

Stochastic gradient methods for machine learning

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Joint work with Eric Moulines, Nicolas Le Roux
and Mark Schmidt - April 2013

Context

Machine learning for “big data”

- **Large-scale machine learning:** large p , large n , large k
 - p : dimension of each observation (input)
 - k : number of tasks (dimension of outputs)
 - n : number of observations
- **Examples:** computer vision, bioinformatics, signal processing
- **Ideal running-time complexity:** $O(pn + kn)$
- **Going back to simple methods**
 - Stochastic gradient methods (Robbins and Monro, 1951)
 - Mixing statistics and optimization

Outline

- **Introduction**

- Supervised machine learning and convex optimization

- **Stochastic approximation algorithms** (Bach and Moulines, 2011; Bach, 2013)

- Stochastic gradient and averaging
- Strongly convex vs. non-strongly convex
- Adaptivity

- **Going beyond stochastic gradient** (Le Roux, Schmidt, and Bach, 2012, 2013)

- More than a single pass through the data
- Linear (exponential) convergence rate for strongly convex functions

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 $\Phi(x) \in \mathcal{F} = \mathbb{R}^p$
- **(regularized) empirical risk minimization:** find $\hat{\theta}$ solution of

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

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 $\hat{\theta}$

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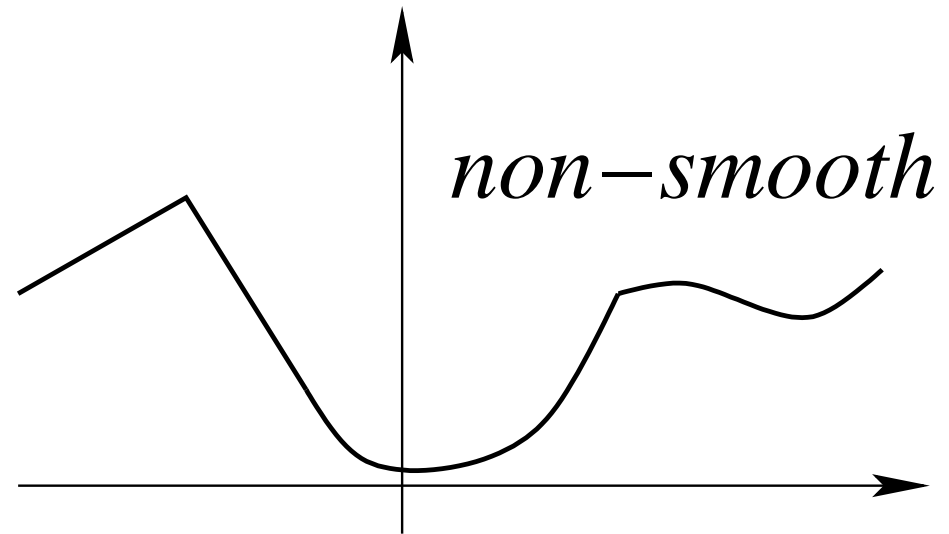
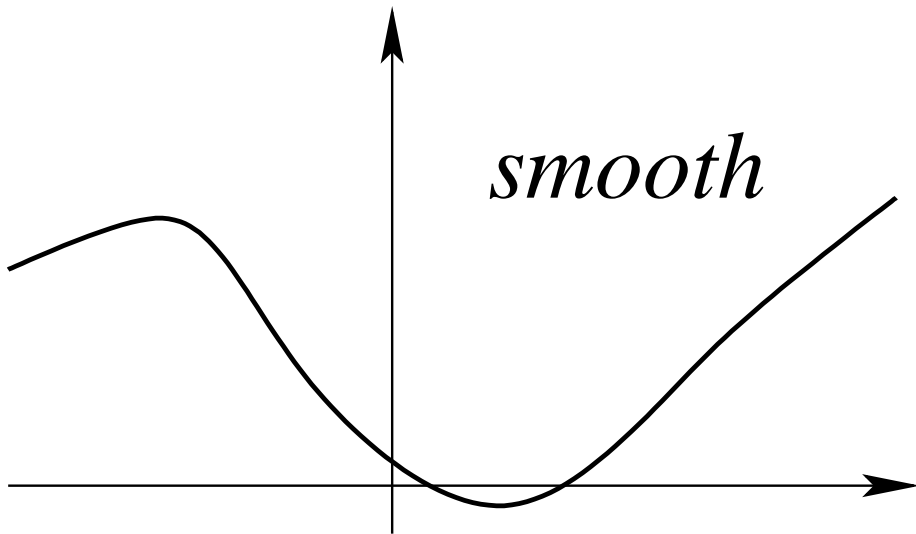
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- **Two fundamental questions:** (1) computing $\hat{\theta}$ and (2) analyzing $\hat{\theta}$
 - **May be tackled simultaneously**

Smoothness and strong convexity

- A function $g : \mathbb{R}^p \rightarrow \mathbb{R}$ is **L -smooth** if and only if it is twice differentiable and

$$\forall \theta \in \mathbb{R}^p, g''(\theta) \preceq L \cdot Id$$



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- **Machine learning**

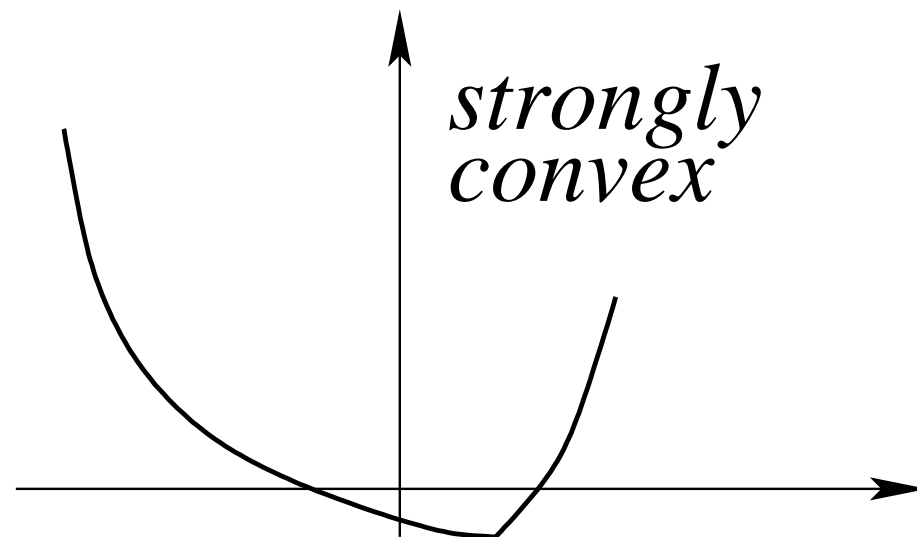
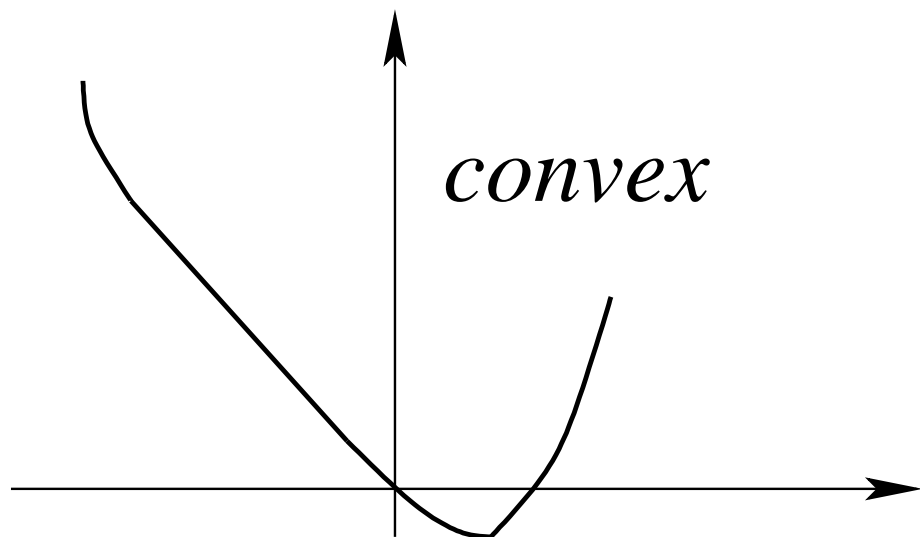
- with $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
- Hessian \approx covariance matrix $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \Phi(x_i)^\top$
- **Bounded data**

Smoothness and **strong convexity**

- A function $g : \mathbb{R}^p \rightarrow \mathbb{R}$ is **μ -strongly convex** if and only if

$$\forall \theta_1, \theta_2 \in \mathbb{R}^p, \quad g(\theta_1) \geq g(\theta_2) + \langle g'(\theta_2), \theta_1 - \theta_2 \rangle + \frac{\mu}{2} \|\theta_1 - \theta_2\|^2$$

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



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- **Machine learning**

- with $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
- Hessian \approx covariance matrix $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \Phi(x_i)^\top$
- **Data with invertible covariance matrix** (low correlation/dimension)
- ... or with added regularization by $\frac{\mu}{2} \|\theta\|^2$

Iterative methods for minimizing smooth functions

- **Assumption:** g convex and smooth on $\mathcal{F} = \mathbb{R}^p$
- **Gradient descent:** $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1})$
 - $O(1/t)$ convergence rate for convex functions
 - $O(e^{-\rho t})$ convergence rate for strongly convex functions
- **Newton method:** $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
 - $O(e^{-\rho 2^t})$ convergence rate
- **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

\Rightarrow **Stochastic approximation**

Stochastic approximation

- **Goal:** Minimizing a function f defined on $\mathcal{F} = \mathbb{R}^p$
 - given only unbiased estimates $f'_n(\theta_n)$ of its gradients $f'(\theta_n)$ at certain points $\theta_n \in \mathcal{F}$
- **Stochastic approximation**
 - Observation of $f'_n(\theta_n) = f'(\theta_n) + \varepsilon_n$, with $\varepsilon_n = \text{i.i.d. noise}$
 - Non-convex problems
- **Machine learning - statistics**
 - loss for a single pair of observations: $f_n(\theta) = \ell(y_n, \theta^\top \Phi(x_n))$
 - $f(\theta) = \mathbb{E} f_n(\theta) = \mathbb{E} \ell(y_n, \theta^\top \Phi(x_n)) = \text{generalization error}$
 - Expected gradient: $f'(\theta) = \mathbb{E} f'_n(\theta) = \mathbb{E} \{ \ell'(y_n, \theta^\top \Phi(x_n)) \Phi(x_n) \}$

Convex smooth stochastic approximation

- **Key assumption:** smoothness and/or strongly convexity
- **Key algorithm:** stochastic gradient descent (a.k.a. Robbins-Monro)

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

– Polyak-Ruppert averaging: $\bar{\theta}_n = \frac{1}{n} \sum_{k=0}^{n-1} \theta_k$

– Which learning rate sequence γ_n ? Classical setting:

$$\gamma_n = Cn^{-\alpha}$$

Convex stochastic approximation

Related work

- **Known global minimax rates of convergence** (Nemirovski and Yudin, 1983; Agarwal et al., 2010)
 - **Strongly convex:** $O(n^{-1})$
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 $\gamma_n \propto n^{-1/2}$
- Bottou and Le Cun (2005); Bottou and Bousquet (2008); Hazan et al. (2007); Shalev-Shwartz and Srebro (2008); Shalev-Shwartz et al. (2007, 2009); Xiao (2010); Duchi and Singer (2009); Nesterov and Vial (2008); Nemirovski et al. (2009)

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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 strongly convex problems

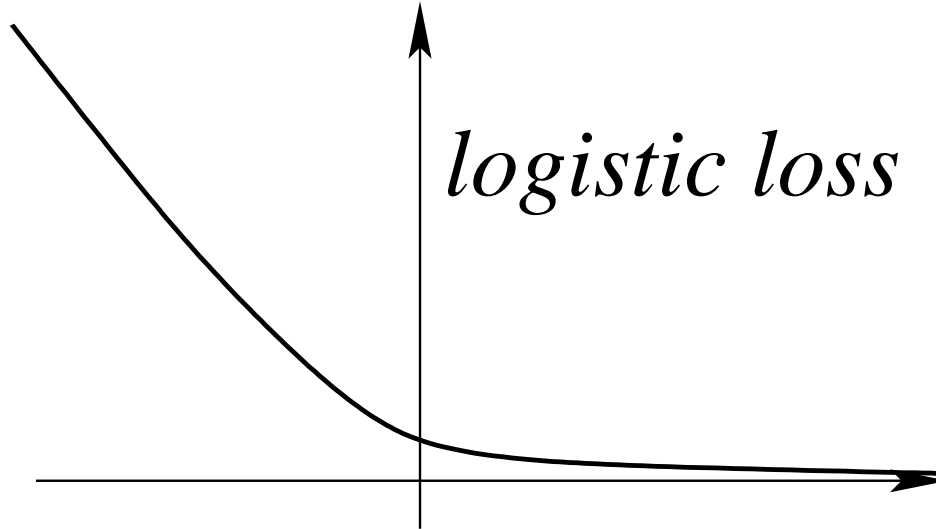
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 - **A single algorithm with global convergence rate?**

Adaptive algorithm for logistic regression

- **Logistic regression:** $(x_n, y_n) \in \mathbb{R}^p \times \{-1, 1\}$
 - Single data point: $f_n(\theta) = \log(1 + \exp(-y_n \theta^\top x_n))$
 - Generalization error: $f(\theta) = \mathbb{E} f_n(\theta)$
- **Cannot be strongly convex** \Rightarrow **local** strong convexity
 - unless restricted to $|\theta^\top x_n| \leq M$
 - μ = lowest eigenvalue of the Hessian at the optimum $f''(\theta_*)$



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 - unless restricted to $|\theta^\top x_n| \leq M$
 - μ = 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):

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

- Proof based on generalized self-concordance (Bach, 2010)

Conclusions / Extensions

Stochastic approximation for machine learning

- **Mixing convex optimization and statistics**
 - Non-asymptotic analysis through moment computations
 - Averaging with longer steps is (more) robust and adaptive
- **Future/current work - open problems**
 - High-probability through all moments $\mathbb{E}\|\theta_n - \theta_*\|^{2d}$
 - Non-random errors (Schmidt, Le Roux, and Bach, 2011)
 - Line search for stochastic gradient
 - Non-parametric stochastic approximation
 - Going beyond a single pass through the data

Going beyond a single pass over the data

- **Stochastic approximation**

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

- **Machine learning practice**

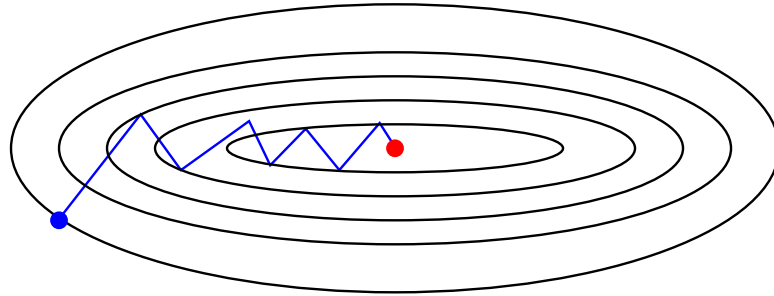
- Finite data set $(x_1, y_1, \dots, x_n, y_n)$
- Multiple passes
- Minimizes **training** cost $\frac{1}{n} \sum_{i=1}^n \ell(y_i, \theta^\top \Phi(x_i))$
- Need to regularize (e.g., by the ℓ_2 -norm) to avoid overfitting

Stochastic vs. deterministic methods

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

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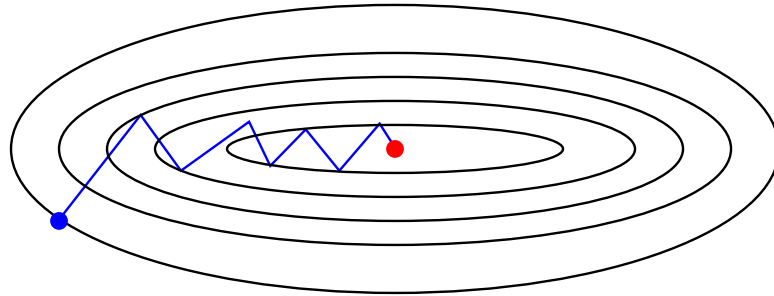


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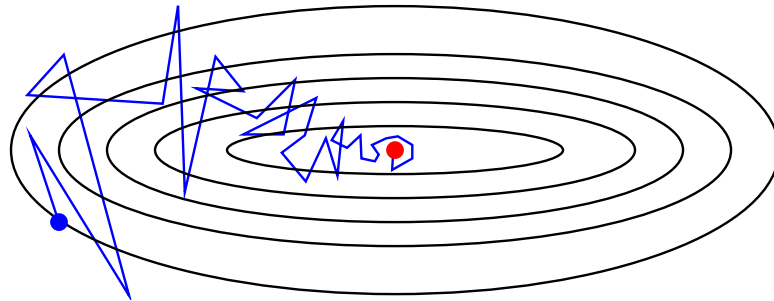
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 - Linear (e.g., exponential) convergence rate
 - Iteration complexity is linear in n
- **Stochastic** gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
 - Sampling with replacement: $i(t)$ random element of $\{1, \dots, n\}$
 - Convergence rate in $O(1/t)$
 - Iteration complexity is independent of n

Stochastic vs. deterministic methods

- Minimizing $g(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$ with $f_i(\theta) = \ell(y_i, \theta^\top \Phi(x_i)) + \mu \Omega(\theta)$
- **Batch** gradient descent: $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1}) = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^n f'_i(\theta_{t-1})$

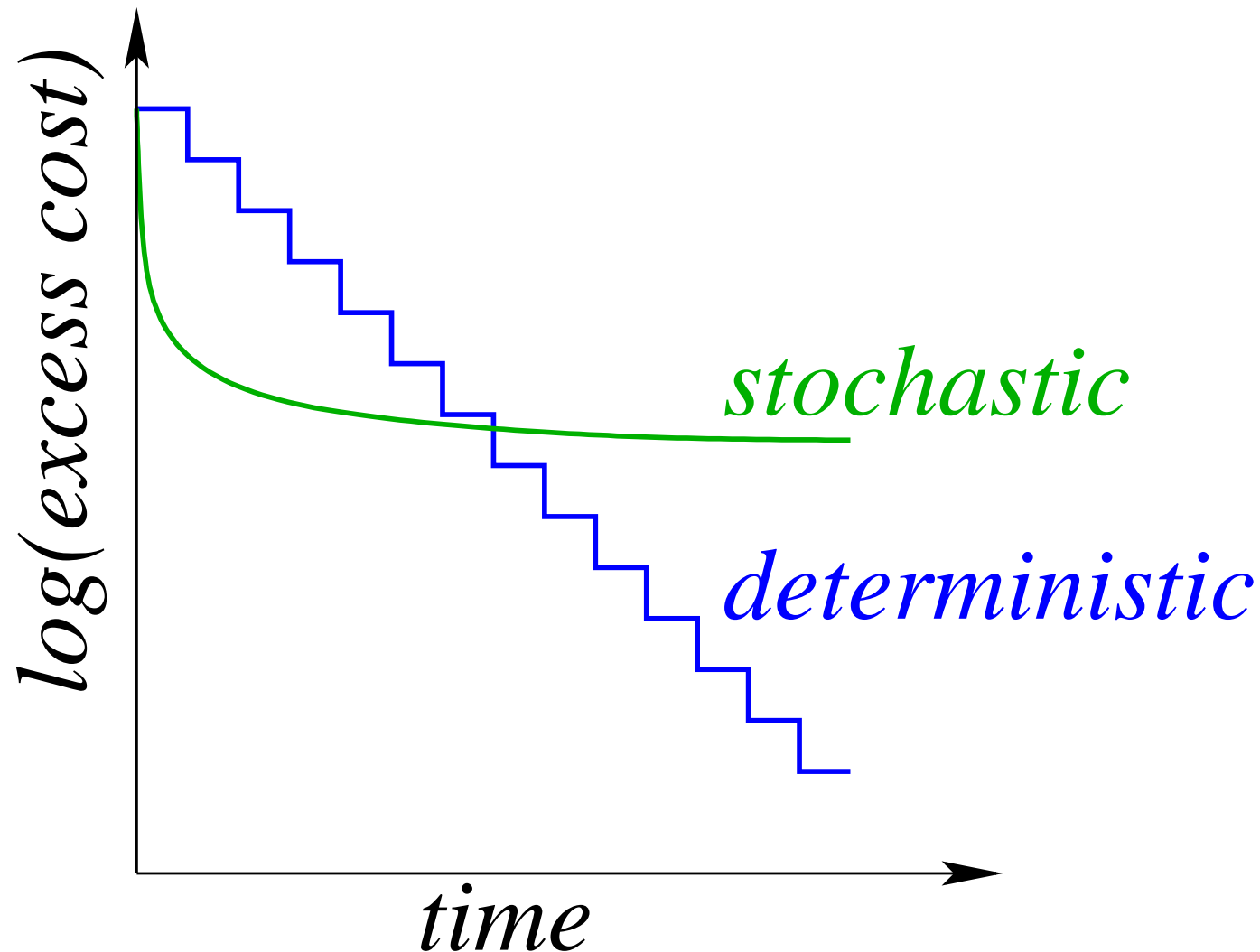


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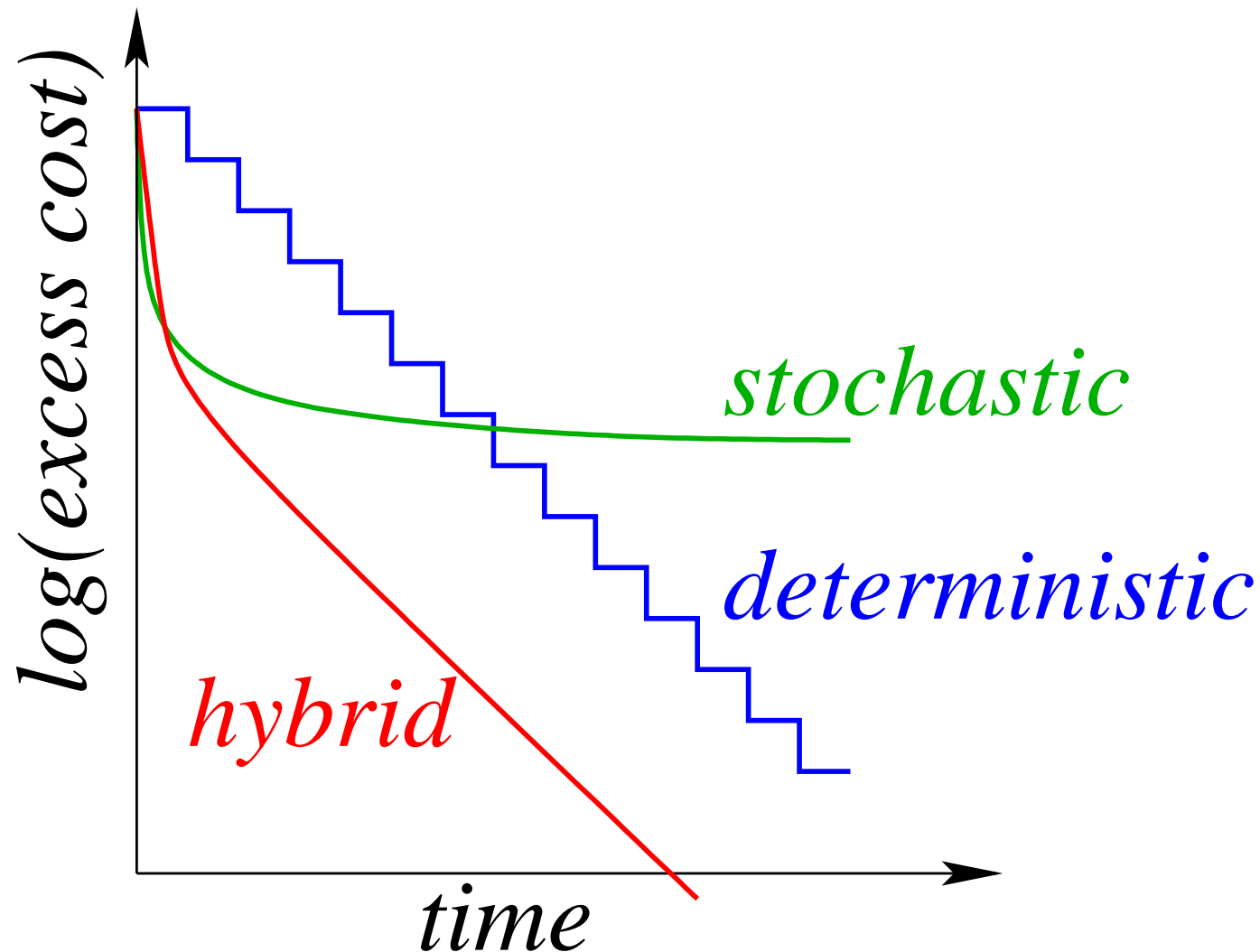
Stochastic vs. deterministic methods

- **Goal** = best of both worlds: linear rate with $O(1)$ iteration cost



Stochastic vs. deterministic methods

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Accelerating gradient methods - Related work

- **Nesterov acceleration**

- Nesterov (1983, 2004)
- Better linear rate but still $O(n)$ iteration cost

- **Hybrid methods, incremental average gradient, increasing batch size**

- Bertsekas (1997); Blatt et al. (2008); Friedlander and Schmidt (2011)
- Linear rate, but iterations make full passes through the data.

Accelerating gradient methods – Related work

- **Momentum, gradient/iterate averaging, stochastic version of accelerated batch gradient methods**
 - Polyak and Juditsky (1992); Tseng (1998); Sunehag et al. (2009); Ghadimi and Lan (2010); Xiao (2010)
 - Can improve constants, but still have sublinear $O(1/t)$ rate
- **Constant step-size stochastic gradient (SG), accelerated SG**
 - Kesten (1958); Delyon and Juditsky (1993); Solodov (1998); Nedic and Bertsekas (2000)
 - Linear convergence, but only up to a fixed tolerance.
- **Stochastic methods in the dual**
 - Shalev-Shwartz and Zhang (2012)
 - Linear rate but limited choice for the f_i 's

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

Stochastic average gradient - Convergence analysis

- **Assumptions**

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

- **Strongly convex case** (Le Roux et al., 2012, 2013)

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

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

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

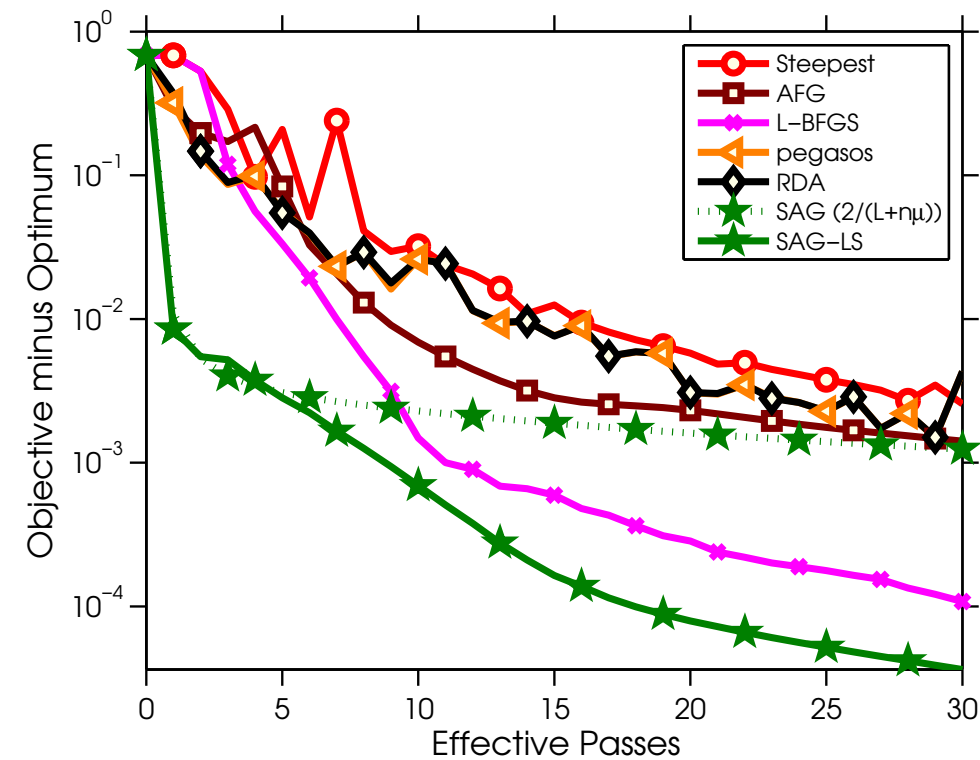
$$\mathbb{E}[g(\theta_t) - g(\theta_*)] \leq 48 \frac{\sigma^2 + L \|\theta_0 - \theta_*\|^2}{\sqrt{n}} \frac{n}{k}$$

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

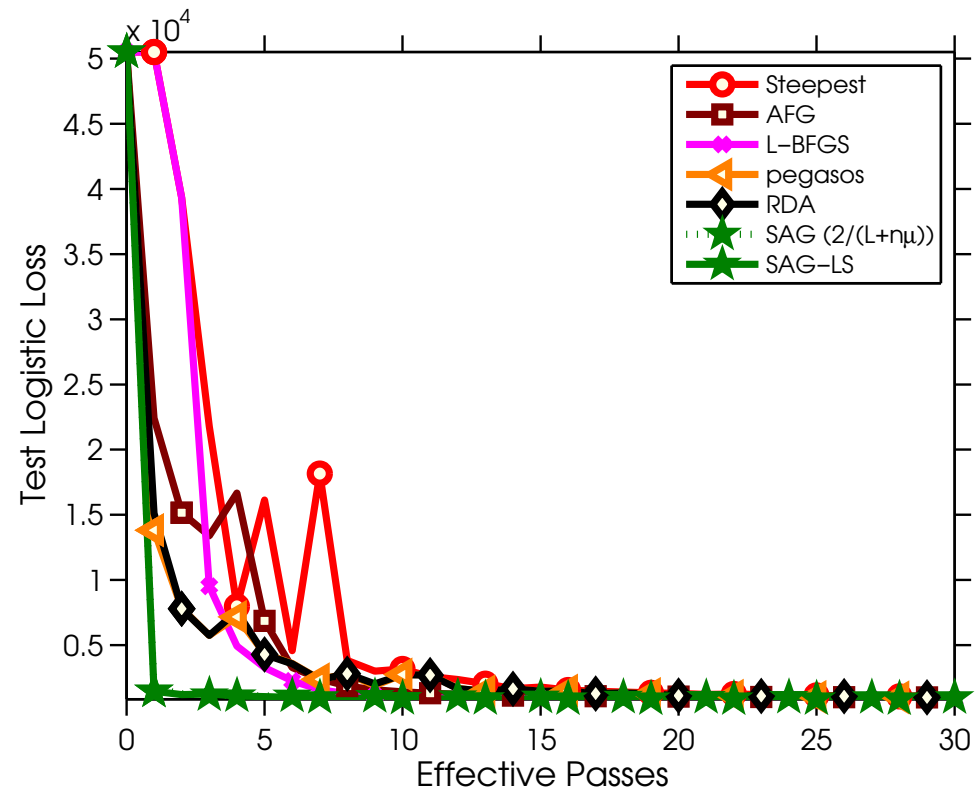
Stochastic average gradient

Simulation experiments

- protein dataset ($n = 145751$, $p = 74$)
- Dataset split in two (training/testing)



Training cost

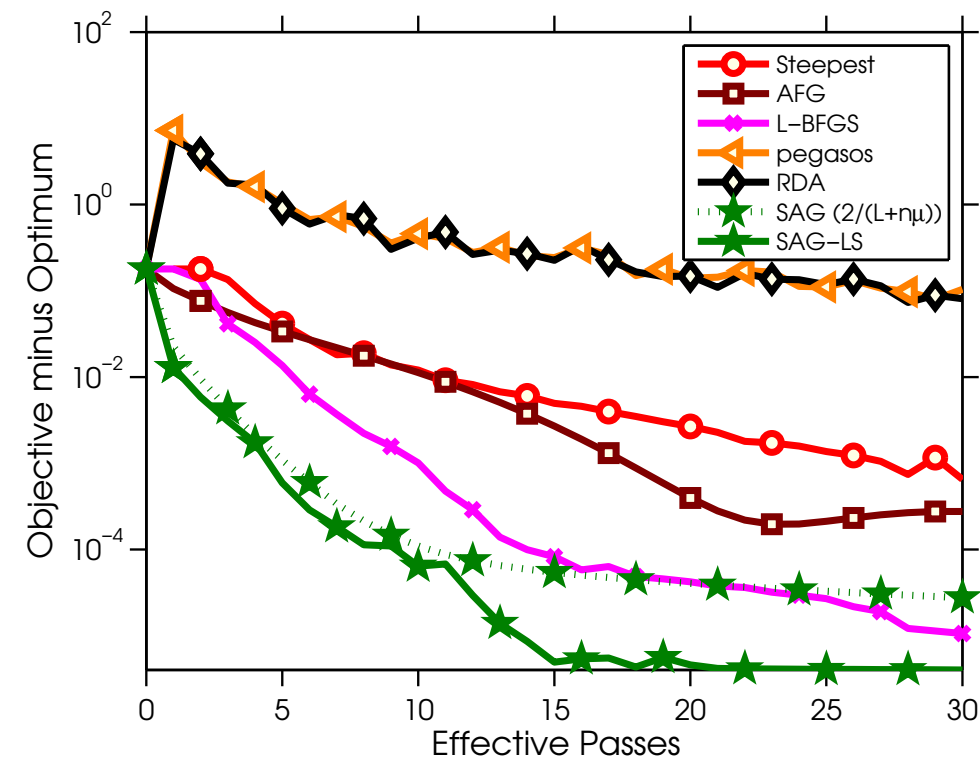


Testing cost

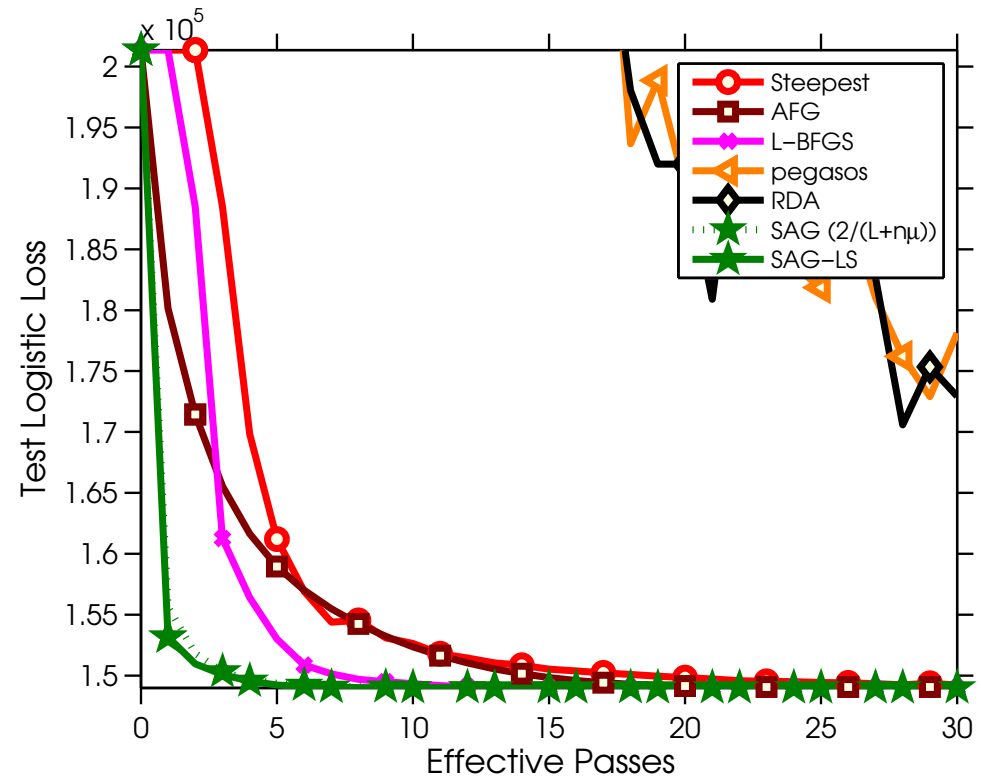
Stochastic average gradient

Simulation experiments

- cover type dataset ($n = 581012$, $p = 54$)
- Dataset split in two (training/testing)



Training cost



Testing cost

Conclusions / Extensions

Stochastic average gradient

- **Going beyond a single pass through the data**
 - Keep memory of all gradients for finite training sets
 - Linear convergence rate with $O(1)$ iteration complexity
 - Randomization leads to easier analysis **and** faster rates
- **Future/current work - open problems**
 - Including a non-differentiable term
 - Line search
 - Using second-order information or non-uniform sampling
 - Distributed optimization
 - Going beyond finite training sets (bound on testing cost)

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