Borkar. Stochastic approximation with two time scales. *Systems & Control Letters*, 29(5): 291–294, 1997.

L. Bottou and O. Bousquet. The tradeoffs of large scale learning. In *Adv. NIPS*, 2008.

L. Bottou and Y. Le Cun. On-line learning for very large data sets. *Applied Stochastic Models in Business and Industry*, 21(2):137–151, 2005.

S. Boucheron and P. Massart. A high-dimensional wilks phenomenon. *Probability theory and related* *fields*, 150(3-4):405–433, 2011.

S. Boucheron, O. Bousquet, G. Lugosi, et al. Theory of classification: A survey of some recent advances. *ESAIM Probability and statistics*, 9:323–375, 2005.

S. Boyd and L. Vandenberghe. *Convex Optimization*. Cambridge University Press, 2003.

S. Bubeck. Convex optimization: Algorithms and complexity. *Foundations and Trends® in Machine Learning*, 8(3-4):231–357, 2015.

N. Cesa-Bianchi, A. Conconi, and C. Gentile. On the generalization ability of on-line learning algorithms. *Information Theory, IEEE Transactions on*, 50(9):2050–2057, 2004.

P. L. Combettes and J.-C. Pesquet. Proximal splitting methods in signal processing. In *Fixed-point algorithms for inverse problems in science and engineering*, pages 185–212. Springer, 2011.

A. d'Aspremont. Smooth optimization with approximate gradient. *SIAM J. Optim.*, 19(3):1171–1183, 2008.

A. Defazio, J. Domke, and T. S. Caetano. Finito: A faster, permutable incremental gradient method for big data problems. In *Proc. ICML*, 2014a.

Aaron Defazio, Francis Bach, and Simon Lacoste-Julien. Saga: A fast incremental gradient method with support for non-strongly convex composite objectives. In *Advances in Neural Information Processing Systems*, pages 1646–1654, 2014b.

A. Défossez and F. Bach. Constant step size least-mean-square: Bias-variance trade-offs and optimal sampling distributions. 2015.

A. Dieuleveut and F. Bach. Non-parametric Stochastic Approximation with Large Step sizes. Technical report, ArXiv, 2014.

A. Dieuleveut, N. Flammarion, and F. Bach. Harder, better, faster, stronger convergence rates for least-squares regression. Technical Report 1602.05419, arXiv, 2016.

J. Duchi and Y. Singer. Efficient online and batch learning using forward backward splitting. *Journal of Machine Learning Research*, 10:2899–2934, 2009. ISSN 1532-4435.

John C. Duchi, Shai Shalev-Shwartz, Yoram Singer, and Ambuj Tewari. Composite objective mirror descent. In *COLT*, pages 14–26. Citeseer, 2010.

M. Duflo. *Algorithmes stochastiques*. Springer-Verlag, 1996.

V. Fabian. On asymptotic normality in stochastic approximation. *The Annals of Mathematical Statistics*, 39(4):1327–1332, 1968.

N. Flammarion and F. Bach. From averaging to acceleration, there is only a step-size. *arXiv preprint arXiv:1504.01577*, 2015.

R. Frostig, R. Ge, S. M. Kakade, and A. Sidford. Competing with the empirical risk minimizer in a single pass. In *Proceedings of the Conference on Learning Theory*, 2015.

S. Ghadimi and G. Lan. Optimal stochastic approximation algorithms for strongly convex stochastic composite optimization. *Optimization Online*, July, 2010.

Saeed Ghadimi and Guanghui Lan. Optimal stochastic approximation algorithms for strongly convex stochastic composite optimization, ii: shrinking procedures and optimal algorithms. *SIAM Journal on Optimization*, 23(4):2061–2089, 2013.

M. Gurbuzbalaban, A. Ozdaglar, and P. Parrilo. On the convergence rate of incremental aggregated gradient algorithms. Technical Report 1506.02081, arXiv, 2015.

L. Györfi and H. Walk. On the averaged stochastic approximation for linear regression. *SIAM Journal* *on Control and Optimization*, 34(1):31–61, 1996.

E. Hazan, A. Agarwal, and S. Kale. Logarithmic regret algorithms for online convex optimization. *Machine Learning*, 69(2):169–192, 2007.

Elad Hazan and Satyen Kale. Beyond the regret minimization barrier: optimal algorithms for stochastic strongly-convex optimization. *The Journal of Machine Learning Research*, 15(1):2489–2512, 2014.

Chonghai Hu, James T Kwok, and Weike Pan. Accelerated gradient methods for stochastic optimization and online learning. In *NIPS*, volume 22, pages 781–789, 2009.

Martin Jaggi. Revisiting Frank-Wolfe: Projection-free sparse convex optimization. In *Proceedings of the 30th International Conference on Machine Learning (ICML-13)*, pages 427–435, 2013.

Rie Johnson and Tong Zhang. Accelerating stochastic gradient descent using predictive variance reduction. In *Advances in Neural Information Processing Systems*, pages 315–323, 2013.

Takafumi Kanamori and Hidetoshi Shimodaira. Active learning algorithm using the maximum weighted log-likelihood estimator. *Journal of statistical planning and inference*, 116(1):149–162, 2003.

H. J. Kushner and G. G. Yin. *Stochastic approximation and recursive algorithms and applications*. Springer-Verlag, second edition, 2003.

S. Lacoste-Julien and M. Jaggi. On the global linear convergence of frank-wolfe optimization variants. In *Advances in Neural Information Processing Systems (NIPS)*, 2015.

S. Lacoste-Julien, M. Schmidt, and F. Bach. A simpler approach to obtaining an o $(1/t)$ convergence rate for projected stochastic subgradient descent. Technical Report 1212.2002, ArXiv, 2012.

Simon Lacoste-Julien, Martin Jaggi, Mark Schmidt, and Patrick Pletscher. Block-coordinate $\{$Frank-Wolfe$\}$ optimization for structural $\{$SVMs$\}$. In *Proceedings of The 30th International Conference* *on Machine Learning*, pages 53–61, 2013.

G. Lan. An optimal method for stochastic composite optimization. *Math. Program.*, 133(1-2, Ser. A): 365–397, 2012.

G. Lan. An optimal randomized incremental gradient method. Technical Report 1507.02000, arXiv, 2015.

Guanghui Lan, Arkadi Nemirovski, and Alexander Shapiro. Validation analysis of mirror descent stochastic approximation method. *Mathematical programming*, 134(2):425–458, 2012.

N. Le Roux, M. Schmidt, and F. Bach. A stochastic gradient method with an exponential convergence rate for strongly-convex optimization with finite training sets. In *Adv. NIPS*, 2012.

N. Le Roux, M. Schmidt, and F. Bach. A stochastic gradient method with an exponential convergence rate for strongly-convex optimization with finite training sets. Technical Report 00674995, HAL, 2013.

R. Leblond, F. Pedregosa, and S. Lacoste-Julien. Asaga: Asynchronous parallel Saga. Technical Report 1606.04809, arXiv, 2016.

H. Lin, J. Mairal, and Z. Harchaoui. A universal catalyst for first-order optimization. In *Advances in Neural Information Processing Systems (NIPS)*, 2015.

O. Macchi. *Adaptive processing: The least mean squares approach with applications in transmission*. Wiley West Sussex, 1995.

J. Mairal. Incremental majorization-minimization optimization with application to large-scale machine learning. *SIAM Journal on Optimization*, 25(2):829–855, 2015.

P. Massart. *Concentration Inequalities and Model Selection: Ecole d'été de Probabilités de Saint-Flour*

23. Springer, 2003.

R. Meir and T. Zhang. Generalization error bounds for bayesian mixture algorithms. *Journal of Machine Learning Research*, 4:839–860, 2003.

A. Nedic and D. Bertsekas. Convergence rate of incremental subgradient algorithms. *Stochastic Optimization: Algorithms and Applications*, pages 263–304, 2000.

A. Nemirovski, A. Juditsky, G. Lan, and A. Shapiro. Robust stochastic approximation approach to stochastic programming. *SIAM Journal on Optimization*, 19(4):1574–1609, 2009.

A. S. Nemirovsky and D. B. Yudin. *Problem complexity and method efficiency in optimization.* Wiley & Sons, 1983.

Y. Nesterov. A method for solving a convex programming problem with rate of convergence $O(1/k^2)$. *Soviet Math. Doklady*, 269(3):543–547, 1983.

Y. Nesterov. *Introductory lectures on convex optimization: a basic course*. Kluwer Academic Publishers, 2004.

Y. Nesterov. Gradient methods for minimizing composite objective function. *Center for Operations Research and Econometrics (CORE), Catholic University of Louvain, Tech. Rep*, 76, 2007.

Y. Nesterov. Primal-dual subgradient methods for convex problems. *Mathematical programming*, 120 (1):221–259, 2009.

Y. Nesterov and A. Nemirovski. *Interior-point polynomial algorithms in convex programming*. SIAM studies in Applied Mathematics, 1994.

Y. Nesterov and J. P. Vial. Confidence level solutions for stochastic programming. *Automatica*, 44(6): 1559–1568, 2008. ISSN 0005-1098.

Yu Nesterov. Efficiency of coordinate descent methods on huge-scale optimization problems. *SIAM Journal on Optimization*, 22(2):341–362, 2012.

A. Nitanda. Stochastic proximal gradient descent with acceleration techniques. In *Advances in Neural Information Processing Systems (NIPS)*, 2014.

N. Parikh and S. P. Boyd. Proximal algorithms. *Foundations and Trends in optimization*, 1(3):127–239, 2014.

I. Pinelis. Optimum bounds for the distributions of martingales in banach spaces. *The Annals of Probability*, 22(4):pp. 1679–1706, 1994. URL `http://www.jstor.org/stable/2244912`.

B. T. Polyak and A. B. Juditsky. Acceleration of stochastic approximation by averaging. *SIAM Journal on Control and Optimization*, 30(4):838–855, 1992.

Maxim Raginsky and Alexander Rakhlin. Information-based complexity, feedback and dynamics in convex programming. *Information Theory, IEEE Transactions on*, 57(10):7036–7056, 2011.

H. Robbins and S. Monro. A stochastic approximation method. *The Annals of Mathematical Statistics*, pages 400–407, 1951a.

H. Robbins and S. Monro. A stochastic approximation method. *Ann. Math. Statistics*, 22:400–407, 1951b.

Herbert Robbins and David Siegmund. A convergence theorem for non negative almost supermartingales and some applications. In *Herbert Robbins Selected Papers*, pages 111–135. Springer, 1985.

R Tyrrell Rockafellar. *Convex Analysis*. Number 28. Princeton University Press, 1997.

D. Ruppert. Efficient estimations from a slowly convergent Robbins-Monro process. Technical Report 781, Cornell University Operations Research and Industrial Engineering, 1988.

M. Schmidt, N. Le Roux, and F. Bach. Optimization with approximate gradients. Technical report, HAL, 2011.

B. Schölkopf and A. J. Smola. *Learning with Kernels*. MIT Press, 2001.

S. Shalev-Shwartz. Sdca without duality, regularization, and individual convexity. Technical Report 1602.01582, arXiv, 2016.

S. Shalev-Shwartz and N. Srebro. SVM optimization: inverse dependence on training set size. In *Proc. ICML*, 2008.

S. Shalev-Shwartz and T. Zhang. Stochastic dual coordinate ascent methods for regularized loss minimization. Technical Report 1209.1873, Arxiv, 2012.

S. Shalev-Shwartz and T. Zhang. Accelerated proximal stochastic dual coordinate ascent for regularized loss minimization. In *Proc. ICML*, 2014.

S. Shalev-Shwartz, Y. Singer, and N. Srebro. Pegasos: Primal estimated sub-gradient solver for svm. In *Proc. ICML*, 2007.

S. Shalev-Shwartz, O. Shamir, N. Srebro, and K. Sridharan. Stochastic convex optimization. In *proc. COLT*, 2009.

O. Shamir. Without-replacement sampling for stochastic gradient methods: Convergence results and application to distributed optimization. Technical Report 1603.00570, arXiv, 2016.

J. Shawe-Taylor and N. Cristianini. *Kernel Methods for Pattern Analysis*. Cambridge University Press, 2004.

Naum Zuselevich Shor, Krzysztof C. Kiwiel, and Andrzej Ruszcay?ski. *Minimization methods for non-differentiable functions*. Springer-Verlag New York, Inc., 1985.

M.V. Solodov. Incremental gradient algorithms with stepsizes bounded away from zero. *Computational Optimization and Applications*, 11(1):23–35, 1998.

K. Sridharan, N. Srebro, and S. Shalev-Shwartz. Fast rates for regularized objectives. 2008.

P. Tseng. An incremental gradient(-projection) method with momentum term and adaptive stepsize rule. *SIAM Journal on Optimization*, 8(2):506–531, 1998.

I. Tsochantaridis, Thomas Joachims, T., Y. Altun, and Y. Singer. Large margin methods for structured and interdependent output variables. *Journal of Machine Learning Research*, 6:1453–1484, 2005.

A. B. Tsybakov. Optimal rates of aggregation. In *Proc. COLT*, 2003.

A. W. Van der Vaart. *Asymptotic statistics*, volume 3. Cambridge Univ. press, 2000.

L. Xiao. Dual averaging methods for regularized stochastic learning and online optimization. *Journal of Machine Learning Research*, 9:2543–2596, 2010. ISSN 1532-4435.

L. Xiao and T. Zhang. A proximal stochastic gradient method with progressive variance reduction. *SIAM Journal on Optimization*, 24(4):2057–2075, 2014.

L. Zhang, M. Mahdavi, and R. Jin. Linear convergence with condition number independent access of full gradients. In *Advances in Neural Information Processing Systems*, 2013.