

# Stochastic optimization: Beyond stochastic gradients and convexity

## Part I

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# Context

## Machine learning for large-scale data

- **Large-scale supervised machine learning:** **large  $d$ , large  $n$** 
  - $d$  : dimension of each observation (input) or number of parameters
  - $n$  : number of observations
- **Examples:** computer vision, advertising, bioinformatics, **etc.**

# Search engines - Advertising - Marketing

The image shows a screenshot of a web browser displaying a Bing search results page for the query "tour de france". The browser's address bar shows the URL: <https://www.bing.com/search?q=tour+de+france&go=Submit&qsn=n&form=QBRE&filt=all&pq=tour+de+france&sc=8>. The search bar contains the text "tour de france".

The search results show 121,000,000 results. The top result is "Tour de France 2014" from [www.letour.fr](http://www.letour.fr). The snippet for this result reads: "tour de picardie 2014 - ... ag2r la mondiale; astana pro team; bigmat - auber 93; bmc racing team; bretagne - seche environnement".

Below the top result are several sub-sections:

- Parcours**: Du samedi 29 juin au dimanche 21 juillet 2013, le 100 e Tour de ...
- Classements**: Classements - Tour de France 2013. Tour de France 2013 - Site officiel ...
- Nice 2013**: Tour de France 2012 - Site officiel de la célèbre course cycliste Le Tour ...
- Tour de France 2011**: Tour de France 2014 - Site officiel de la célèbre course cycliste Le Tour ...
- Étape 14**: Étape 14 - Saint-Pourçain-sur-Sioule > Lyon - Tour de ...
- Étape 18**: Étape 18 - Gap > Alpe-d'Huez - Tour de France 2013

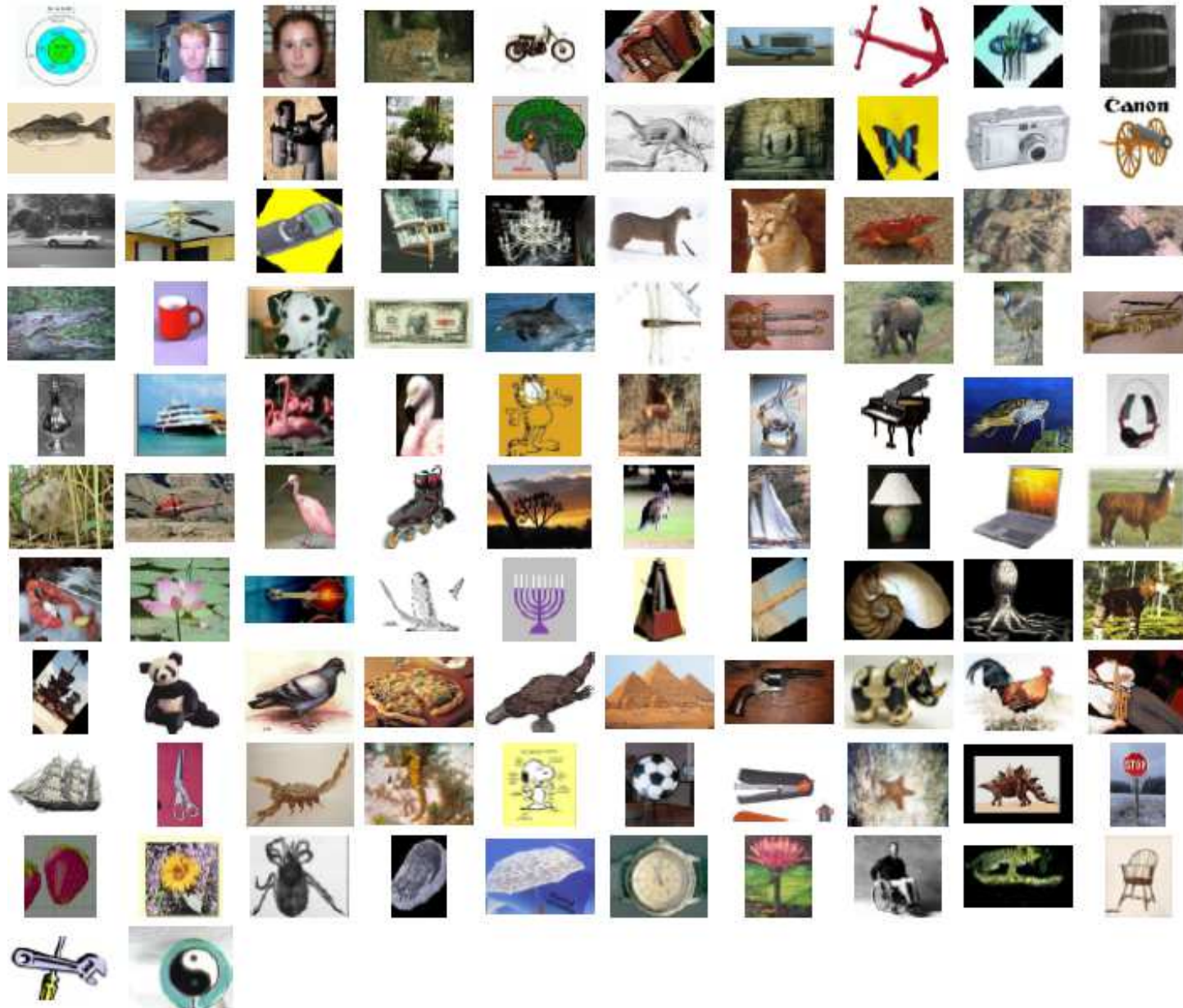
On the right side of the page, there is a "Related searches" section with the following links:

- Tracé Tour de France 2014
- Regarder Tour de France Direct
- Classement Général Tour de France
- Itinéraire Tour de France
- Étape Du Tour
- France 2
- Tour de France Cyclisme
- Tour de France Online

At the bottom of the page, there is another result for "Tour de France 2013" from [www.letour.fr/le-tour/2013/fr](http://www.letour.fr/le-tour/2013/fr). The snippet reads: "Tour de France 2013 - Site officiel de la célèbre course cycliste Le Tour de France. Contient les itinéraires, coureurs, équipes et les infos des Tours passés."

Finally, there is a result for "Tour de France (cyclisme) — Wikipédia" from [fr.wikipedia.org/wiki/Tour\\_de\\_France\\_\(cyclisme\)](http://fr.wikipedia.org/wiki/Tour_de_France_(cyclisme)). The snippet reads: "Le Tour de France est une compétition cycliste par étapes créée en 1903 par Henri Desgrange et Géo Lefèvre, chef de la rubrique cyclisme du journal L'Auto. Histoire · Médiatisation du ... · Équipes et participation".

# Visual object recognition



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- **Ideal running-time complexity:**  $O(dn)$
- **Going back to simple methods**
  - Stochastic gradient methods (Robbins and Monro, 1951)
- **Goal: Present recent progress**

# Outline

## 1. Introduction/motivation: Supervised machine learning

- Optimization of finite sums
- Existing optimization methods for finite sums

## 2. Convex finite-sum problems

- Linearly-convergent stochastic gradient method
- SAG, SAGA, SVRG, SDCA, MISO, etc.
- From lazy gradient evaluations to variance reduction

## 3. Non-convex problems

## 4. Parallel and distributed settings

## 5. Perspectives

# References

- **Textbooks and tutorials**

- Nesterov (2004): *Introductory lectures on convex optimization*
- Bubeck (2015): *Convex Optimization: Algorithms and Complexity*
- Bertsekas (2016): *Nonlinear programming*
- Bottou et al. (2016): *Optimization methods for large-scale machine learning*

- **Research papers**

- See end of slides
- Slides available at [www.ens.fr/~fbach/](http://www.ens.fr/~fbach/)



# Parametric supervised machine learning

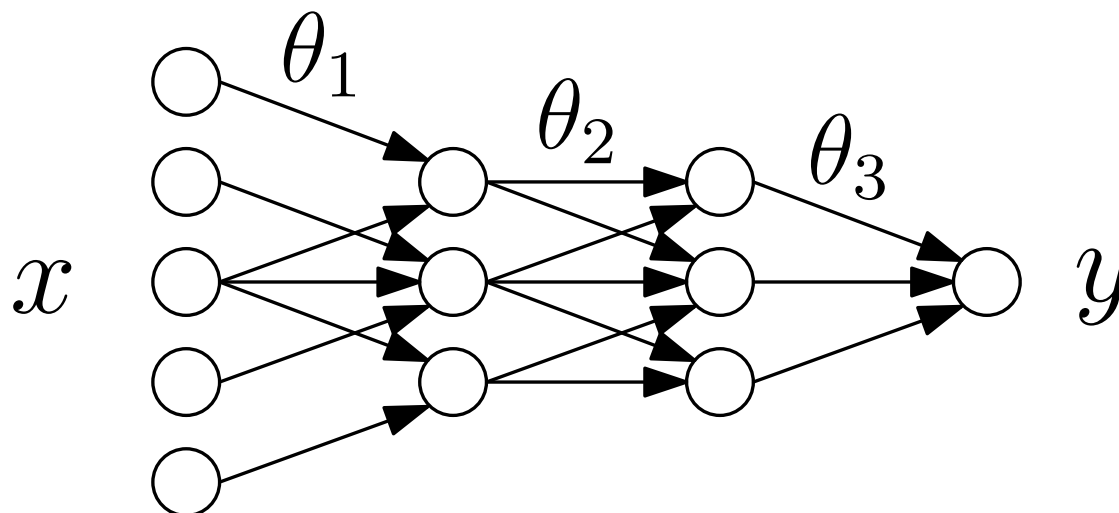
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  - Neural networks:  $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\dots \theta_2^\top \sigma(\theta_1^\top x))$



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- **(regularized) empirical risk minimization:** find  $\hat{\theta}$  solution of

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

data fitting term + regularizer

# Usual losses

- **Regression:**  $y \in \mathbb{R}$ 
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- **Structured prediction**
  - Complex outputs  $y$  ( $k$  classes/labels, graphs, trees, or  $\{0, 1\}^k$ , etc.)
  - Prediction function  $h(x, \theta) \in \mathbb{R}^k$
  - Conditional random fields (Lafferty et al., 2001)
  - Max-margin (Taskar et al., 2003; Tsochantaridis et al., 2005)

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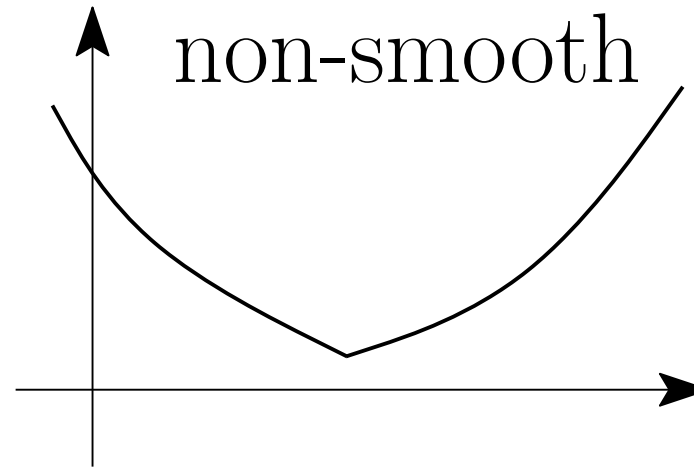
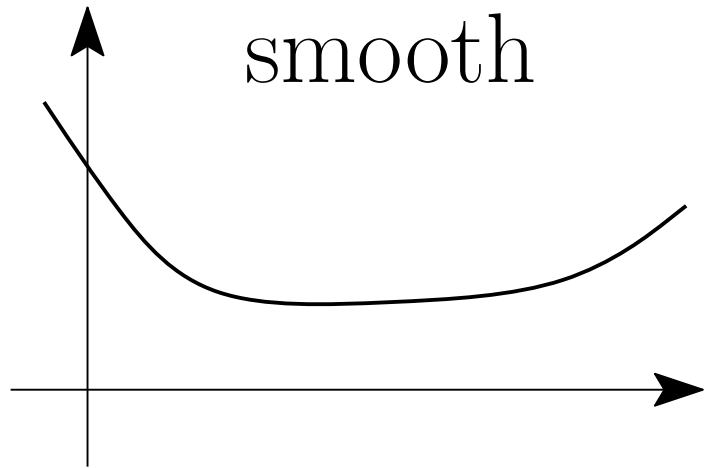
data fitting term + regularizer

- **Optimization:** optimization of regularized risk      training cost
- **Statistics:** guarantees on  $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$       testing cost

# Smoothness and (strong) convexity

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

$$\forall \theta \in \mathbb{R}^d, |\text{eigenvalues}[g''(\theta)]| \leq L$$



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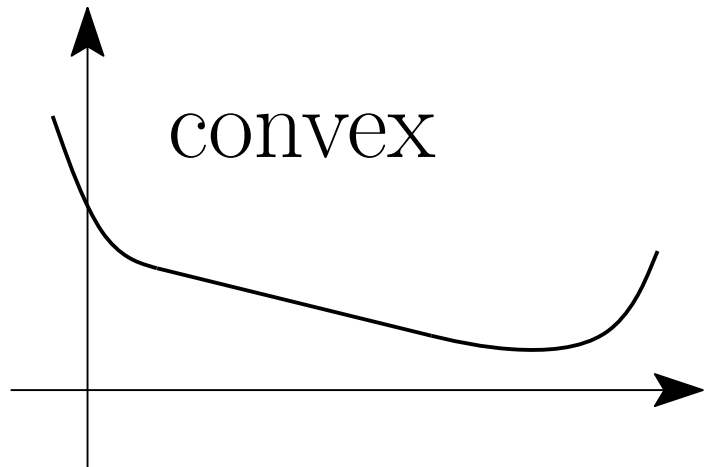
- **Machine learning**

- with  $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
- Smooth prediction function  $\theta \mapsto h(x_i, \theta) + \text{smooth loss}$

# Smoothness and (strong) convexity

- A twice differentiable function  $g : \mathbb{R}^d \rightarrow \mathbb{R}$  is **convex** if and only if

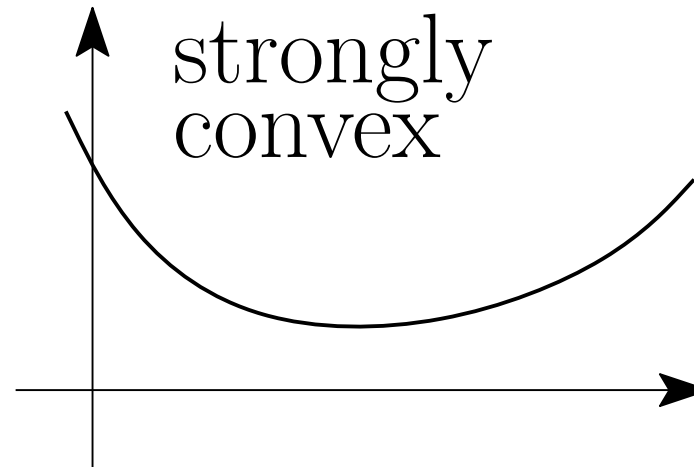
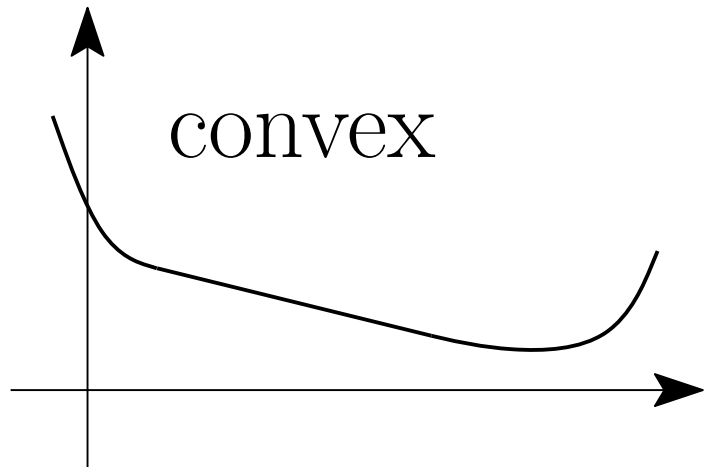
$$\forall \theta \in \mathbb{R}^d, \text{ eigenvalues}[g''(\theta)] \geq 0$$



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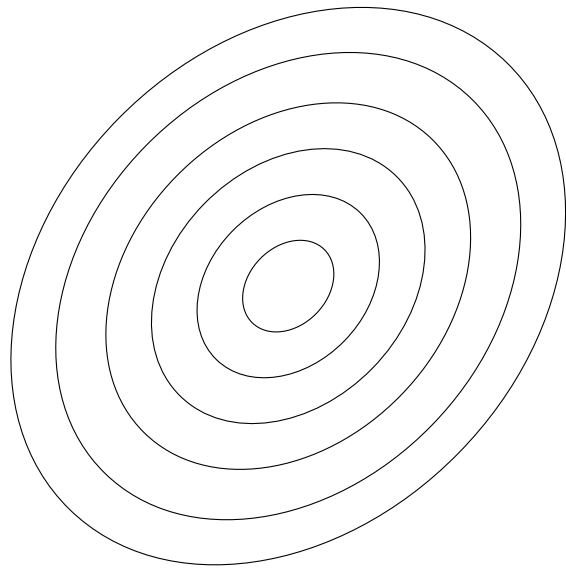


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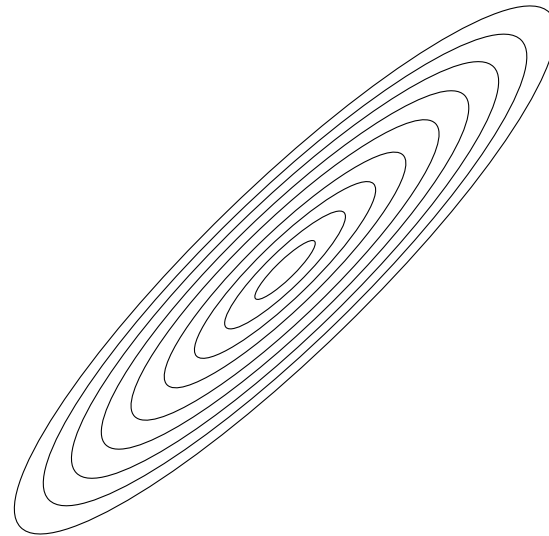
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- Condition number  $\kappa = L/\mu \geq 1$



(small  $\kappa = L/\mu$ )



(large  $\kappa = L/\mu$ )



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- **Convexity in machine learning**

- With  $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
- Convex loss and linear predictions  $h(x, \theta) = \theta^\top \Phi(x)$

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- **Relevance of convex optimization**

- Easier design and analysis of algorithms
- Global minimum vs. local minimum vs. stationary points
- Gradient-based algorithms only need convexity for their analysis

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- **Strong convexity in machine learning**

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- Invertible covariance matrix  $\frac{1}{n} \sum_{i=1}^n \Phi(x_i) \Phi(x_i)^\top \Rightarrow n \geq d$
- Even when  $\mu > 0$ ,  $\mu$  may be arbitrarily small!

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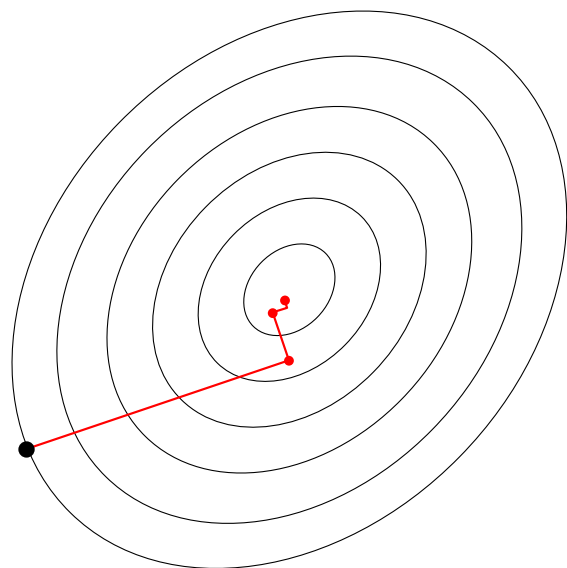
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- **Adding regularization by  $\frac{\mu}{2} \|\theta\|^2$**

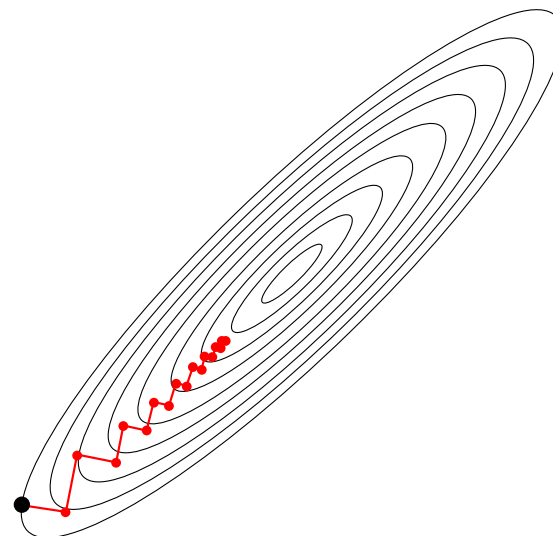
- creates additional bias unless  $\mu$  is small, but reduces variance
- Typically  $L/\sqrt{n} \geq \mu \geq L/n$

# 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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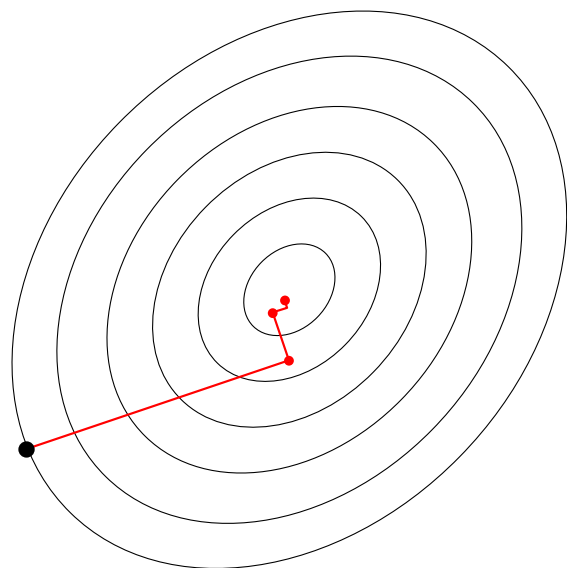
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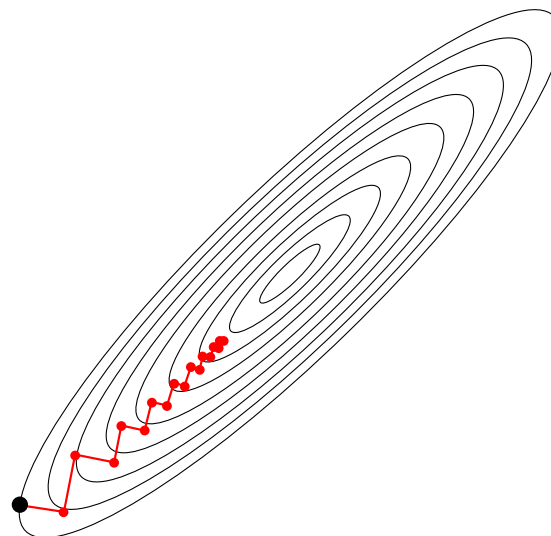
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$$g(\theta_t) - g(\theta_*) \leq O(1/t)$$

$$g(\theta_t) - g(\theta_*) \leq O((1 - \mu/L)^t) = O(e^{-t(\mu/L)}) \text{ if } \mu\text{-strongly convex}$$



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  - $O(1/t)$  convergence rate for convex functions
  - $O(e^{-t/\kappa})$  *linear* if strongly-convex
- **Newton method:**  $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1}g'(\theta_{t-1})$ 
  - $O(e^{-\rho 2^t})$  *quadratic* rate



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  - $O(e^{-\rho 2^t})$  *quadratic* rate  $\Leftrightarrow$  **complexity** =  $O((nd^2 + d^3) \cdot \log \log \frac{1}{\epsilon})$

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  1. No need to optimize below statistical error
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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:**  $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$ 
  - Sampling with replacement:  $i(t)$  random element of  $\{1, \dots, n\}$
  - Polyak-Ruppert averaging:  $\bar{\theta}_t = \frac{1}{t+1} \sum_{u=0}^t \theta_u$

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  - Polyak-Ruppert averaging:  $\bar{\theta}_t = \frac{1}{t+1} \sum_{u=0}^t \theta_u$
- **Convergence rate** if each  $f_i$  is convex  $L$ -smooth and  $g$   $\mu$ -strongly-convex:

$$\mathbb{E}g(\bar{\theta}_t) - g(\theta_*) \leq \begin{cases} O(1/\sqrt{t}) & \text{if } \gamma_t = 1/(L\sqrt{t}) \\ O(L/(\mu t)) = O(\kappa/t) & \text{if } \gamma_t = 1/(\mu t) \end{cases}$$

- No adaptivity to strong-convexity in general
- Adaptivity with self-concordance assumption (Bach, 2014)
- Running-time complexity:  $O(d \cdot \kappa/\varepsilon)$

# Outline

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## 2. Convex finite-sum problems

- Linearly-convergent stochastic gradient method
- SAG, SAGA, SVRG, SDCA, etc.
- From lazy gradient evaluations to variance reduction

## 3. Non-convex problems

## 4. Parallel and distributed settings

## 5. Perspectives

## Stochastic vs. deterministic methods

- Minimizing  $g(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$  with  $f_i(\theta) = \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta)$

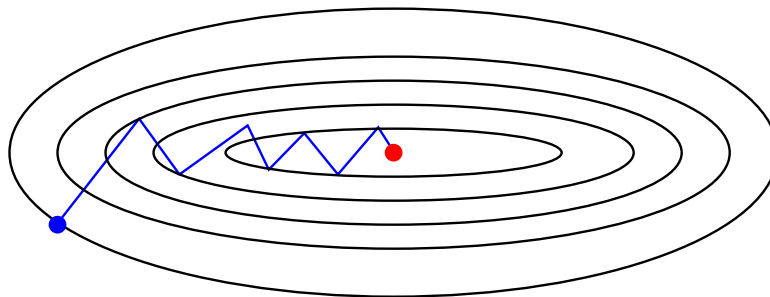


# Stochastic vs. deterministic methods

- Minimizing  $g(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$  with  $f_i(\theta) = \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta)$
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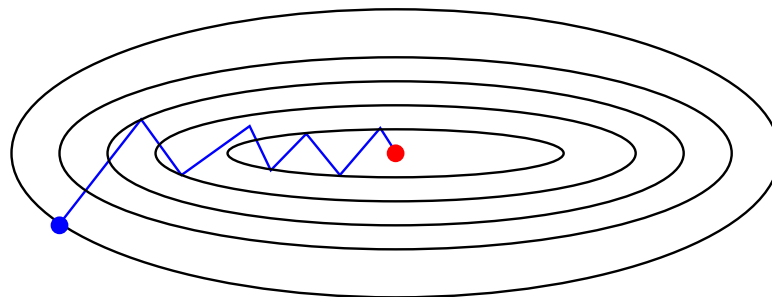


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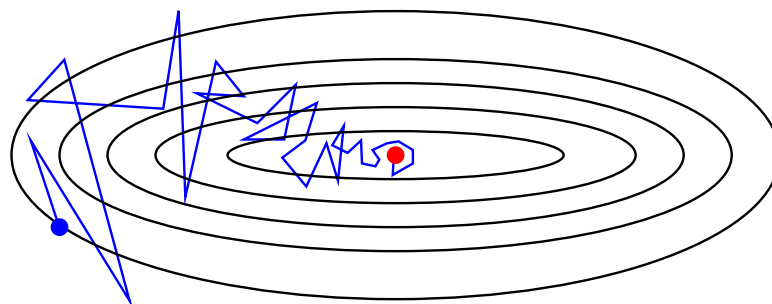
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  - Sampling with replacement:  $i(t)$  random element of  $\{1, \dots, n\}$
  - Convergence rate in  $O(\kappa/t)$
  - Iteration complexity is independent of  $n$

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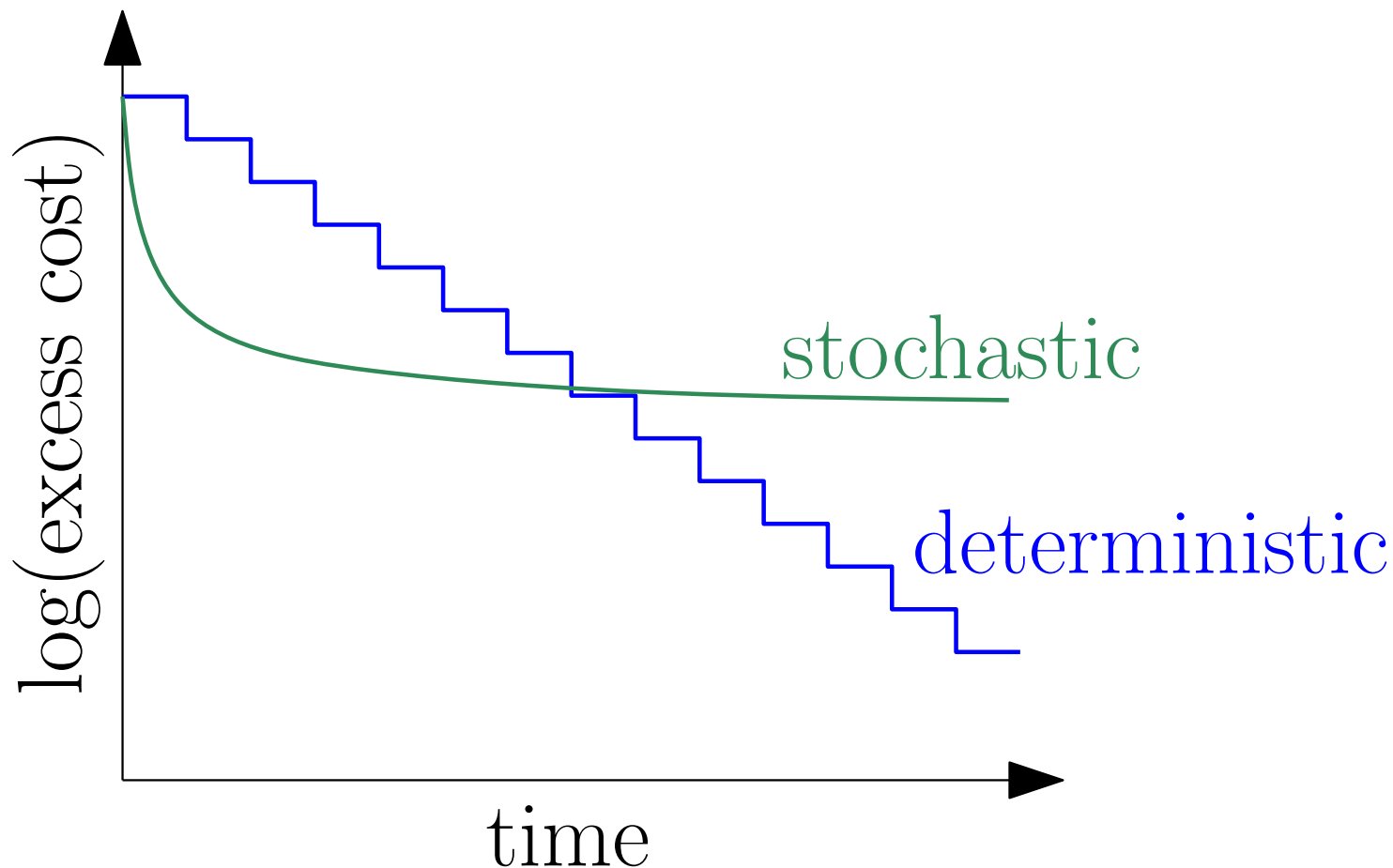


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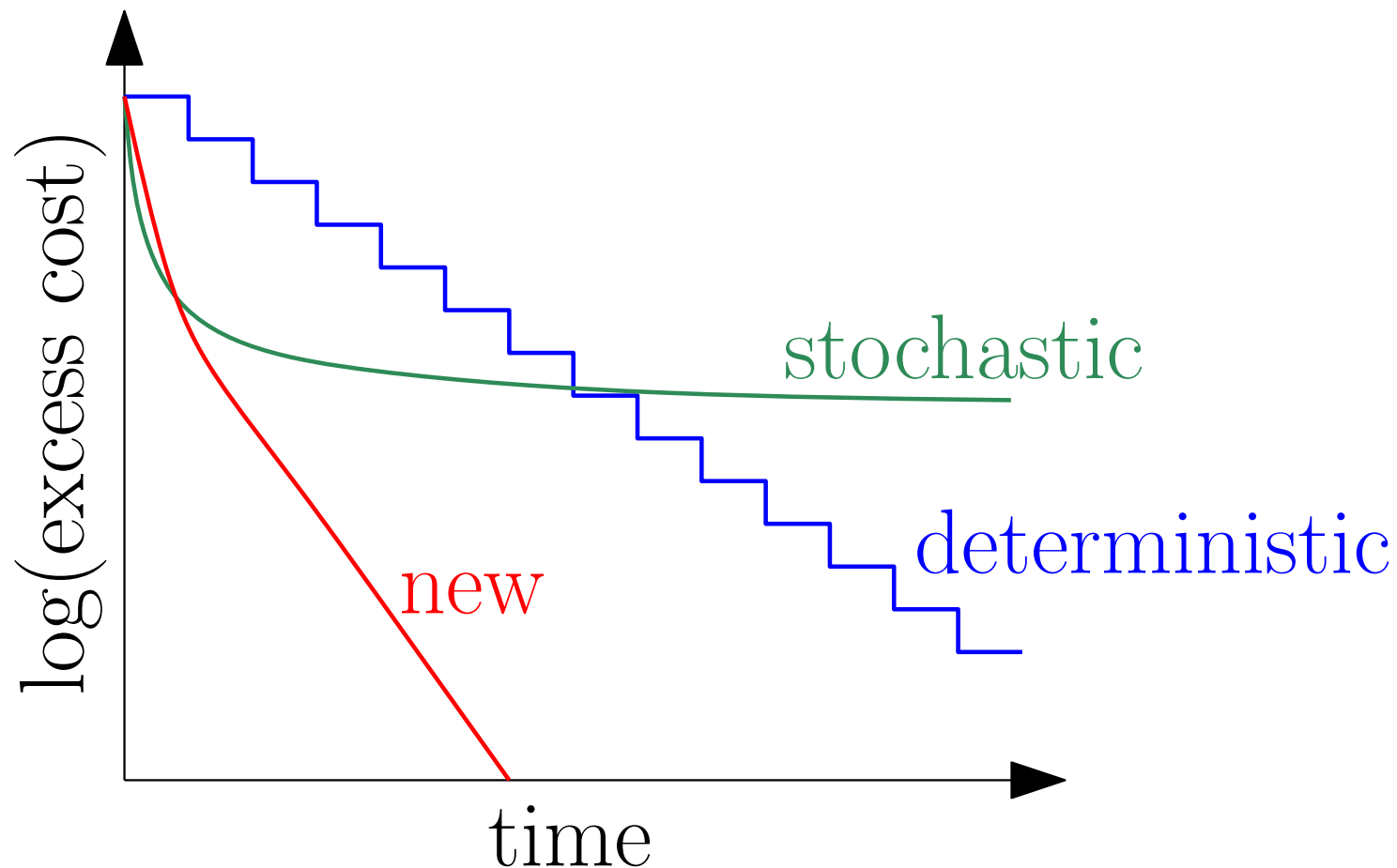
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Simple choice of step size



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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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$$g(\theta_t) - g(\theta_*) \leq O(1/t^2)$$

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- Still  $O(nd)$  iteration cost: complexity =  $O(nd \cdot \sqrt{\kappa} \log \frac{1}{\epsilon})$

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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  $f_i, i = 1, \dots, n$
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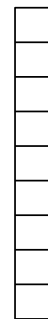
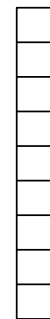
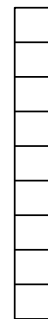
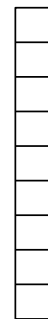
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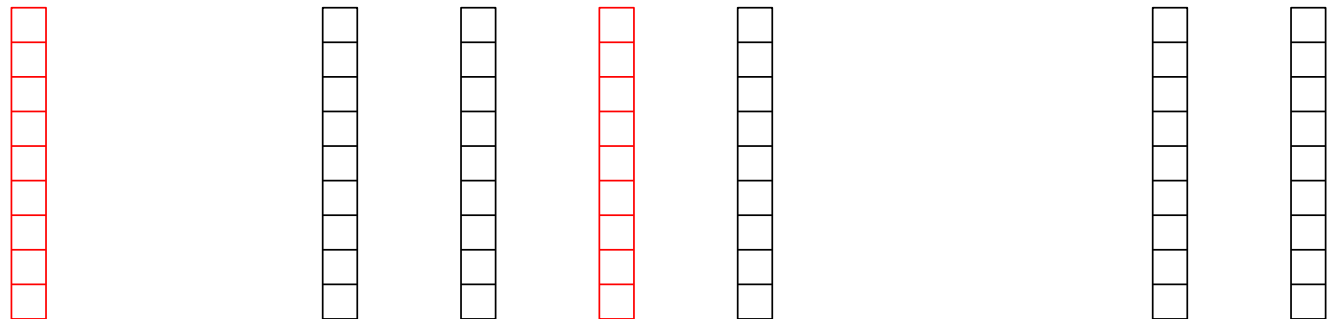
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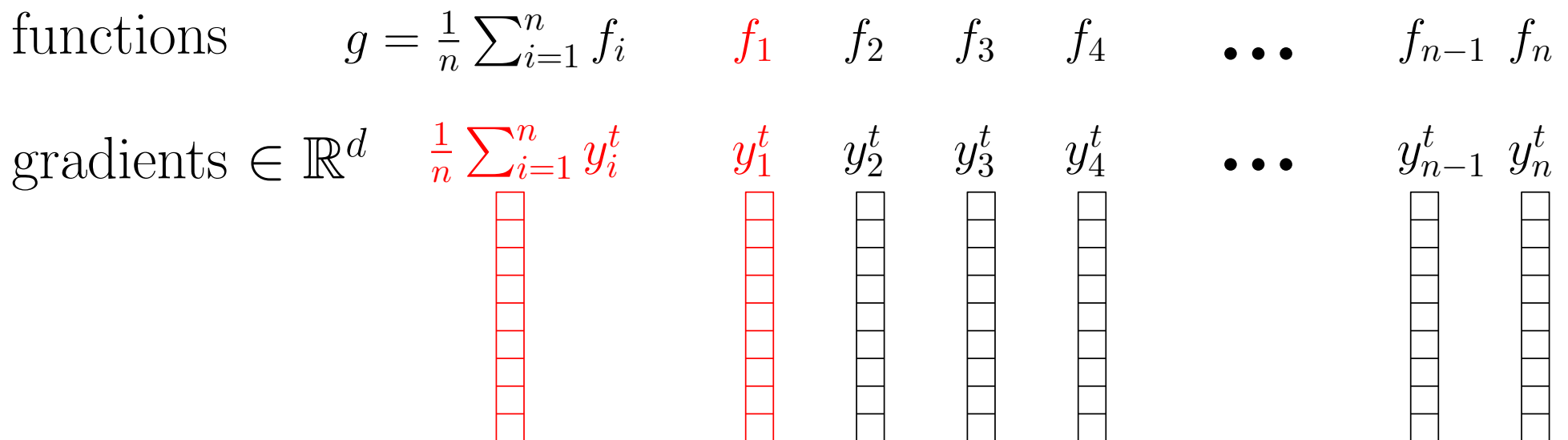
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- Stochastic version of incremental average gradient (Blatt et al., 2008)
- **Extra memory requirement:**  $n$  gradients in  $\mathbb{R}^d$  in general
- **Linear supervised machine learning:** only  $n$  real numbers
  - If  $f_i(\theta) = \ell(y_i, \Phi(x_i)^\top \theta)$ , 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,  $i = 1, \dots, n$
- $g = \frac{1}{n} \sum_{i=1}^n f_i$  is  $\mu$ -strongly convex
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- **Strongly convex case** (Le Roux et al., 2012; Schmidt et al., 2016)

$$\mathbb{E}[g(\theta_t) - g(\theta_*)] \leq \text{cst} \times \left(1 - \min\left\{\frac{1}{8n}, \frac{\mu}{16L}\right\}\right)^t$$

- Linear (exponential) convergence rate with  $O(d)$  iteration cost
- After one pass, reduction of cost by  $\exp\left(-\min\left\{\frac{1}{8}, \frac{n\mu}{16L}\right\}\right)$
- NB: in machine learning, may often restrict to  $\mu \geq L/n$   
 $\Rightarrow$  constant error reduction after each effective pass

# 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  $g$   $\mu$ -strongly convex

Stochastic gradient descent	$d \times \frac{L}{\mu} \times \frac{1}{\epsilon}$
Gradient descent	$d \times n \frac{L}{\mu} \times \log \frac{1}{\epsilon}$
Accelerated gradient descent	$d \times n \sqrt{\frac{L}{\mu}} \times \log \frac{1}{\epsilon}$
SAG	$d \times \left(n + \frac{L}{\mu}\right) \times \log \frac{1}{\epsilon}$

– 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

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- **Beating two lower bounds** (Nemirovski 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	$d \times n/\varepsilon$
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**

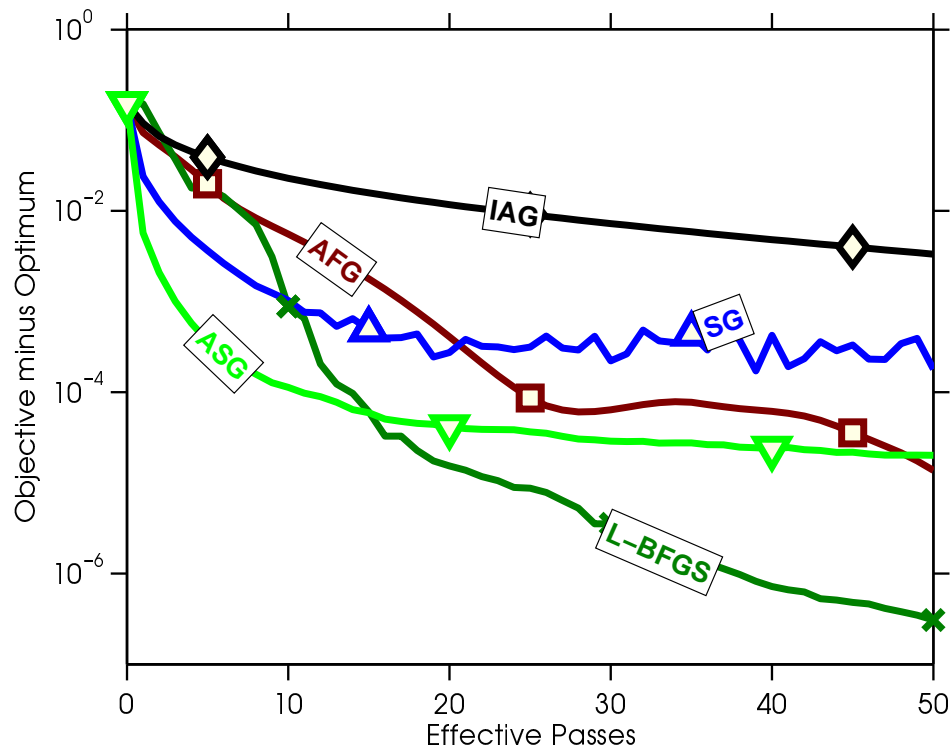
- Favors functions with large variations

- See [www.cs.ubc.ca/~schmidtm/Software/SAG.html](http://www.cs.ubc.ca/~schmidtm/Software/SAG.html)

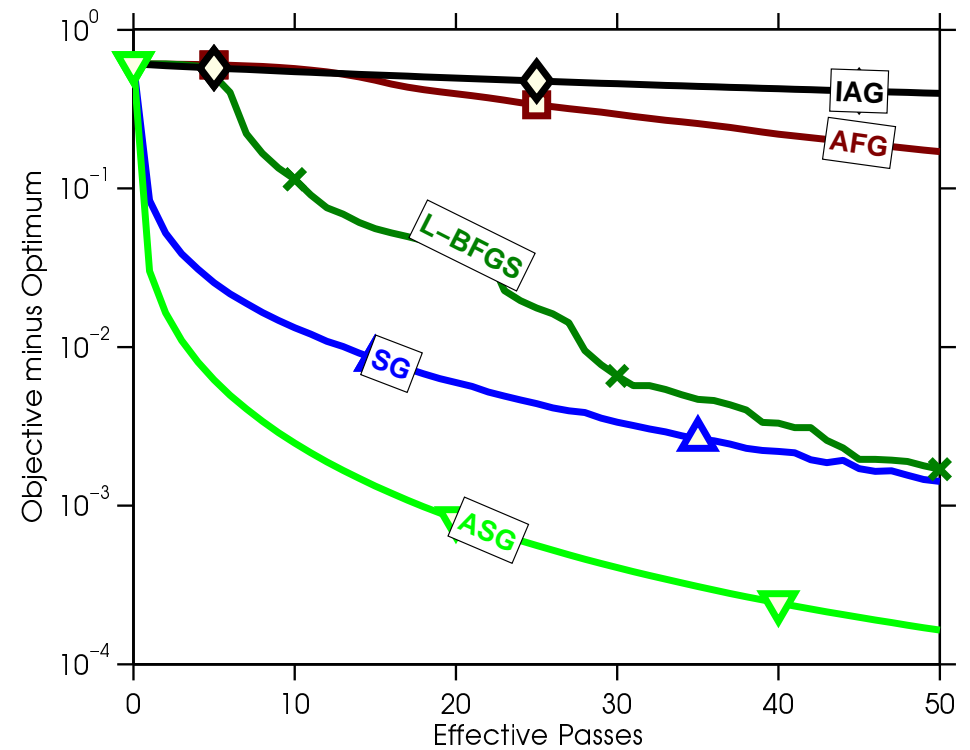


# Experimental results (logistic regression)

quantum dataset  
( $n = 50\,000$ ,  $d = 78$ )

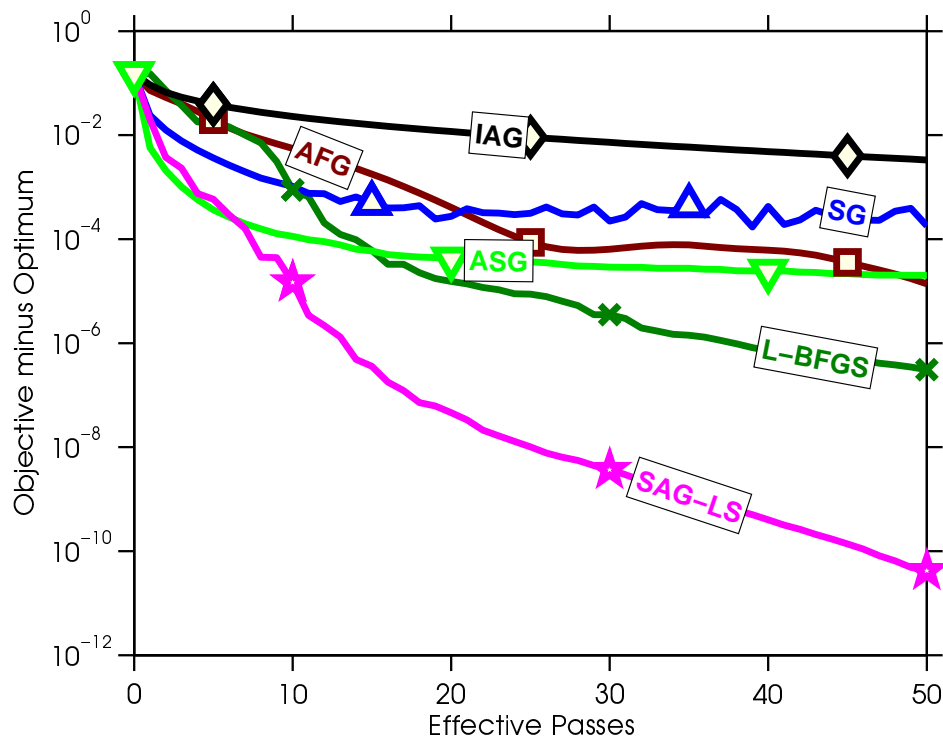


rcv1 dataset  
( $n = 697\,641$ ,  $d = 47\,236$ )

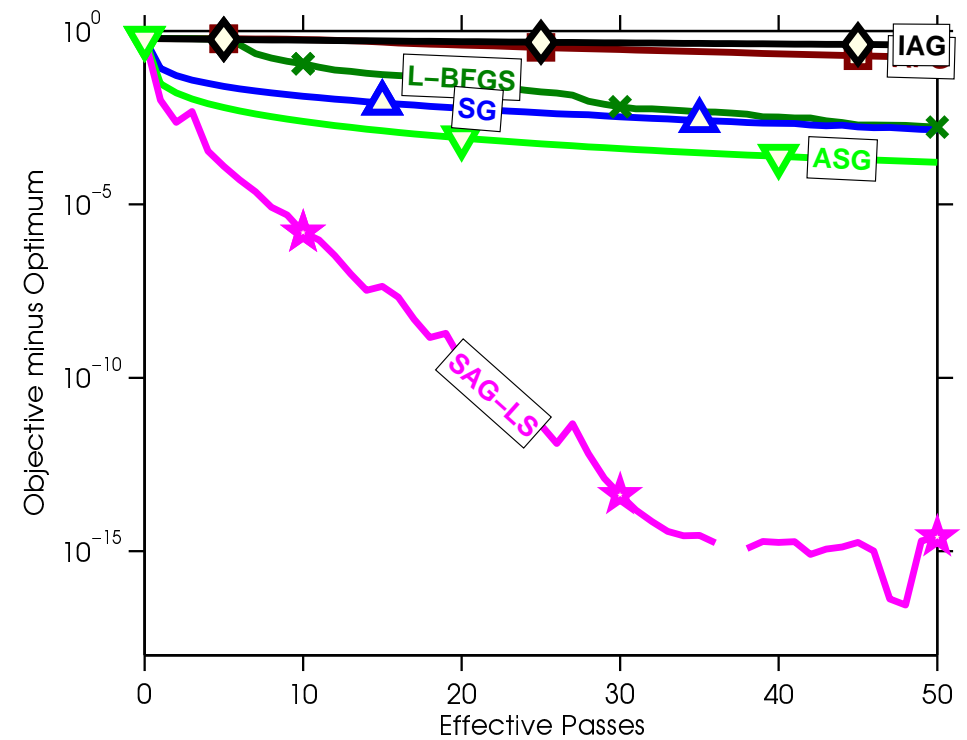


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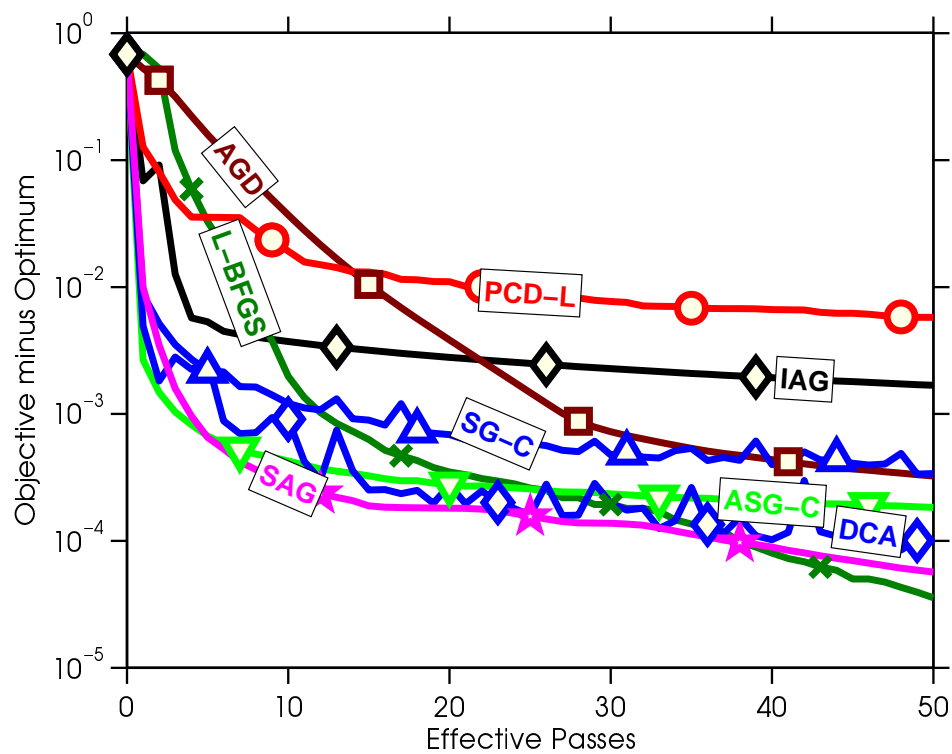


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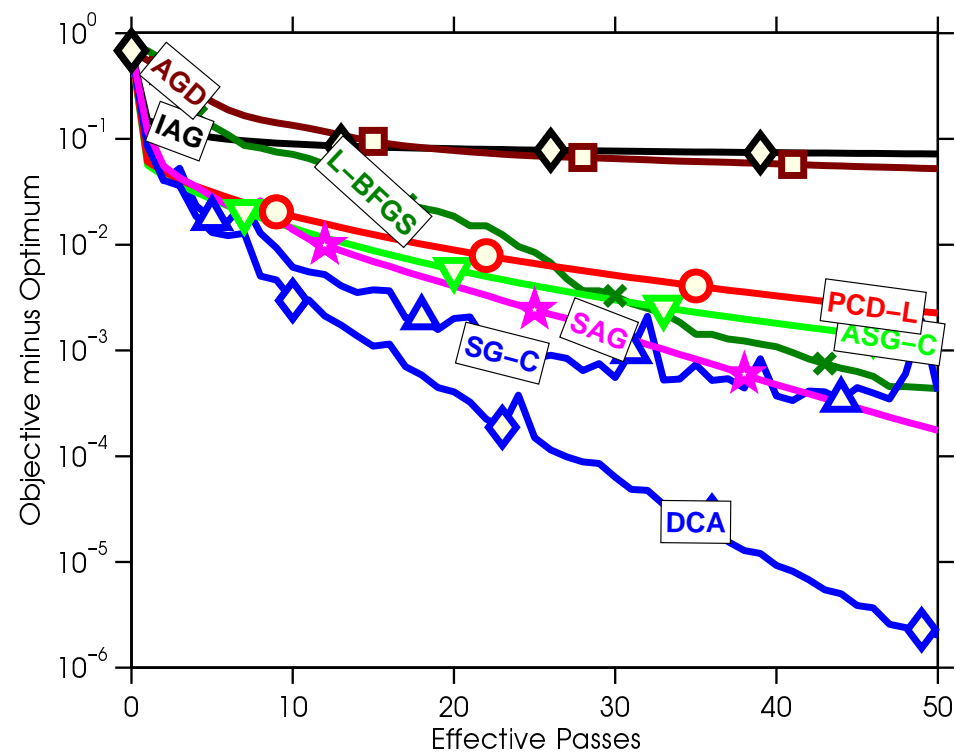


# Before non-uniform sampling

protein dataset  
( $n = 145\,751$ ,  $d = 74$ )

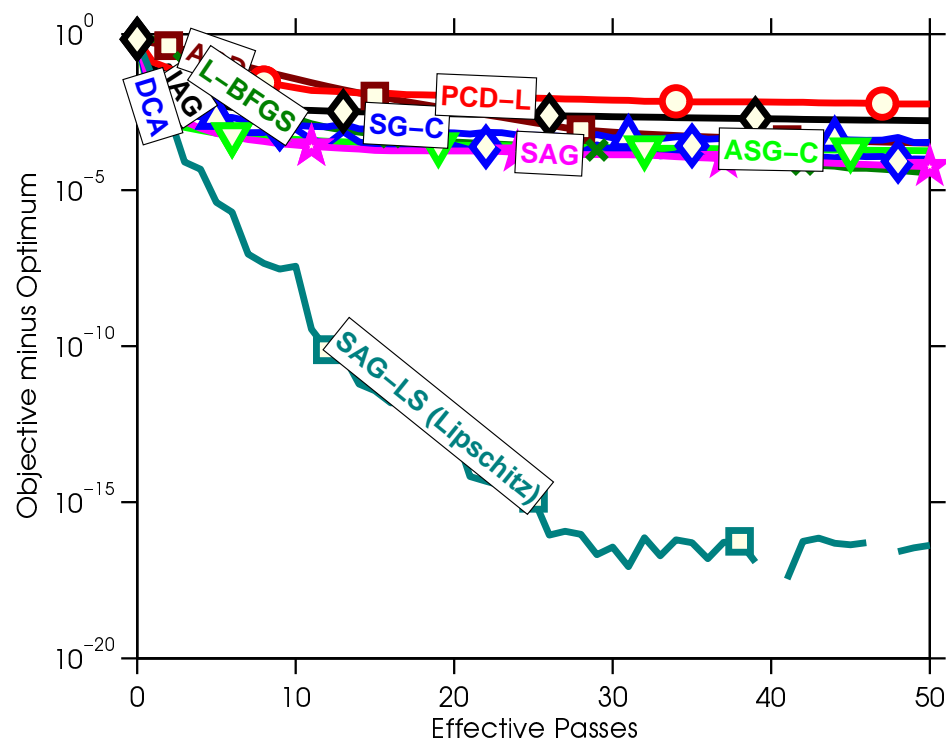


sido dataset  
( $n = 12\,678$ ,  $d = 4\,932$ )

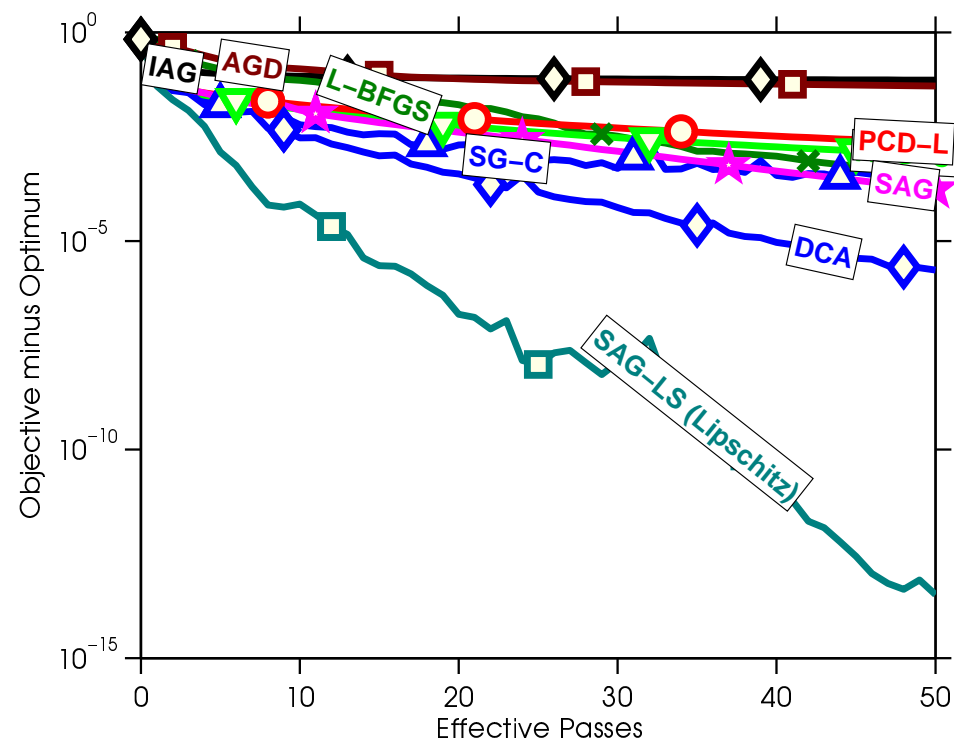


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# Linearly convergent stochastic gradient algorithms

- **Many related algorithms**

- SAG (Le Roux, Schmidt, and Bach, 2012)
- SDCA (Shalev-Shwartz and Zhang, 2013)
- SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
- MISO (Mairal, 2015)
- Finito (Defazio et al., 2014b)
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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

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

- $\mathbb{E}Z_\alpha = \alpha\mathbb{E}X + (1 - \alpha)\mathbb{E}Y$
- $\text{var}(Z_\alpha) = \alpha^2 [\text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y)]$
- $\alpha = 1$ : no bias,  $\alpha < 1$ : potential bias (but reduced variance)
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  - Useful if  $Y$  positively correlated with  $X$
- **Application to gradient estimation** (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**
    - $$\theta_t = \theta_{t-1} - \gamma \left[ g'(\tilde{\theta}) + (f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\tilde{\theta})) \right]$$
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- **No need to store gradients** - two gradient evaluations per inner step
- Two parameters: length of epochs + step-size  $\gamma$
- Same linear convergence rate as SAG, simpler proof

# 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:**  $\theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^n y_i^{t-1} + (f'_{i(t)}(\theta_{t-1}) - y_{i(t)}^{t-1}) \right]$ 
  - Defazio, Bach, and Lacoste-Julien (2014a)
  - Unbiased update without epochs

## SVRG vs. SAGA

- **SAGA** update:  $\theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^n y_i^{t-1} + (f'_{i(t)}(\theta_{t-1}) - y_{i(t)}^{t-1}) \right]$
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	SAGA	SVRG
<b>Storage of gradients</b>	<b>yes</b>	<b>no</b>
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	$d \times$	$n \frac{L}{\mu}$	$\times \log \frac{1}{\epsilon}$
Accelerated gradient descent	$d \times$	$n \sqrt{\frac{L}{\mu}}$	$\times \log \frac{1}{\epsilon}$
SAG(A), SVRG, SDCA, MISO	$d \times$	$(n + \frac{L}{\mu})$	$\times \log \frac{1}{\epsilon}$

# Acceleration

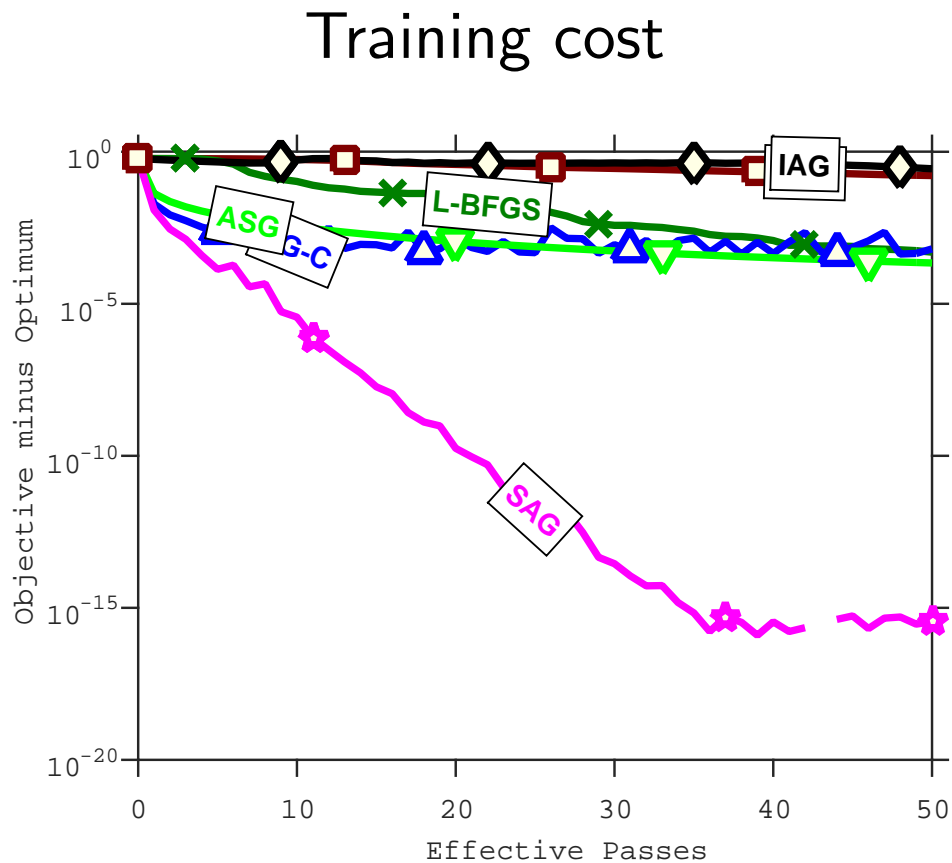
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<b>Accelerated versions</b>	$d \times (n + \sqrt{n \frac{L}{\mu}}) \times \log \frac{1}{\epsilon}$

- **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

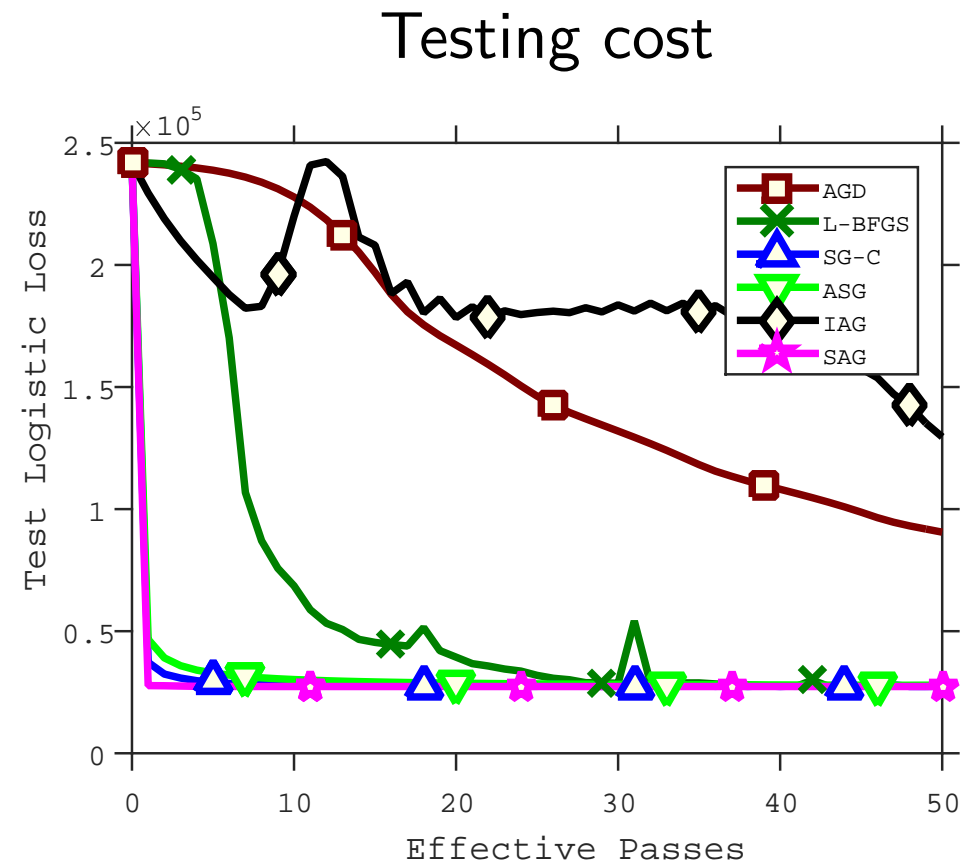
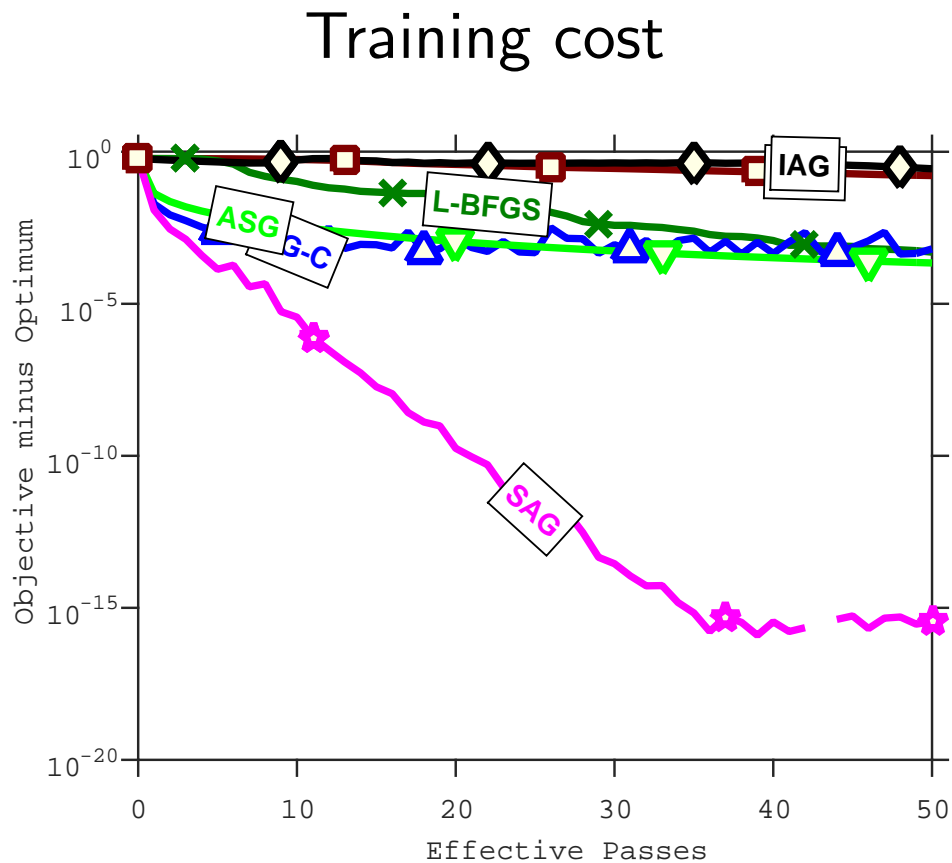
# From training to testing errors

- rcv1 dataset ( $n = 697\,641$ ,  $d = 47\,236$ )
  - NB: IAG, SG-C, ASG with optimal step-sizes in hindsight



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- **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
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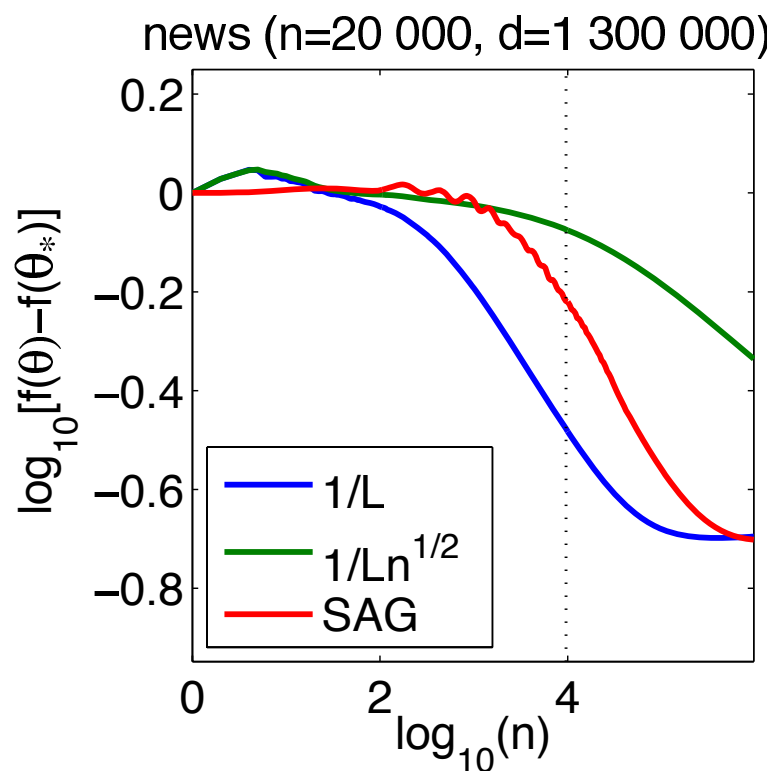
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- **Constant-step-size SGD**
  - Linear convergence up to the noise level for strongly-convex problems (Solodov, 1998; Nedic and Bertsekas, 2000)
  - **Full convergence and robustness to ill-conditioning?**

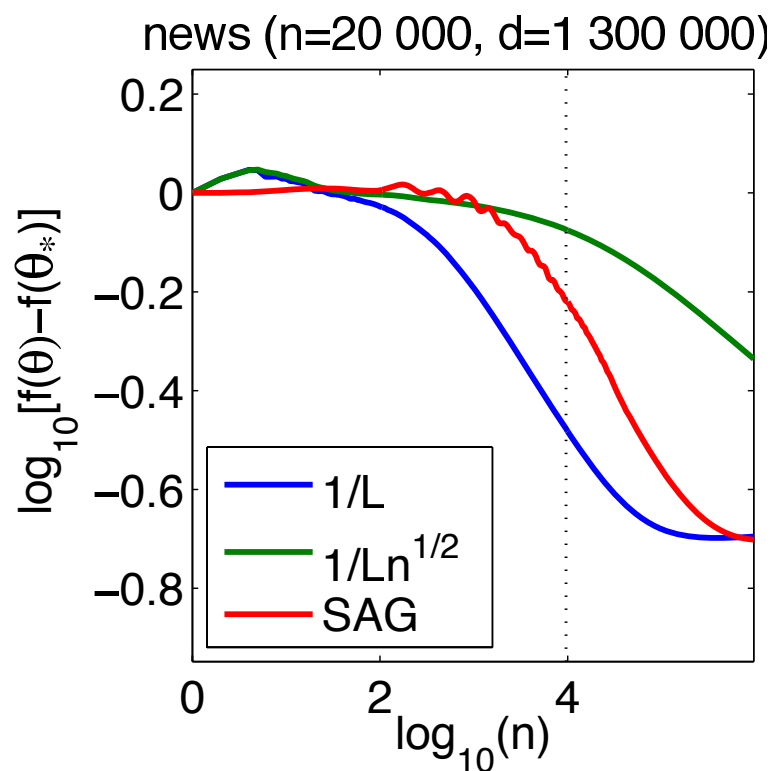
# Robust averaged stochastic gradient (Bach and Moulines, 2013)

- **Constant-step-size SGD is convergent for least-squares**
  - Convergence rate in  $O(1/n)$  without any dependence on  $\mu$
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- Convergence in  $O(1/n)$  for smooth losses with  $O(d)$  online Newton step

# Conclusions - Convex optimization

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  - Provable and precise rates
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- **What's next: non-convexity, parallelization, extensions/perspectives**



# Postdoc opportunities in **downtown Paris**



- **Machine learning group at INRIA - Ecole Normale Supérieure**
  - Two postdoc positions (2 years)
  - One junior researcher position (4 years)

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