Stochastic Variance-Reduced Optimization for Machine Learning
Part I

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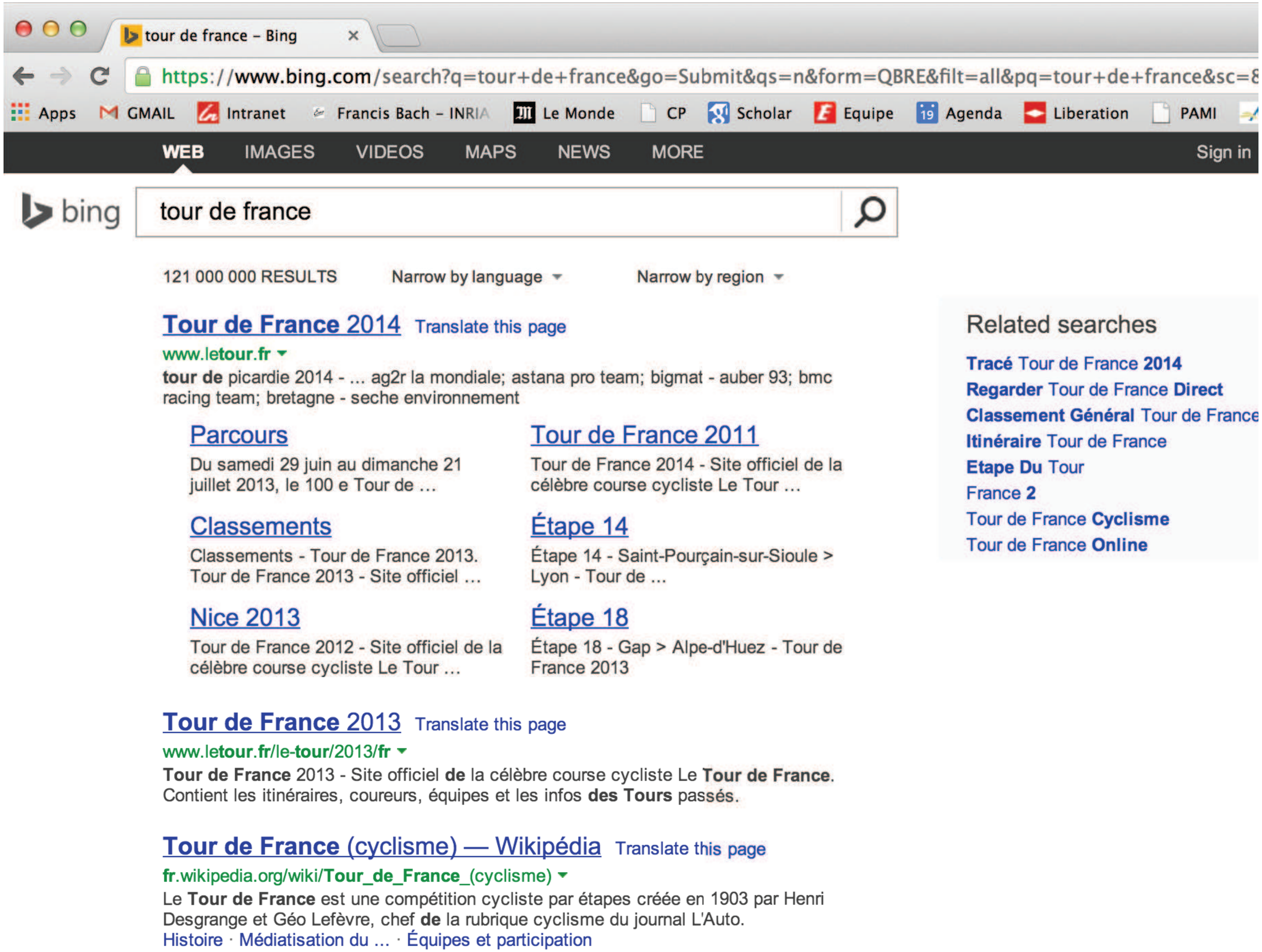
Joint tutorial with Mark Schmidt, UBC - *SIOPT - 2017*

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



Visual object recognition

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- **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. **Non-independent and identically distributed**
5. **Non-stochastic: other types of structures**
6. **Non-serial: parallel and distributed settings**

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/`

Parametric supervised machine learning

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

- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$

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  - Linear predictions: $h(x, \theta) = \theta^\top \Phi(x)$ with features $\Phi(x) \in \mathbb{R}^d$

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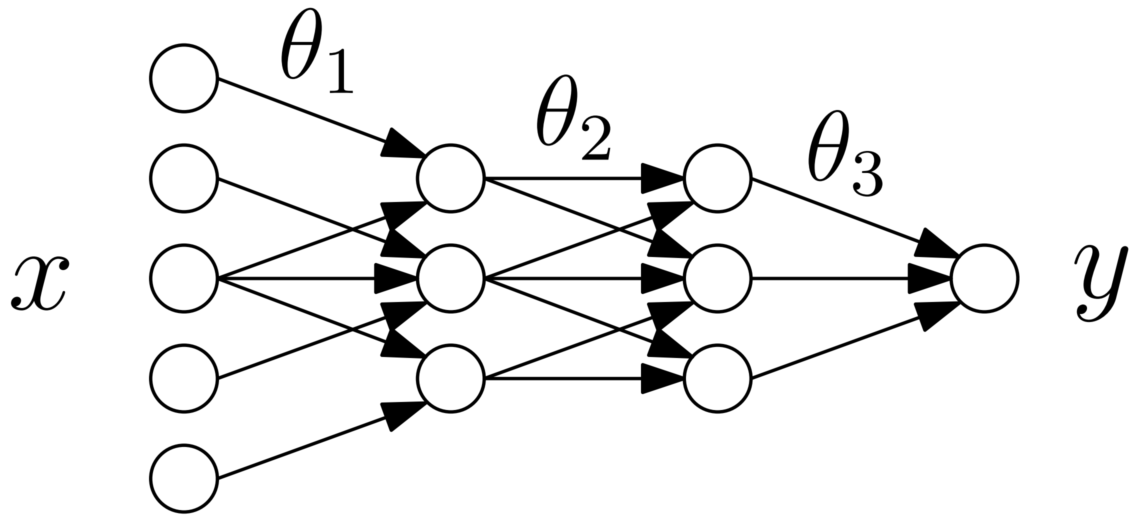
  - Neural networks: $h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))$



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

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

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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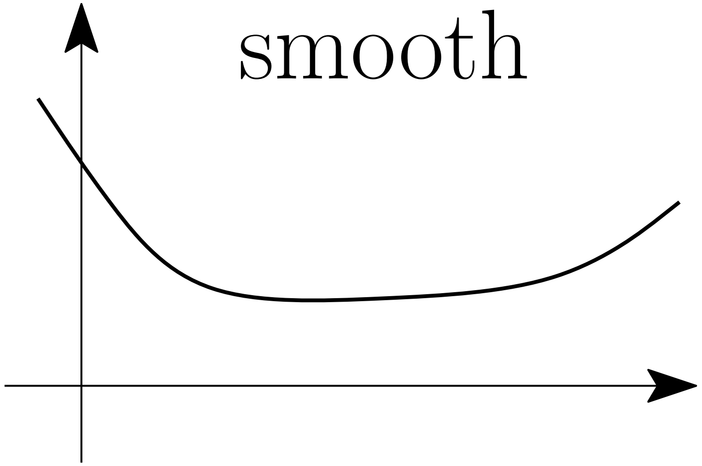
- Optimization: optimization of regularized risk training cost

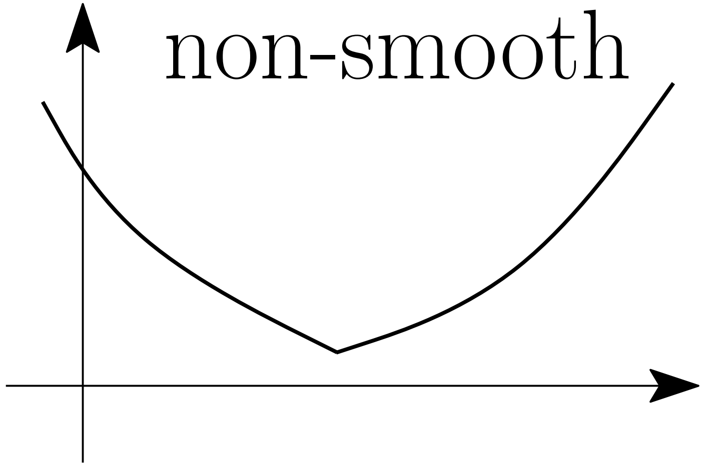
- Statistics: guarantees on $\mathbb{E}_{p(x,y)} \ell(y, h(x, \theta))$ testing cost

Smoothness and (strong) convexity

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

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





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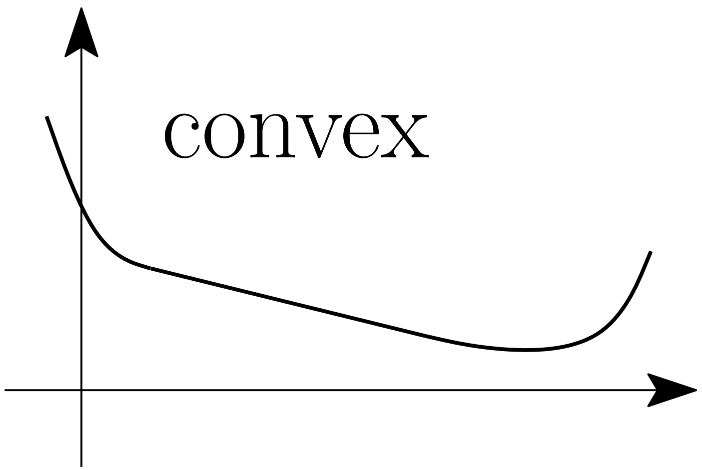
- **Machine learning**
  - with $g(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i, \theta))$
  - Smooth prediction function $\theta \mapsto h(x_i, \theta)$ + smooth loss

Smoothness and (strong) convexity

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

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



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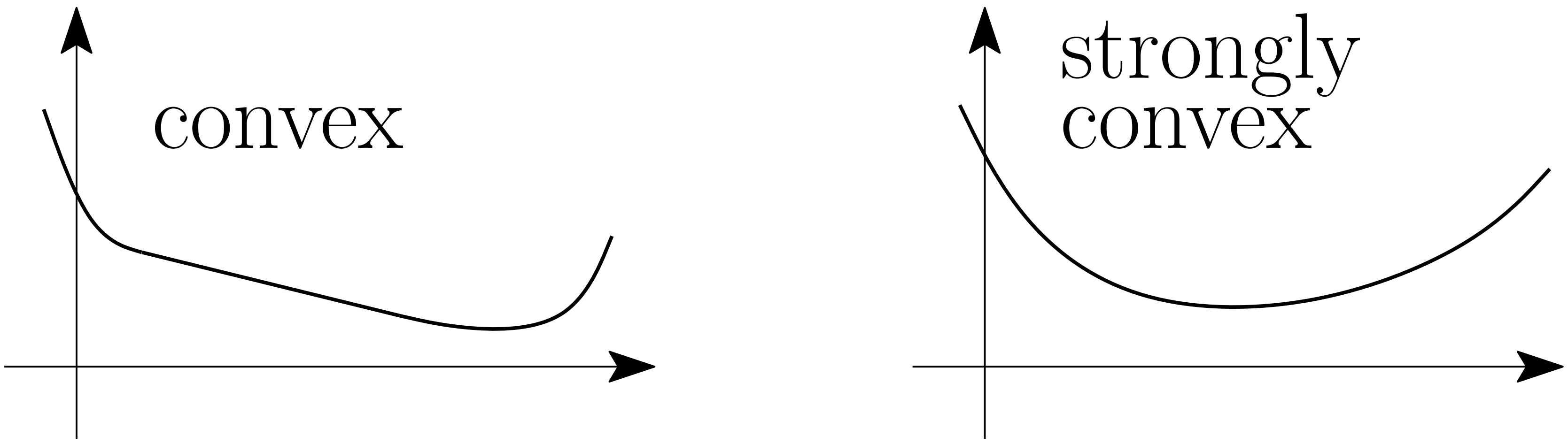

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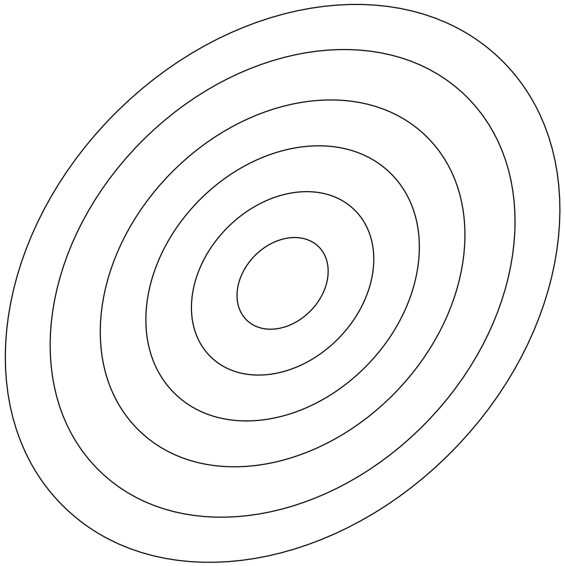
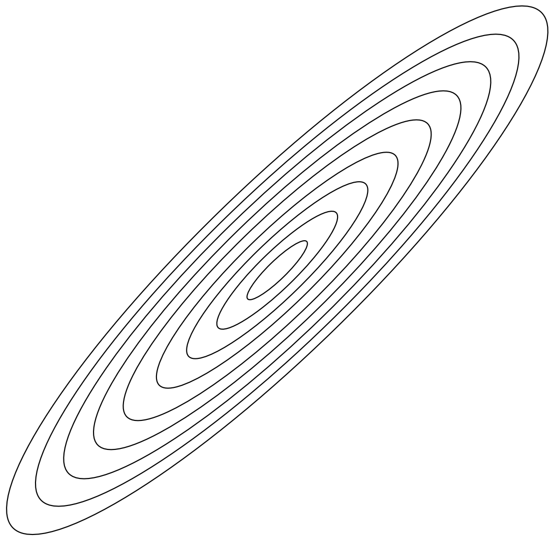
  - Condition number $\kappa = L/\mu \geqslant 1$



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



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- **Convexity in machine learning**
  - With $g(\theta) = \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta))$
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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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  - Invertible covariance matrix $\frac{1}{n}\sum_{i=1}^n \Phi(x_i)\Phi(x_i)^\top \Rightarrow n \geqslant d$
  - Even when $\mu > 0$, μ may be arbitrarily small!

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- **Adding regularization by $\frac{\mu}{2}\|\theta\|^2$**
  - creates additional bias unless μ is small, but reduces variance
  - Typically $L/\sqrt{n} \geqslant \mu \geqslant L/n$

Iterative methods for minimizing smooth functions

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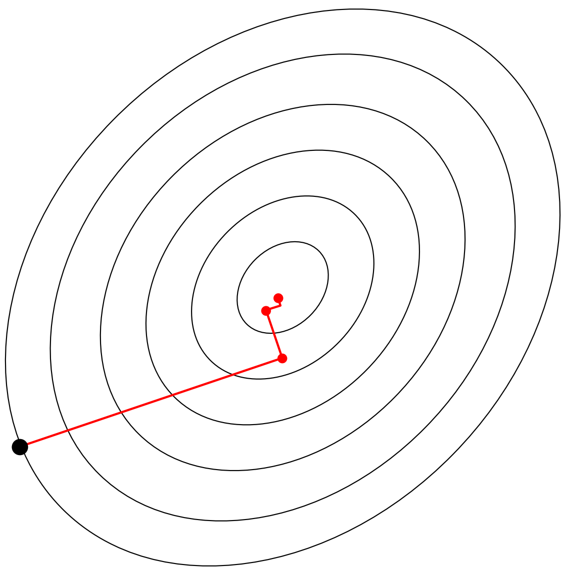
- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t \, g'(\theta_{t-1})$



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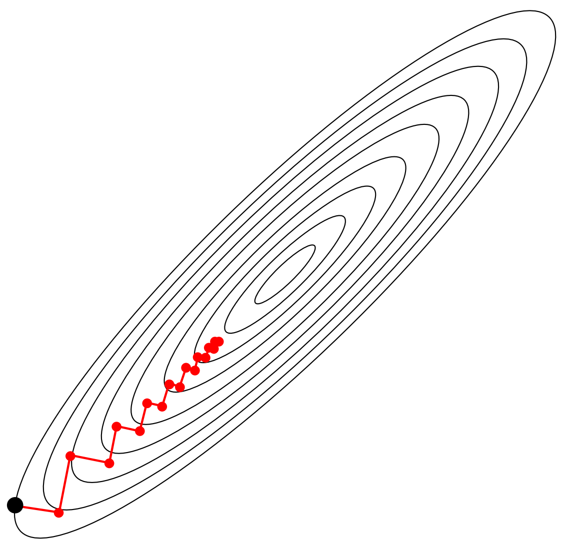

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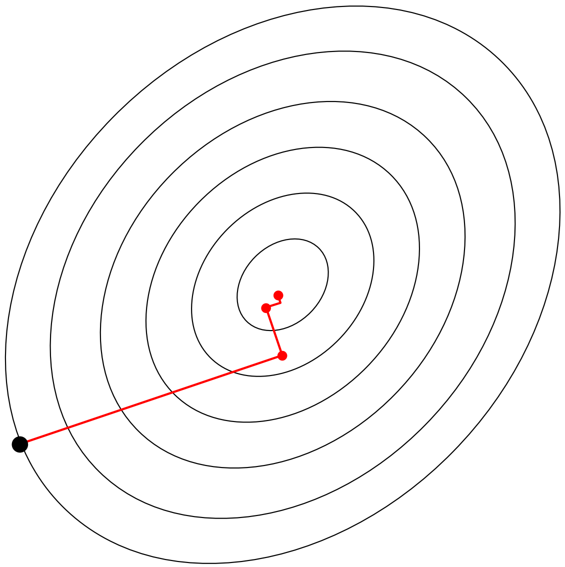
$$g(\theta_t) - g(\theta_*) \leqslant O(1/t)$$
$$g(\theta_t) - g(\theta_*) \leqslant O((1-\mu/L)^t) = O(e^{-t(\mu/L)}) \text{ if } \mu\text{-strongly convex}$$



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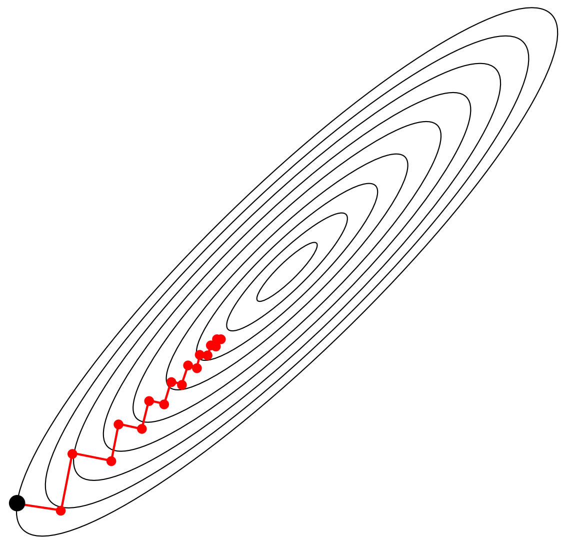

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- **Newton method**: $\theta_t = \theta_{t-1} - g''(\theta_{t-1})^{-1} g'(\theta_{t-1})$
  - $O\big(e^{-\rho 2^t}\big)$ *quadratic* rate

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- **Key insights for machine learning (Bottou and Bousquet, 2008)**
  1. No need to optimize below statistical error
  2. Cost functions are averages
  3. Testing error is more important than training 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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- **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, 2014)
  - Running-time complexity: $O(d \cdot \kappa/\varepsilon)$

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   – 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 $f_i(\theta) = \ell\big(y_i, h(x_i,\theta)\big) + \lambda\Omega(\theta)$

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

  – Linear (e.g., exponential) convergence rate in $O(e^{-t/\kappa})$

  – Iteration complexity is linear in n

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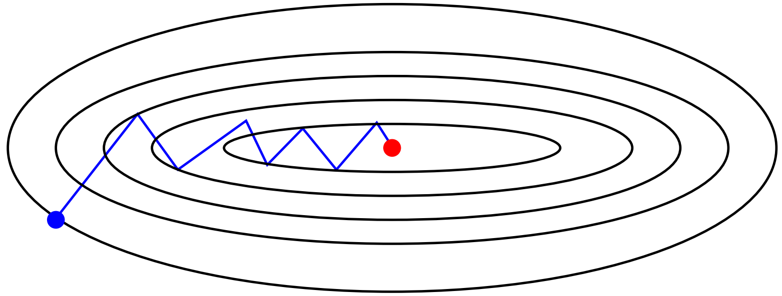

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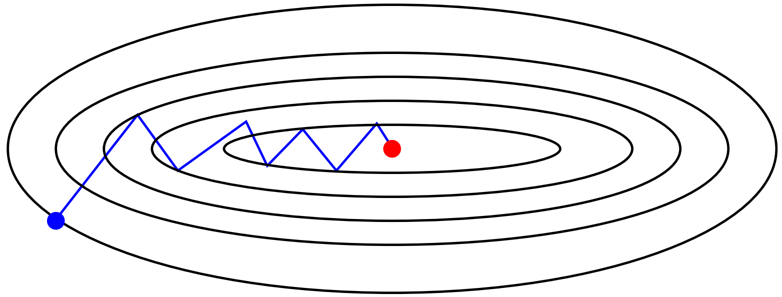
- Stochastic gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f'_{i(t)}(\theta_{t-1})$
  - Sampling with replacement: $i(t)$ random element of $\{1, \dots, n\}$
  - Convergence rate in $O(\kappa/t)$
  - Iteration complexity is independent of n

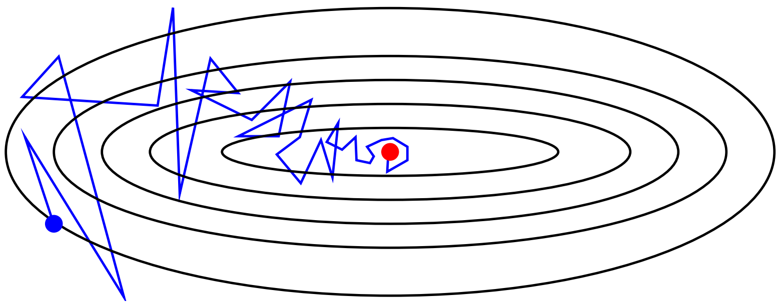
Stochastic vs. deterministic methods

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

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

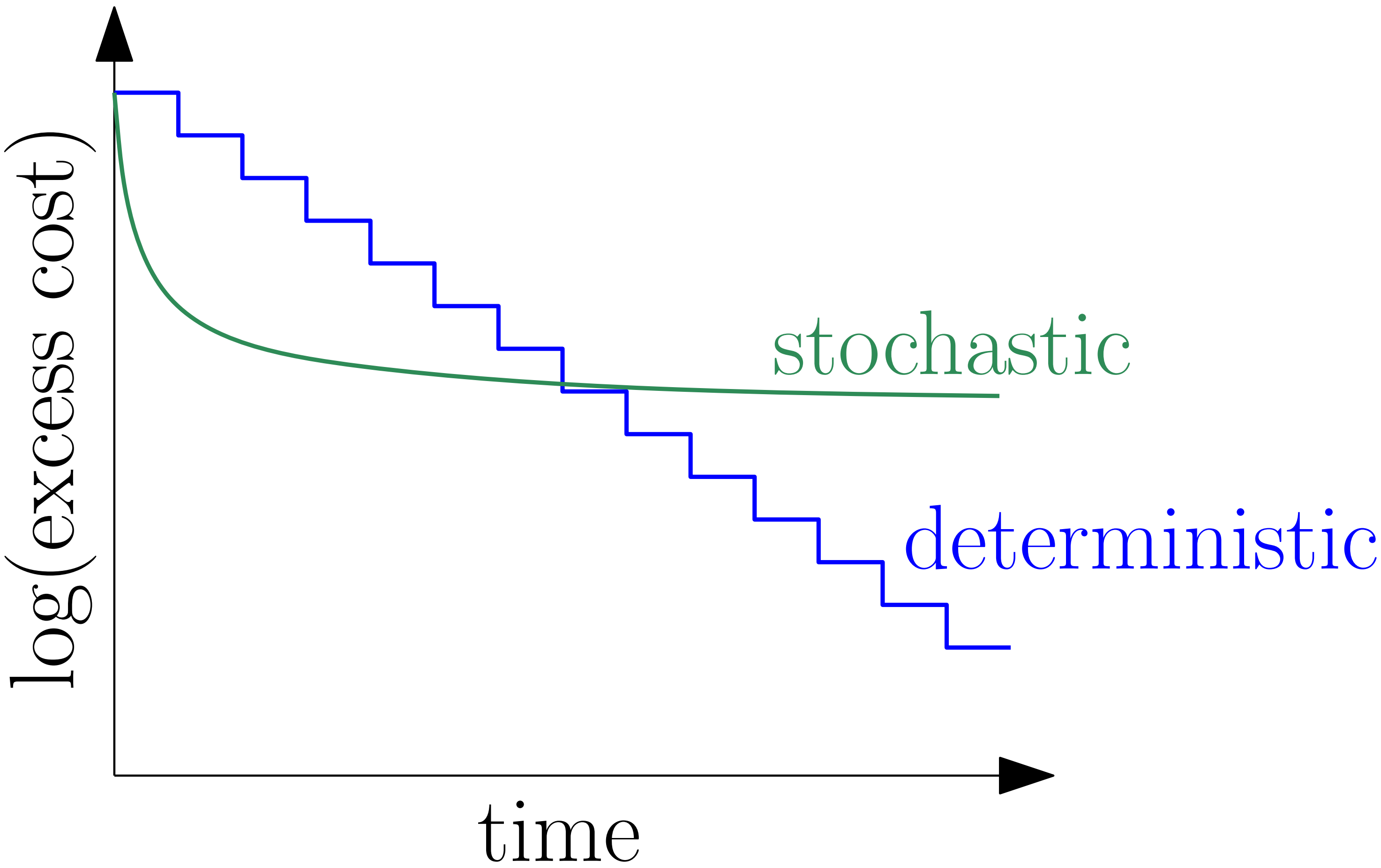


- Stochastic gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f_{i(t)}'(\theta_{t-1})$



Stochastic vs. deterministic methods

- **Goal** = **best of both worlds**: Linear rate with $O(d)$ iteration cost
  Simple choice of step size



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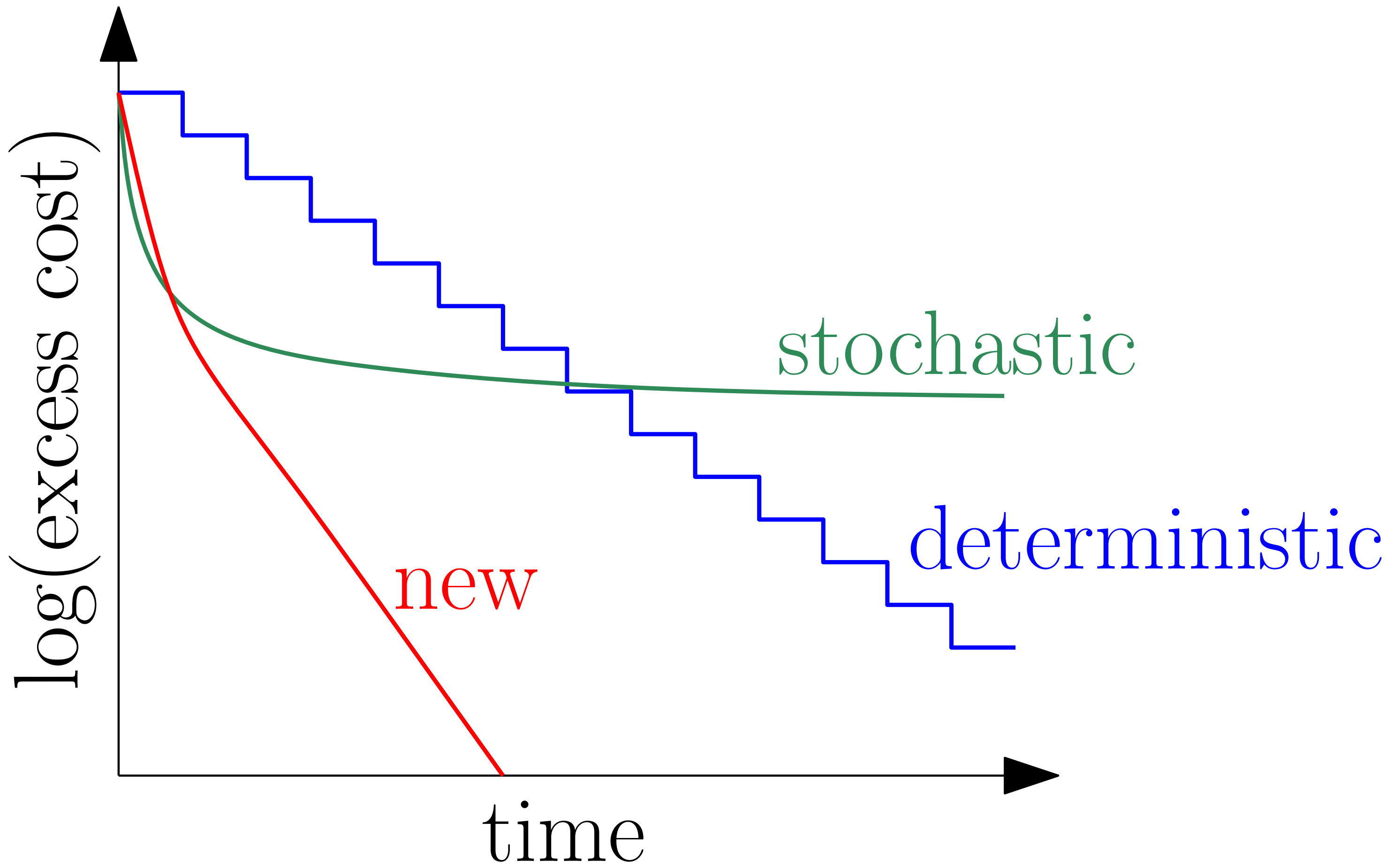

Accelerating gradient methods - Related work

- **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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  – Good choice of momentum term $\delta_t \in [0, 1)$

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

  $g(\theta_t) - g(\theta_*) \leqslant O(e^{-t\sqrt{\mu/L}}) = O(e^{-t/\sqrt{\kappa}})$ if μ-strongly convex

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  - Optimal rates after $t = O(d)$ iterations (Nesterov, 2004)
  - Still $O(nd)$ iteration cost: complexity $= O(nd \cdot \sqrt{\kappa} \log \frac{1}{\varepsilon})$

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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
  - 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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functions	$g = \frac{1}{n} \sum_{i=1}^{n} f_i$	f_1	f_2	f_3	f_4	$\bullet\bullet\bullet$	f_{n-1}	f_n
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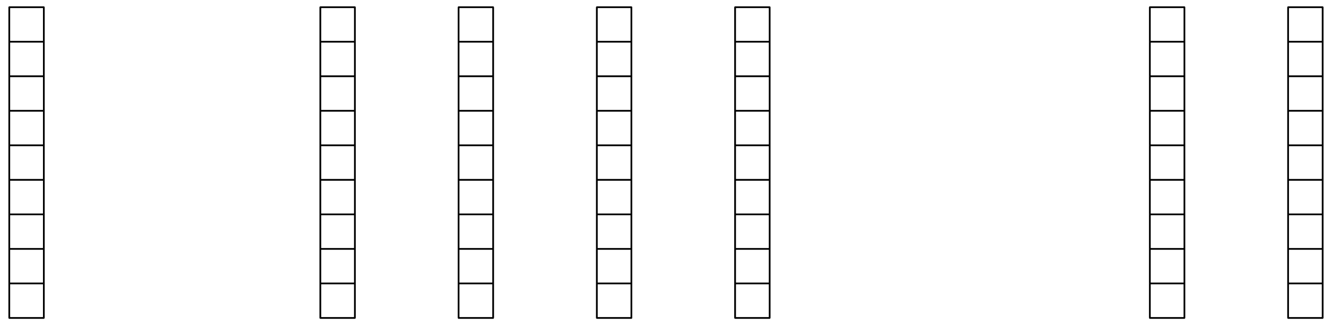

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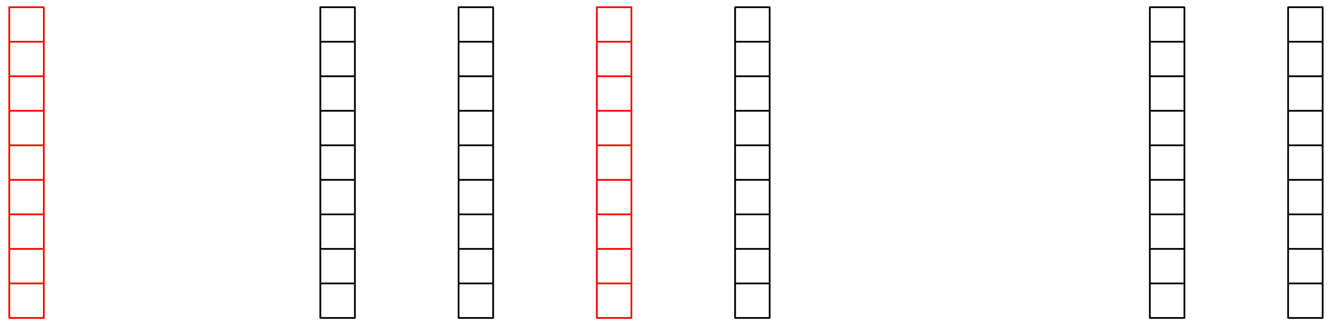

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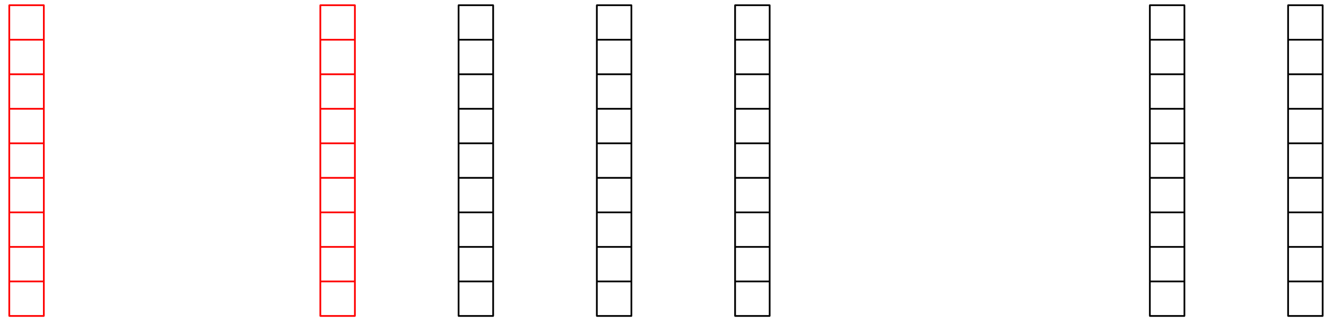

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- **Extra memory requirement**: n gradients in $\mathbb{R}^d$ in general

- **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 μ-strongly convex
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- **Strongly convex case** (Le Roux et al., 2012; Schmidt et al., 2016)

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

  - 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

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

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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/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

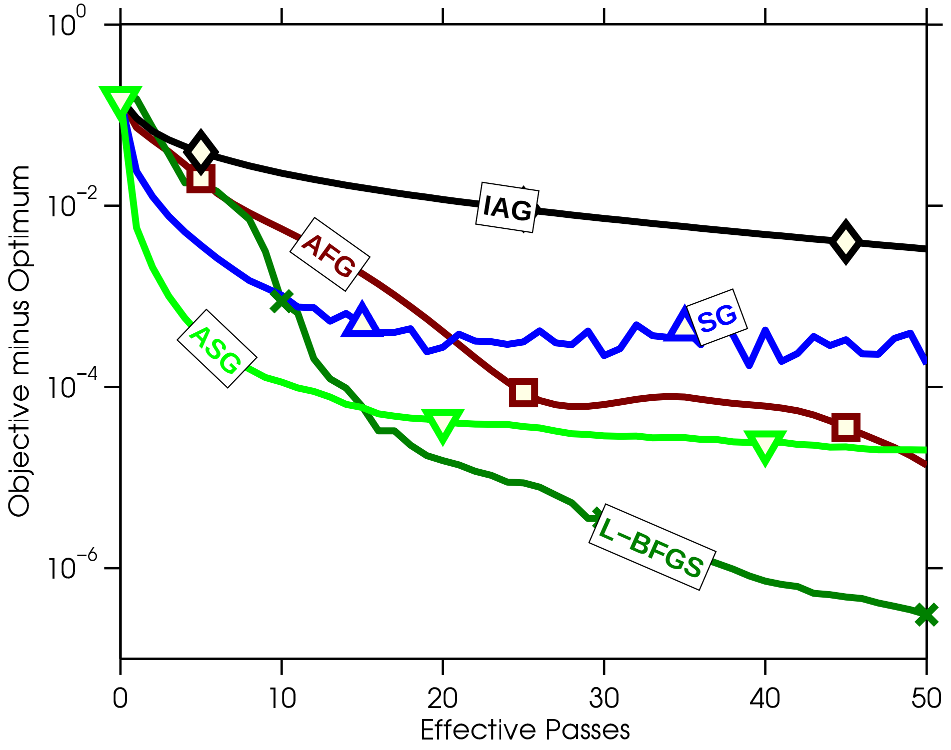
Stochastic average gradient
Implementation details and extensions

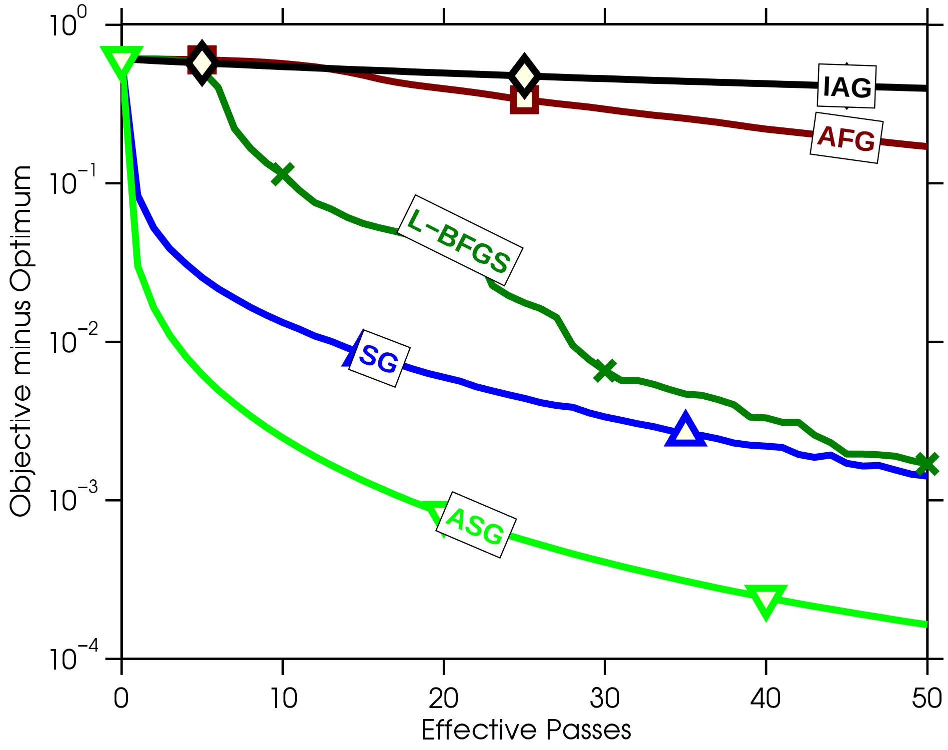
- **Sparsity in the features**
  - Just-in-time updates $\Rightarrow$ replace $O(d)$ by number of non zeros
  - See also Leblond, Pedregosa, and Lacoste-Julien (2016)
- **Mini-batches**
  - Reduces the memory requirement + block access to data
- **Line-search**
  - Avoids knowing L in advance
- **Non-uniform 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
$(n = 697\,641,\ d = 47\,236)$





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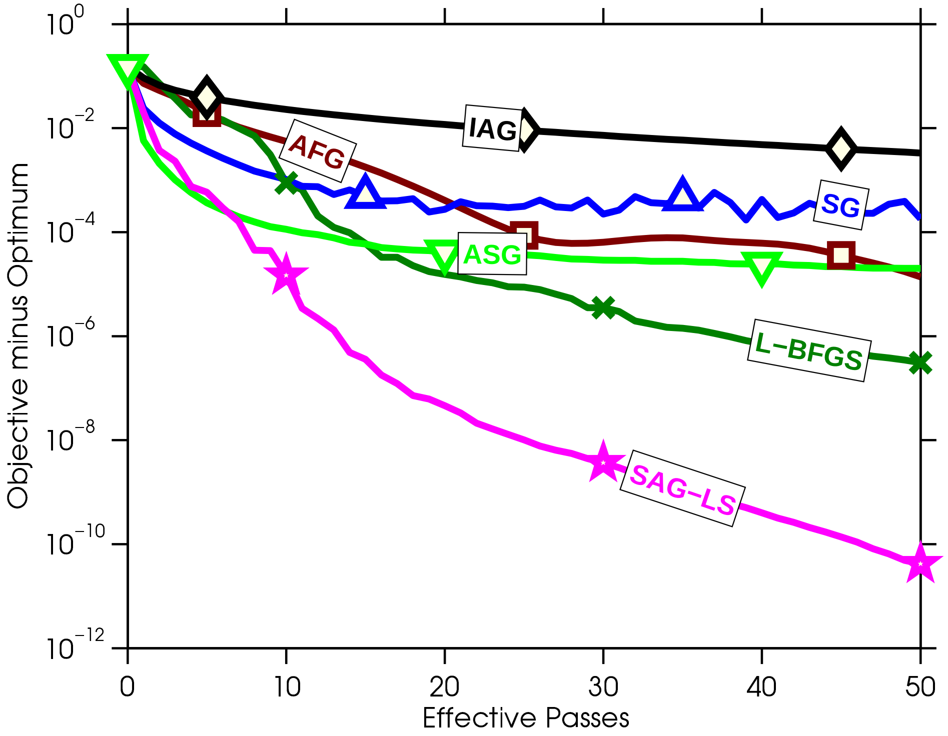

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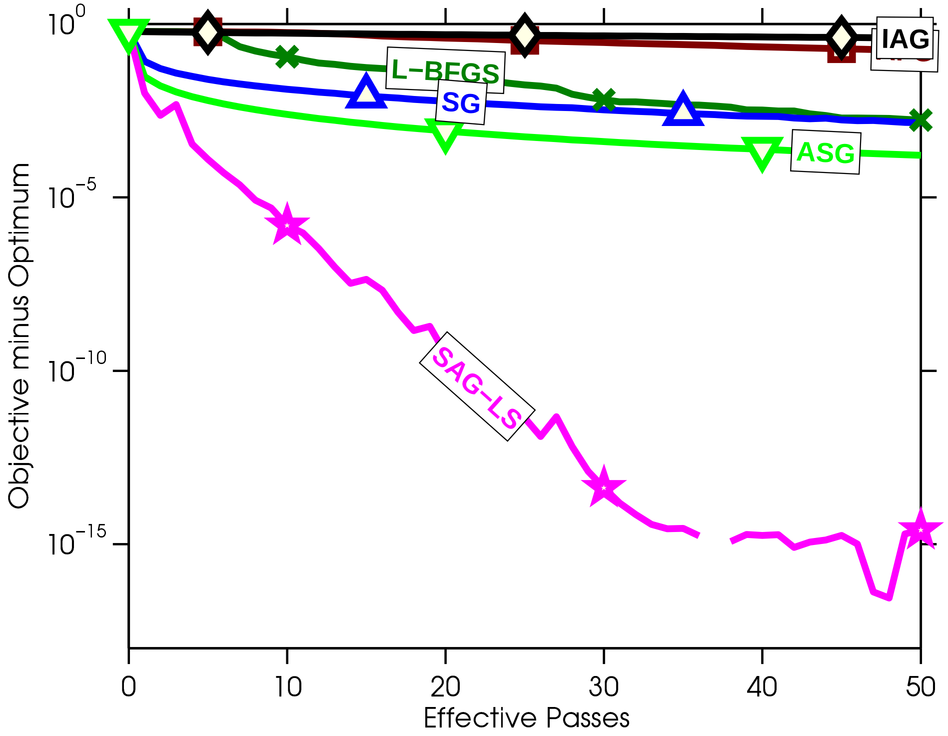

Before non-uniform sampling

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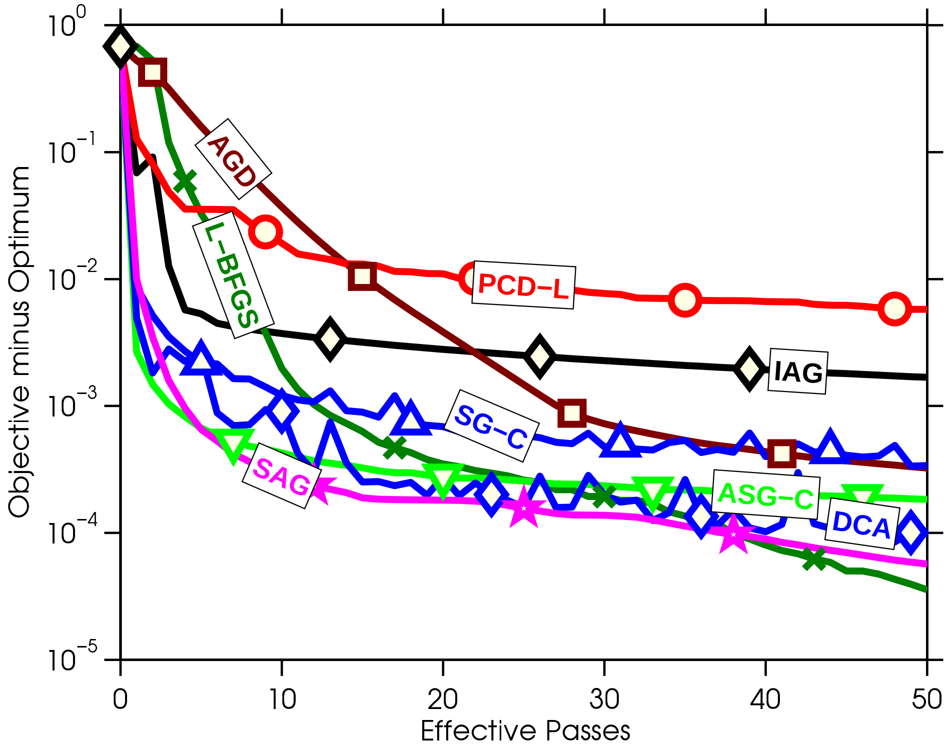

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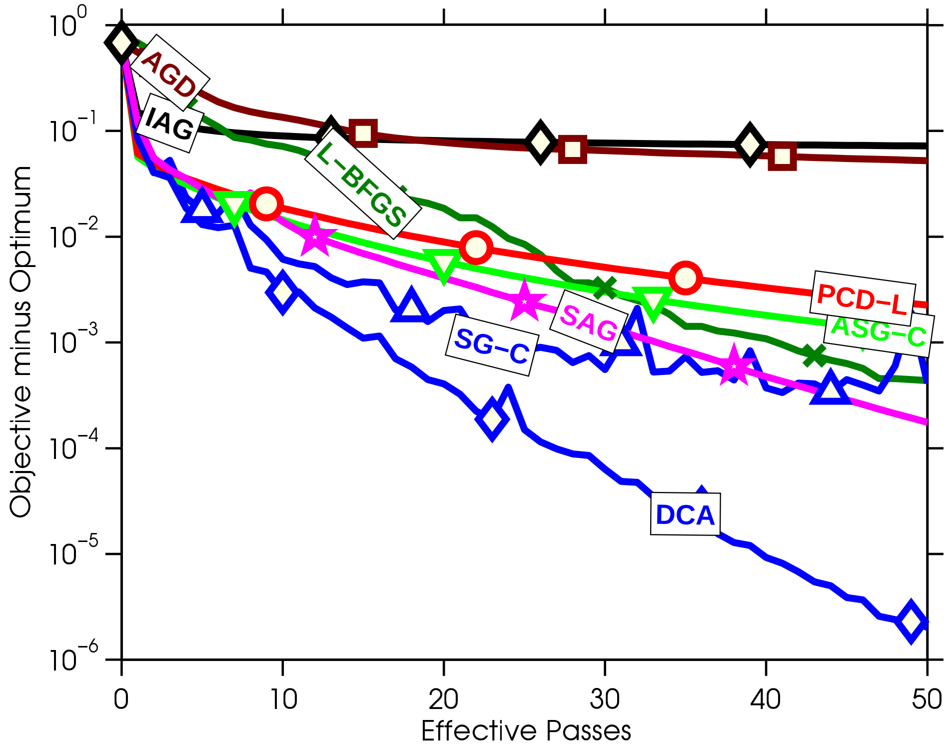

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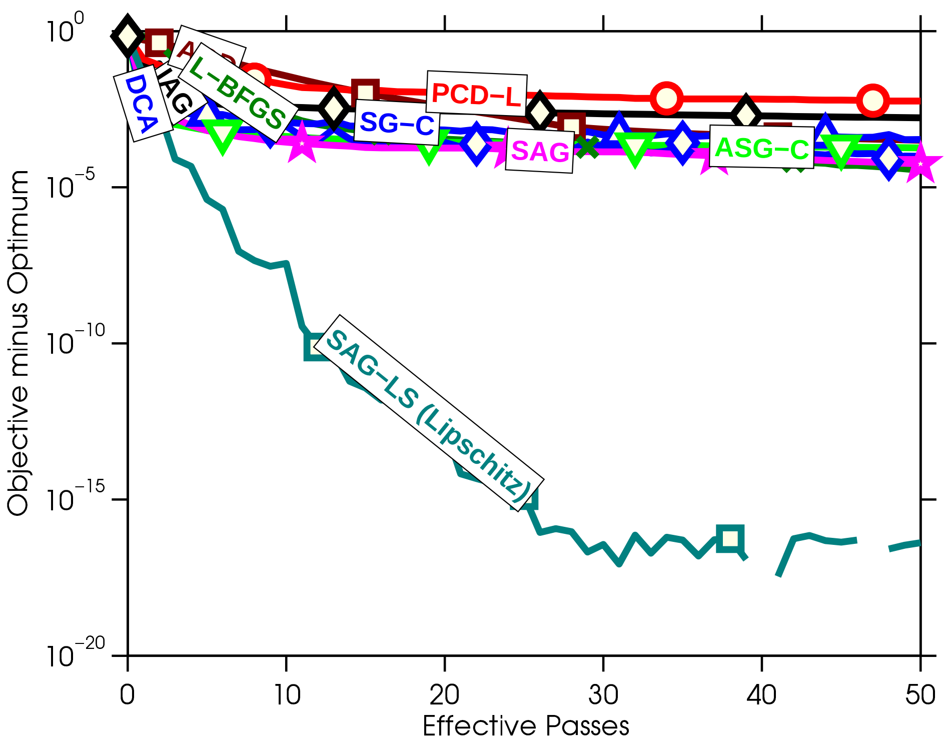

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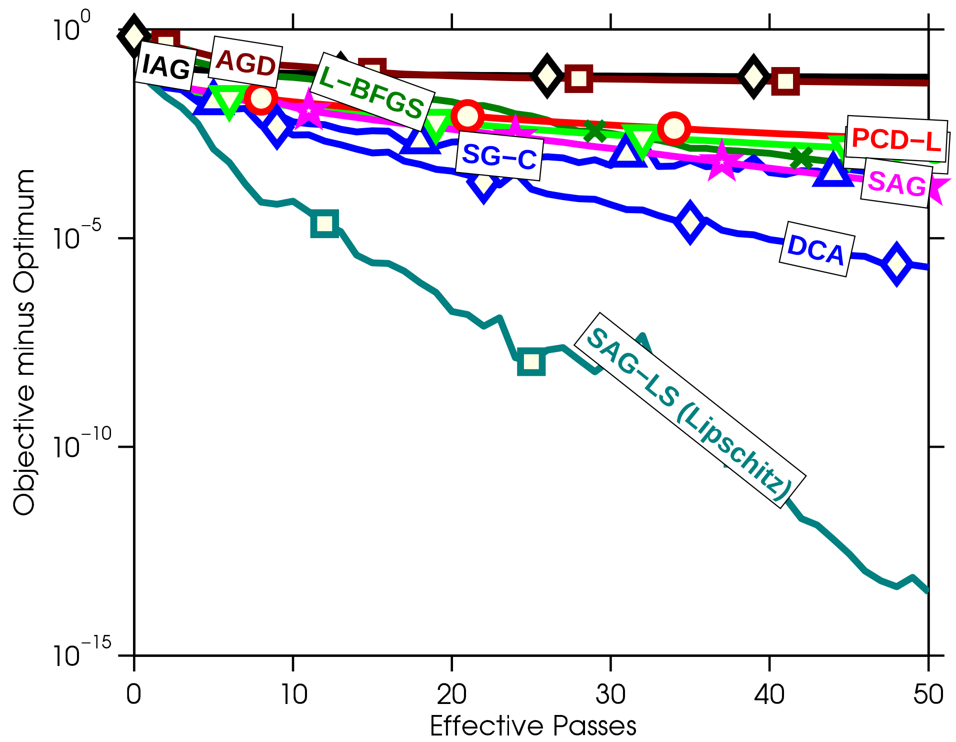

Linearly convergent stochastic gradient algorithms

- **Many related algorithms**
  - SAG (Le Roux, Schmidt, and Bach, 2012)
  - SDCA (Shalev-Shwartz and Zhang, 2013)
  - SVRG (Johnson and Zhang, 2013; Zhang et al., 2013)
  - MISO (Mairal, 2015)
  - Finito (Defazio et al., 2014b)
  - SAGA (Defazio, Bach, and Lacoste-Julien, 2014a)
  - $\ldots$

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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

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

  - $\mathbb{E}Z_\alpha = \alpha\mathbb{E}X + (1-\alpha)\mathbb{E}Y$
  - $\text{var}(Z_\alpha) = \alpha^2\big[\,\text{var}(X) + \text{var}(Y) - 2\text{cov}(X,Y)\big]$
  - $\alpha = 1$: 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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– 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

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 (2014a)
  - 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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  - Extra projection / soft thresholding step after gradient update
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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	$d\times \quad (n+\sqrt{n\frac{L}{\mu}}) \quad \times \log\frac{1}{\varepsilon}$

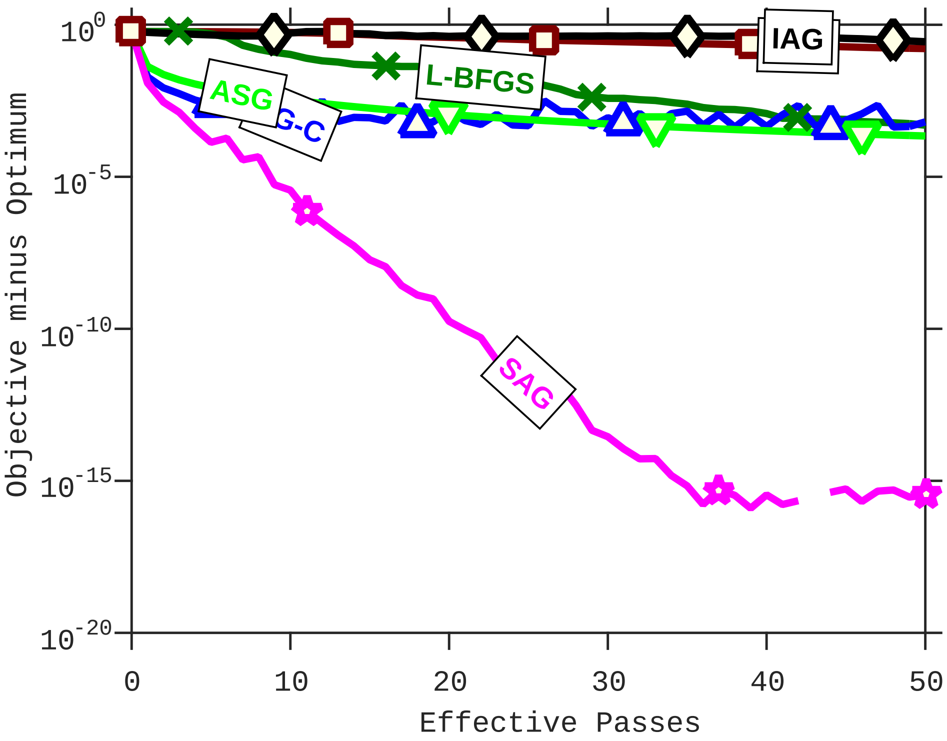
- **Acceleration for special algorithms** (e.g., Shalev-Shwartz and Zhang, 2014; Nitanda, 2014; Lan, 2015; Defazio, 2016)

- **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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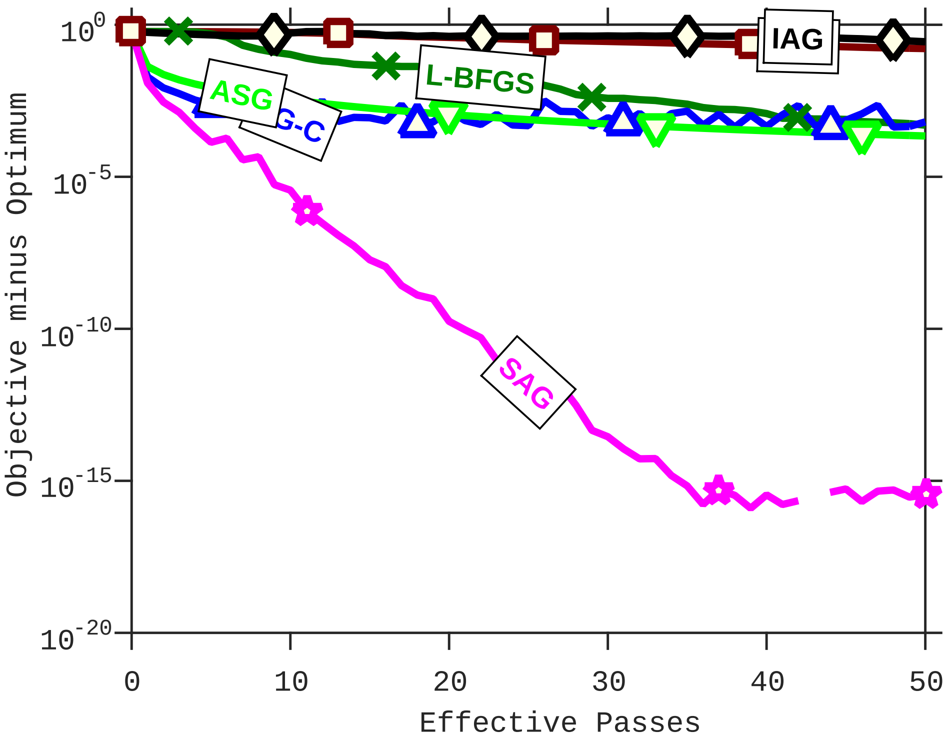

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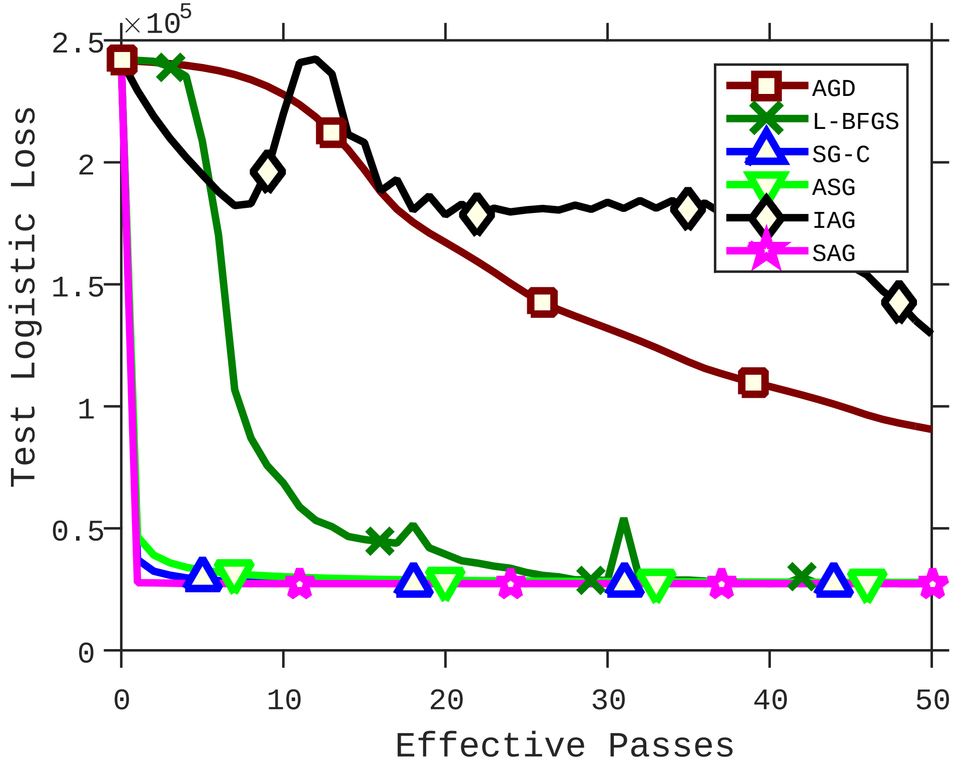

SGD minimizes the testing cost!

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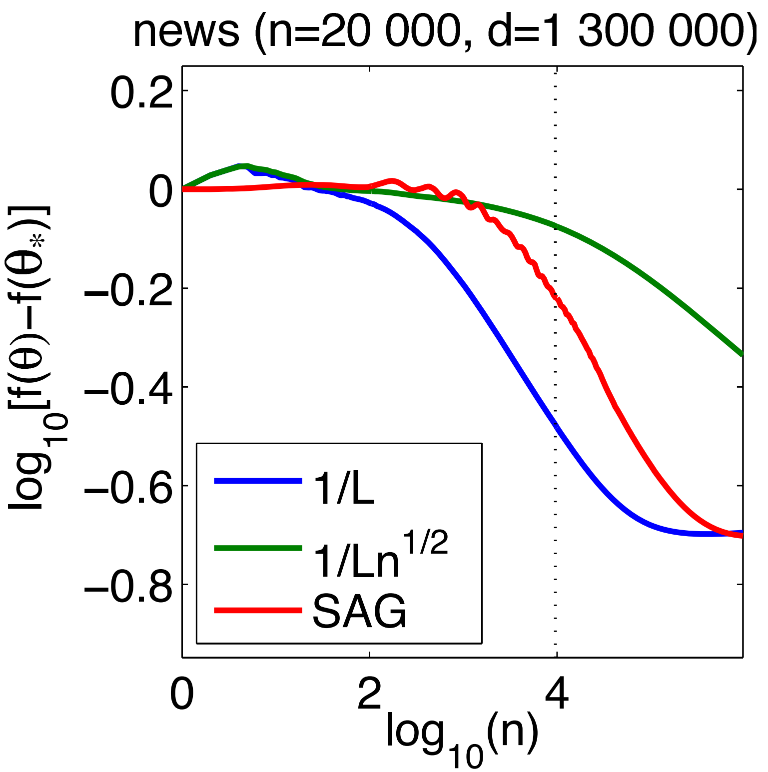
- **Constant-step-size SGD**
  - Linear convergence up to the noise level for strongly-convex problems (Solodov, 1998; Nedic and Bertsekas, 2000)
  - Full convergence and robustness to ill-conditioning?

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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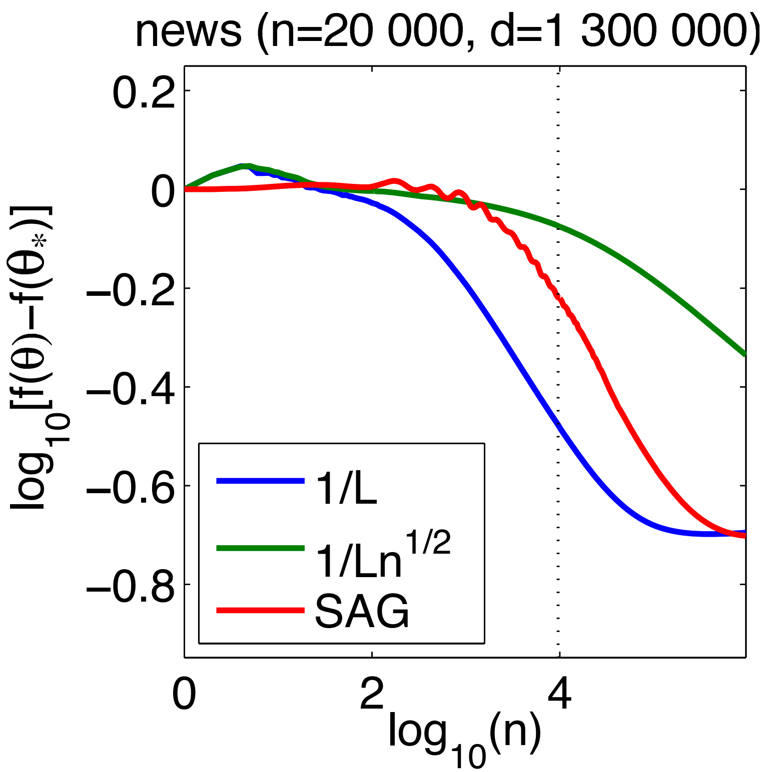

- Convergence in $O(1/n)$ for smooth losses with $O(d)$ online Newton step

Conclusions - Convex optimization

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  - Provable and precise rates
  - Improves on two known lower-bounds (by using structure)
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- **What's next: non-convex, non-i.i.d., non-serial**

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