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**: $O(pn + kn)$

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- **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

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

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- Expected risk: $f(\theta) = \mathbb{E}_{(x,y)} \ell(y, \theta^\top \Phi(x))$ testing cost
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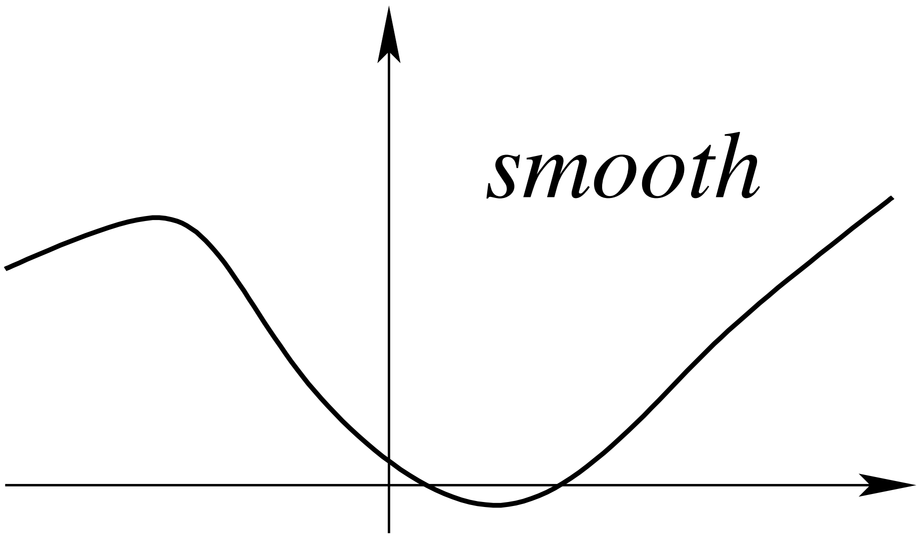
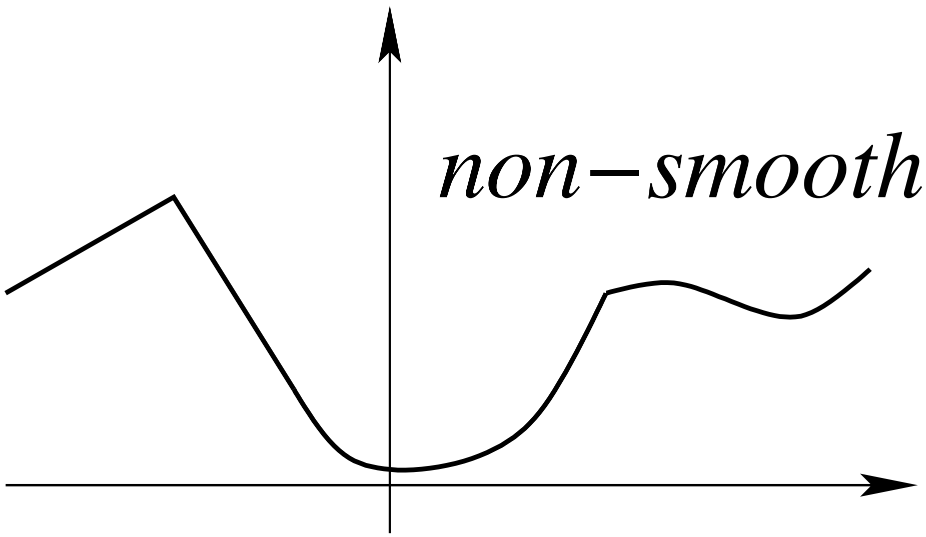
  - **May be tackled simultaneously**

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

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





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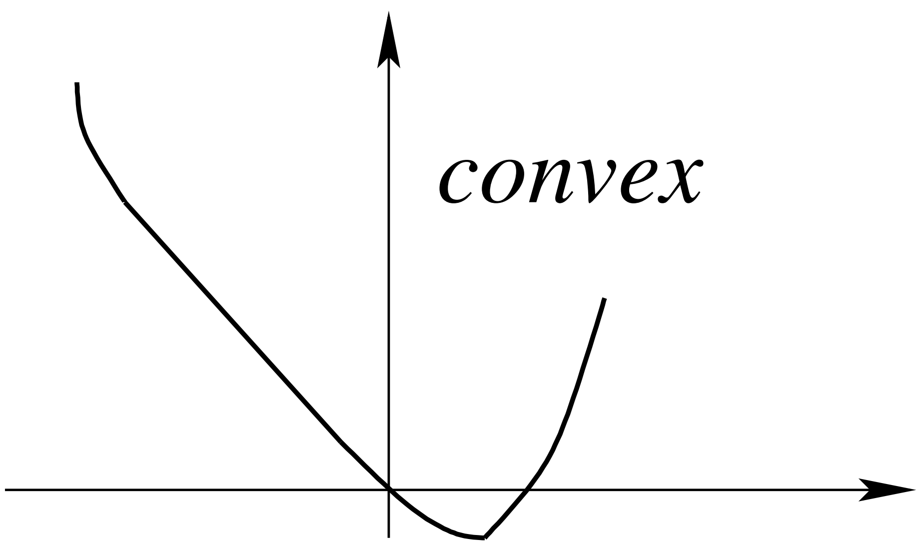
- **Machine learning**
  - with $g(\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \theta^\top \Phi(x_i))$
  - Hessian $\approx$ covariance matrix $\frac{1}{n}\sum_{i=1}^{n} \Phi(x_i)\Phi(x_i)^\top$
  - Bounded data

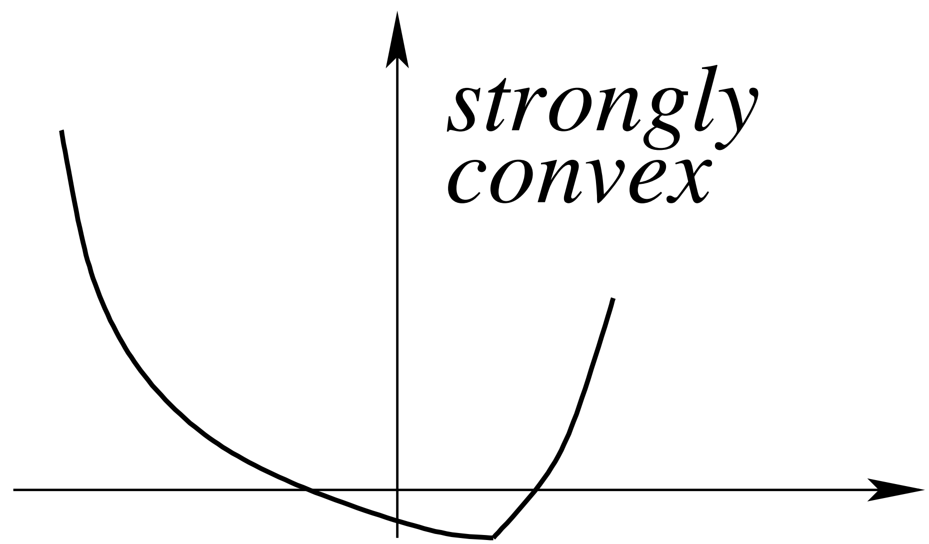
Smoothness and strong convexity

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

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

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





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  - Hessian $\approx$ covariance matrix $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \Phi(x_i)^\top$
  - Data with invertible covariance matrix (low correlation/dimension)
  - ... 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**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ convergence rate

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- **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 ε_n = i.i.d. noise
  - Non-convex problems

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- **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: $f'(\theta) = \mathbb{E} f_n'(\theta) = \mathbb{E}\left\{ \ell'(y_n, \theta^\top \Phi(x_n))\, \Phi(x_n) \right\}$

Convex smooth stochastic approximation

- **Key assumption**: smoothness and/or strongly convexity

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- **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: $\bar{\theta}_n = \frac{1}{n}\sum_{k=0}^{n-1}\theta_k$

  – Which learning rate sequence γ_n? Classical setting: $\boxed{\gamma_n = Cn^{-\alpha}}$

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 $\gamma_n \propto (\mu n)^{-1}$
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- Bottou and Le Cun (2005); Bottou and Bousquet (2008); Hazan et al. (2007); Shalev-Shwartz and Srebro (2008); Shalev-Shwartz et al. (2007, 2009); Xiao (2010); Duchi and Singer (2009); Nesterov and Vial (2008); Nemirovski et al. (2009)

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- **Asymptotic analysis of averaging** (Polyak and Juditsky, 1992; Ruppert, 1988)
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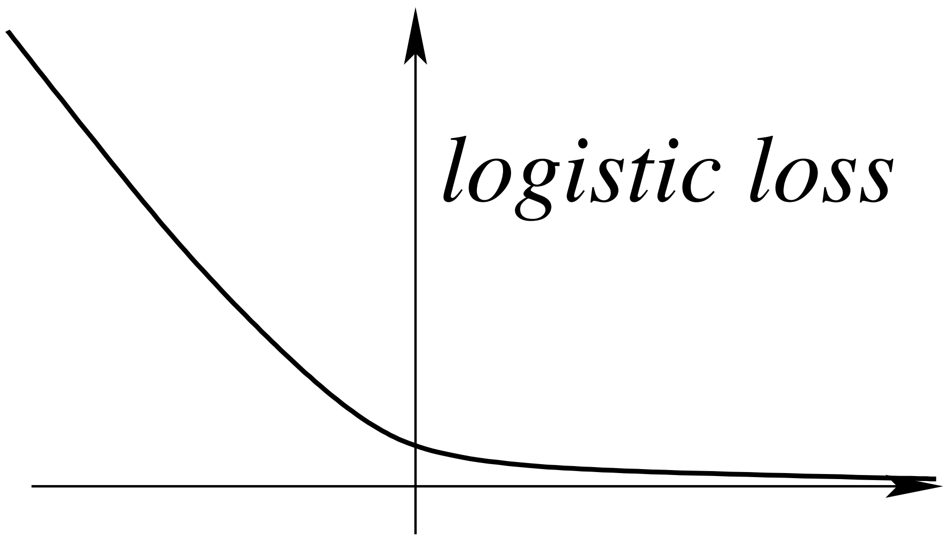
  - **A single algorithm with global convergence rate?**

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 $|\theta^\top x_n| \leqslant M$
  - $\mu =$ lowest eigenvalue of the Hessian at the optimum $f''(\theta_*)$



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

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

  - 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

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- **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 $\mathbb{E}_{(x,y)}\, \ell(y, \theta^\top \Phi(x))$

Going beyond a single pass over the data

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- **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 $f_i(\theta) = \ell\big(y_i, \theta^\top \Phi(x_i)\big) + \mu\Omega(\theta)$

- Batch gradient descent: $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1}) = \theta_{t-1} - \frac{\gamma_t}{n}\sum_{i=1}^{n} f_i'(\theta_{t-1})$

  – Linear (e.g., exponential) convergence rate

  – Iteration complexity is linear in n

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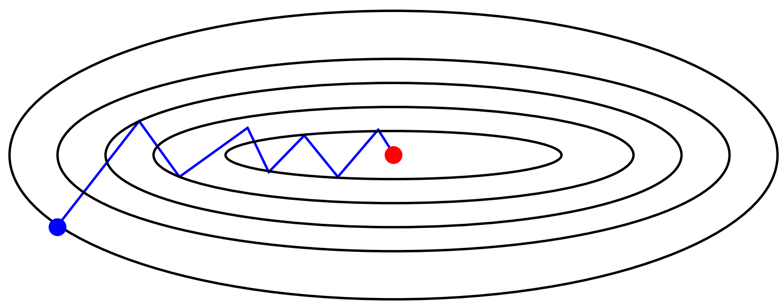

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- Stochastic gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
  - Sampling with replacement: $i(t)$ random element of $\{1, \dots, n\}$
  - Convergence rate in $O(1/t)$
  - Iteration complexity is independent of n

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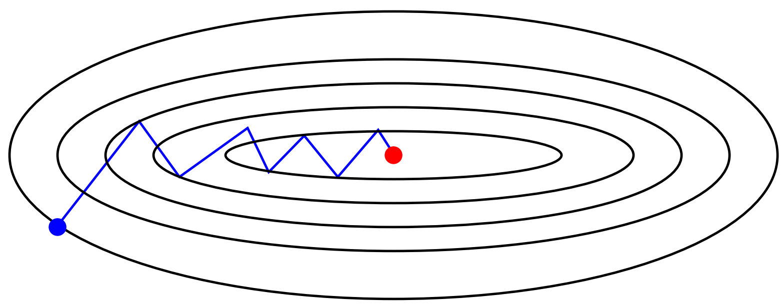

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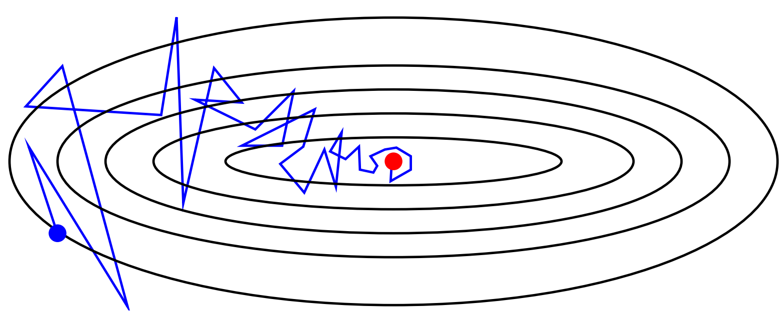

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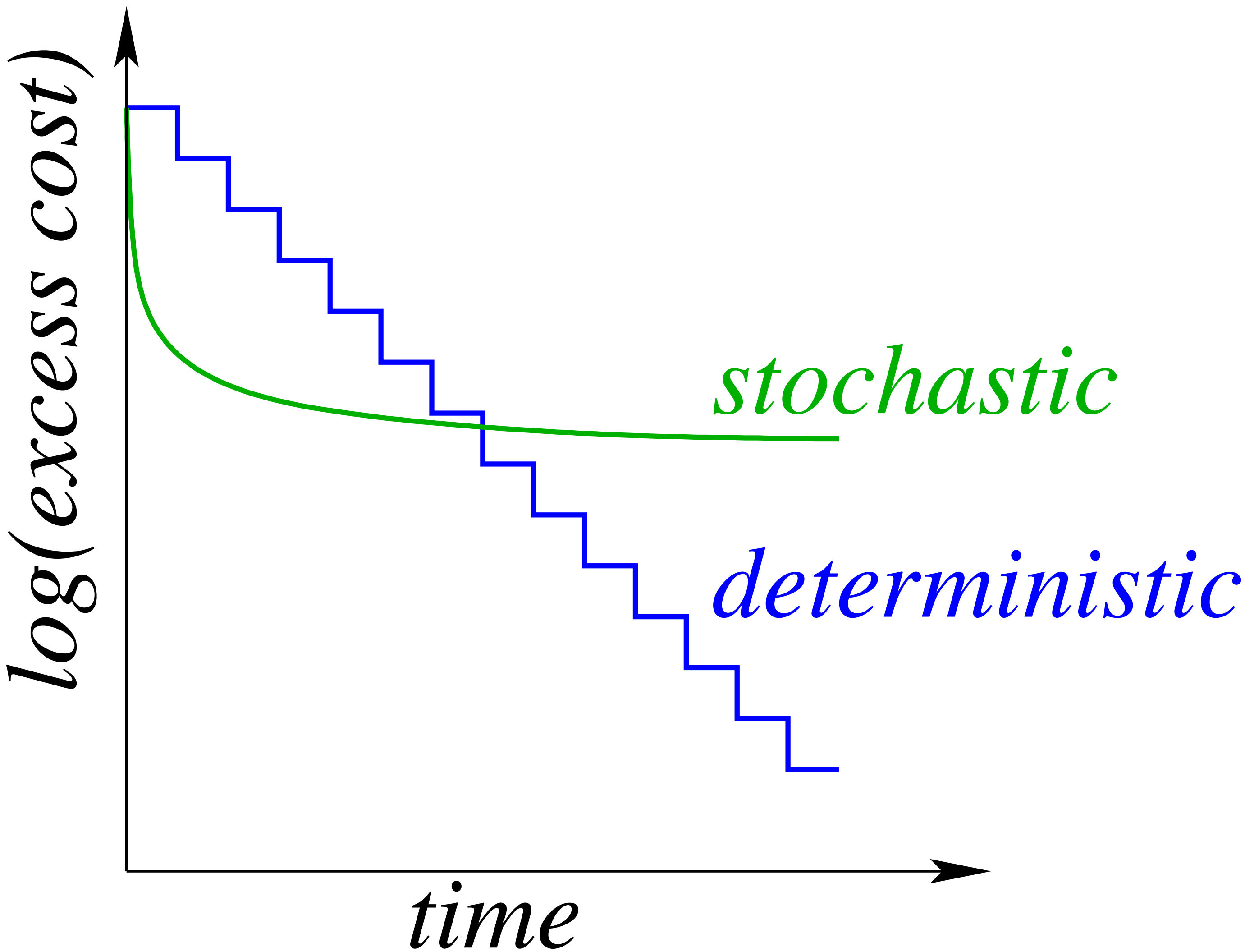

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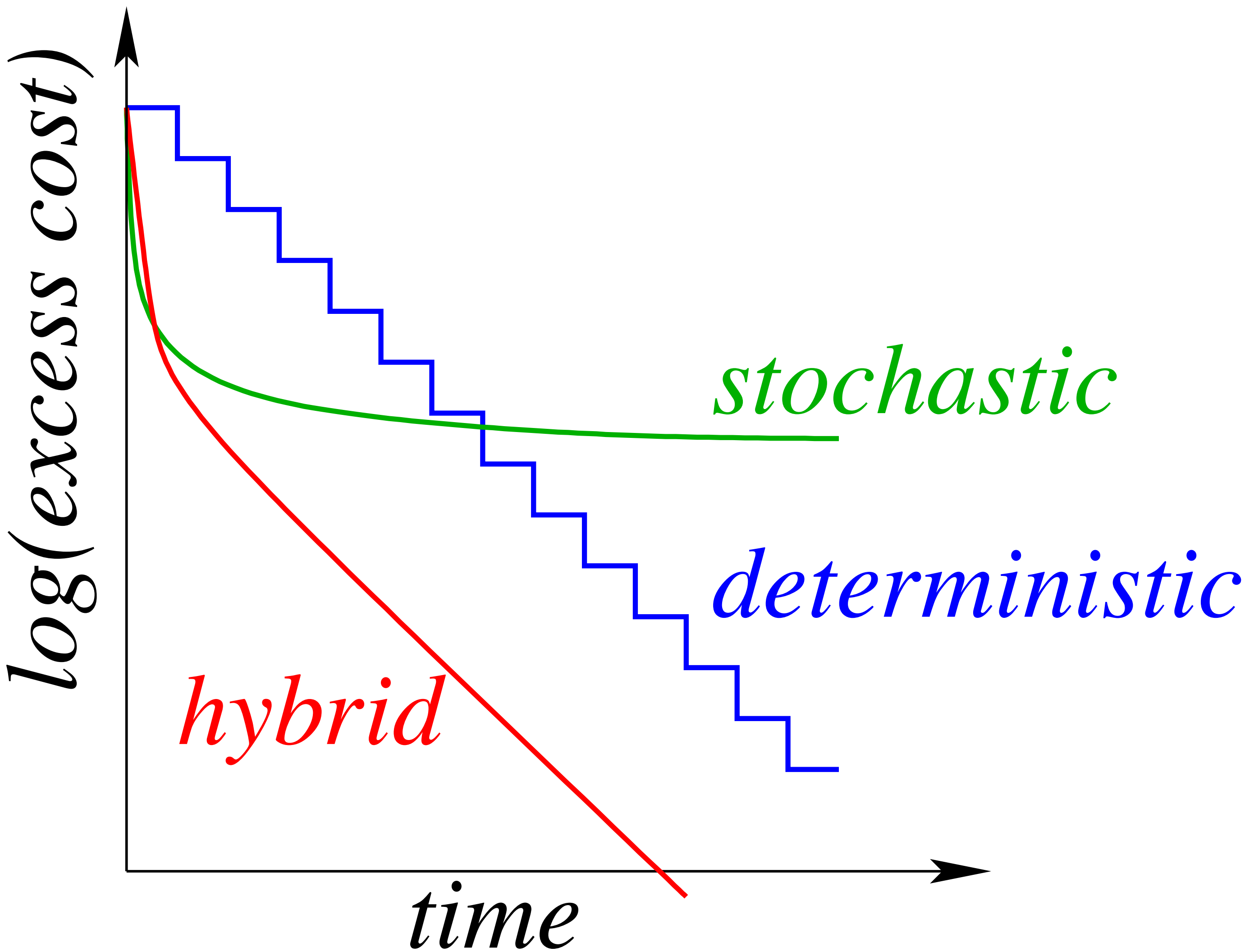

Accelerating gradient methods - Related work

- **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 $y_i^t = \begin{cases} f_i'(\theta_{t-1}) & \text{if } i = i(t) \\ y_i^{t-1} & \text{otherwise} \end{cases}$

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- Stochastic version of incremental average gradient (Blatt et al., 2008)

- Extra memory requirement
  - Supervised machine learning
    - If $f_i(\theta) = \ell_i(y_i, \Phi(x_i)^\top \theta)$, then $f_i'(\theta) = \ell_i'(y_i, \Phi(x_i)^\top \theta)\, \Phi(x_i)$
    - Only need to store n real numbers

Stochastic average gradient - Convergence analysis

- **Assumptions**
  - Each f_i is 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

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

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

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

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

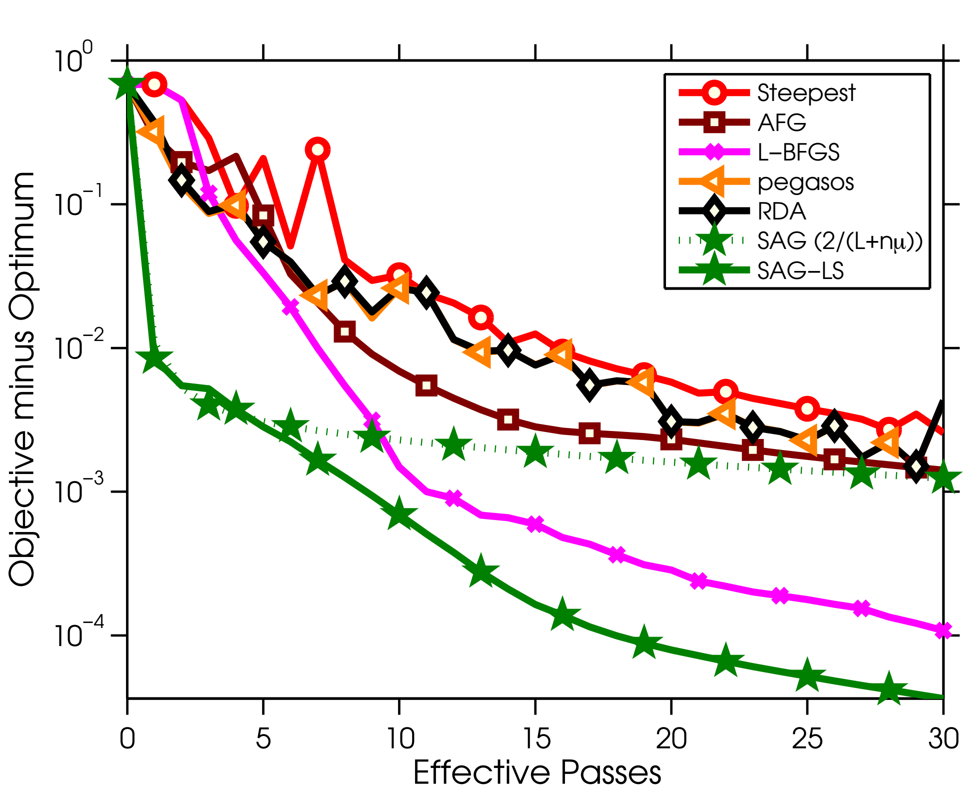
$$\mathbb{E}\big[g(\theta_t) - g(\theta_*)\big] \leqslant 48 \frac{\sigma^2 + L\|\theta_0 - \theta_*\|^2}{\sqrt{n}} \frac{n}{k}$$

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

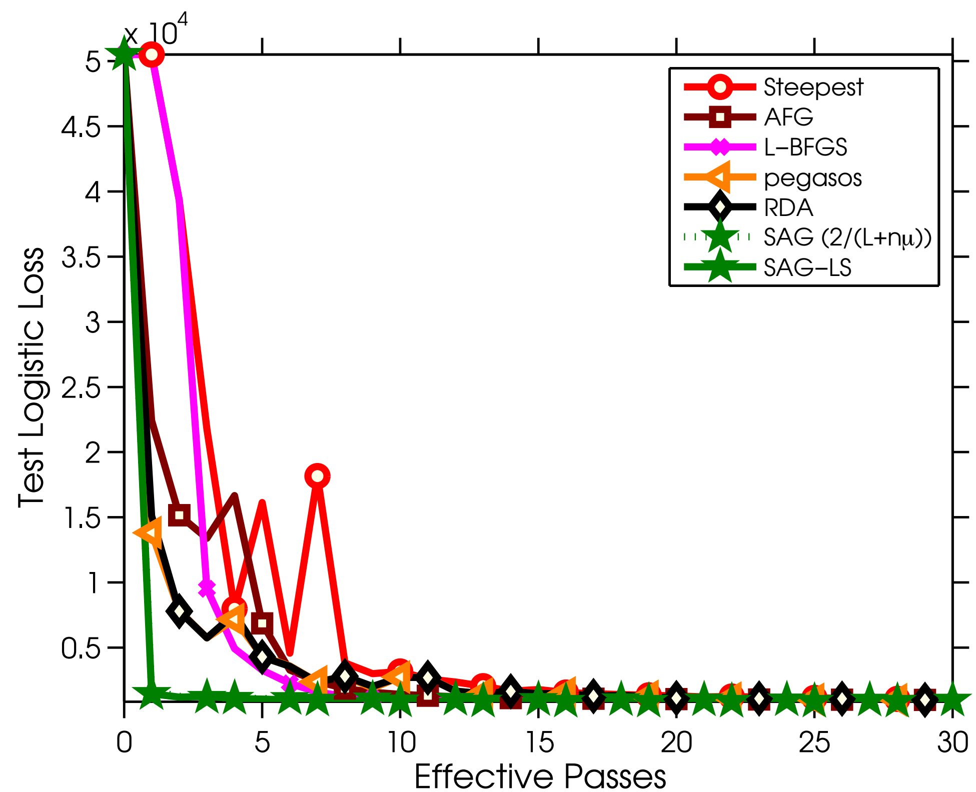
Stochastic average gradient
Simulation experiments

- `protein` dataset ($n = 145751$, $p = 74$)

- Dataset split in two (training/testing)



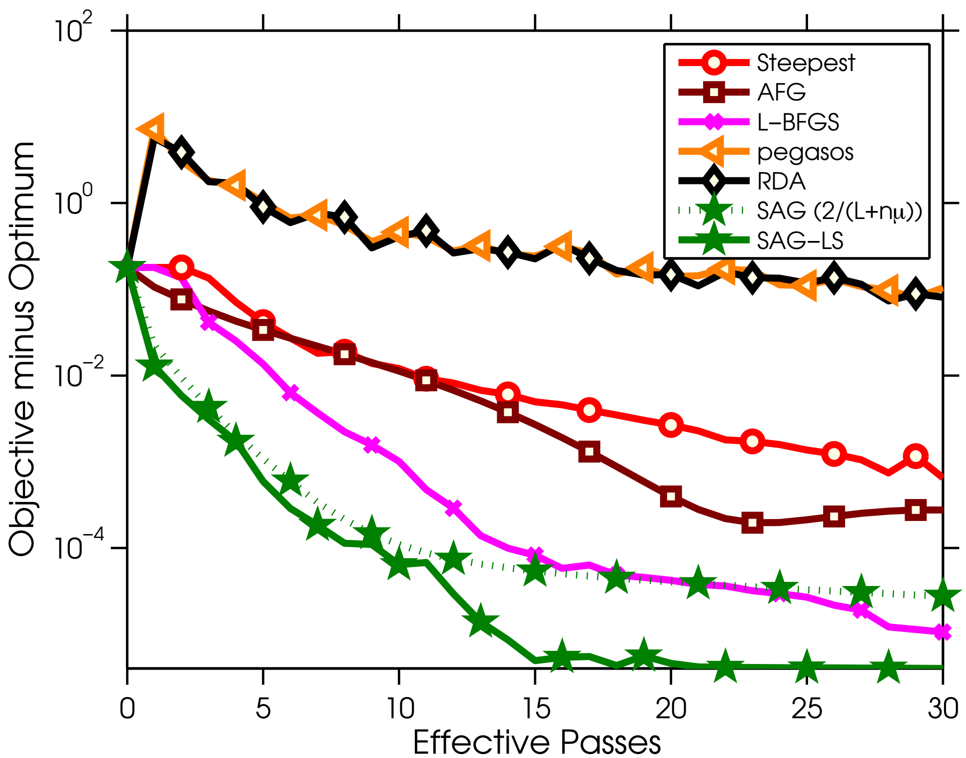
Training cost



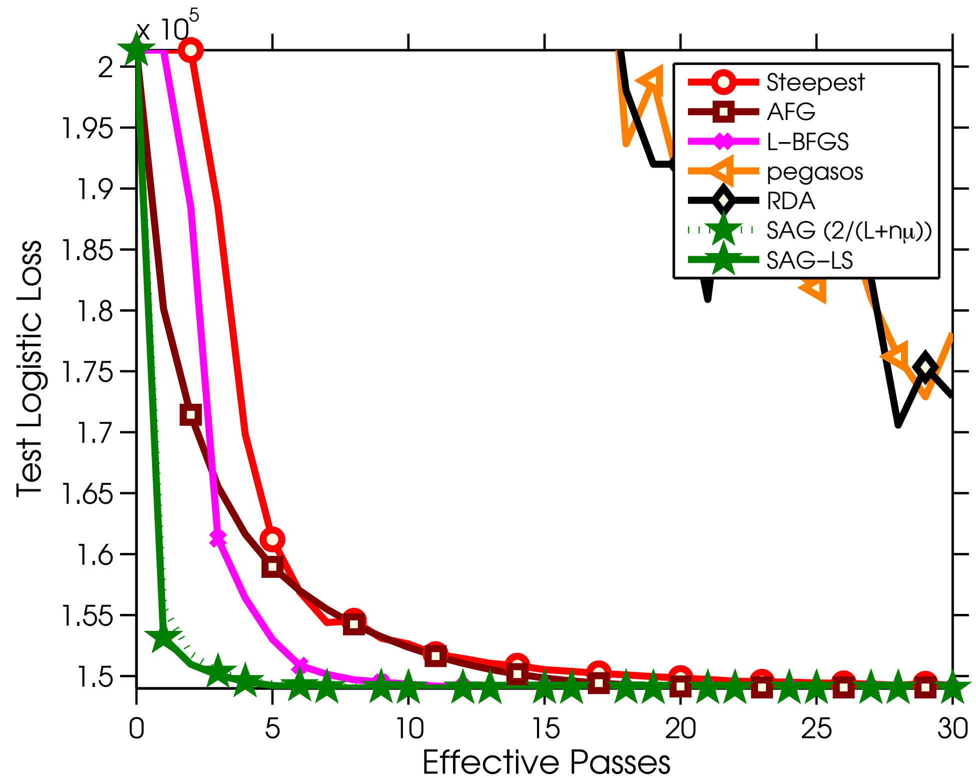
Testing cost

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
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  - Randomization leads to easier analysis and faster rates

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- **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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