Linearly-Convergent Stochastic Gradient Algorithms

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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

Tour de France 2014  Translate this page
www.letour.fr  
Tour de France 2014 - Site officiel de la célèbre course cycliste Le Tour de France.
Contient les itinéraires, coureurs, équipes et les infos des Tours passés.

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Tour de France (cyclisme) — Wikipédia  Translate this page
fr.wikipedia.org/wiki/Tour_de_France_(cyclisme)  
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 LAuto.
Histoire  Médiation du … Equipes et participation
Visual object recognition
**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
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- **Examples**: computer vision, advertising, bioinformatics, etc.

- **Ideal running-time complexity**: $O(dn)$
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Machine learning for large-scale data

- Large-scale supervised machine learning: \textit{large }$d$, \textit{large }$n$
  - $d$: dimension of each observation (input), or number of parameters
  - $n$: number of observations

- Examples: computer vision, advertising, bioinformatics, etc.

- 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. Stochastic average gradient (SAG)
   - Linearly-convergent stochastic gradient method
   - Precise convergence rates

3. Extensions
   - Link with variance reduction
   - Acceleration
   - Saddle-point problems
Parametric supervised machine learning

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

- **Prediction function** $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
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- **Motivating examples**
  - Linear predictions: $h(x, \theta) = \theta^\top \Phi(x)$ with features $\Phi(x) \in \mathbb{R}^d$
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- **Motivating examples**
  - Linear predictions: \( h(x, \theta) = \theta^\top \Phi(x) \) with features \( \Phi(x) \in \mathbb{R}^d \)
  - Neural networks: \( h(x, \theta) = \theta_m^\top \sigma(\theta_{m-1}^\top \sigma(\cdots \theta_2^\top \sigma(\theta_1^\top x))) \)
Parametric supervised machine learning

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

- **(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**: $y \in \mathbb{R}$
  - Quadratic loss $\ell(y, h(x, \theta)) = \frac{1}{2}(y - h(x, \theta))^2$
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### Usual losses

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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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\]

\( f_i(\theta) \) = data fitting term + regularizer
Parametric supervised machine learning

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$$

- **Optimization**: optimization of regularized risk

- **training cost**
Parametric supervised machine learning

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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
Finite sums in signal processing

- Model fitting

  \[ \min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta) \]
Finite sums in signal processing

- Model fitting

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

  - Differences: (1) Typically need high precision for \( \theta \)
    (2) Data \((x_i, y_i)\) may not be i.i.d.
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• Model fitting

  - *Same optimization problem:* \[
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  - *Differences:* 
    (1) Typically need high precision for \(\theta\)
    (2) Data \((x_i, y_i)\) may not be i.i.d.

• Structured regularization

  - E.g., total variation \(\sum_{i \sim j} |\theta_i - \theta_j|\)
A function $g : \mathbb{R}^d \rightarrow \mathbb{R}$ is $L$-smooth if and only if it is twice differentiable and

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

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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 $g : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if
  $$\forall \theta \in \mathbb{R}^d, \text{ eigenvalues } [g''(\theta)] \geq 0$$

convex
**Smoothness and (strong) convexity**

- A twice differentiable function $g : \mathbb{R}^d \to \mathbb{R}$ is $\mu$-strongly convex if and only if
  \[
  \forall \theta \in \mathbb{R}^d, \text{ eigenvalues} [g''(\theta)] \geq \mu
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- Condition number $\kappa = L/\mu \geq 1$

(small $\kappa = L/\mu$)  
(large $\kappa = L/\mu$)
Smoothness and (strong) convexity

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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
Smoothness and (strong) convexity

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- **Strong 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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  - 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!
**Smoothness and (strong) convexity**

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

\[ g(\theta_t) - g(\theta^*) \leq O\left(\frac{1}{t}\right) \]

\[ g(\theta_t) - g(\theta^*) \leq O\left(e^{-\frac{t}{\kappa}}\right) = O\left(e^{-\frac{t}{L/\mu}}\right) \]

(small $\kappa = L/\mu$) \hspace{2cm} (large $\kappa = L/\mu$)
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  $g(\theta_t) - g(\theta_*) \leq O\left(\frac{1}{t}\right)$
  
  $g(\theta_t) - g(\theta_*) \leq O\left((1-\mu/L)^t\right) = O\left(e^{-t(\mu/L)}\right)$ if $\mu$-strongly convex

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

- **Assumption:** $g$ convex and $L$-smooth on $\mathbb{R}^d$

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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 \( \{1, \ldots, n\} \)
  - Polyak-Ruppert averaging: \( \bar{\theta}_t = \frac{1}{t+1} \sum_{u=0}^{t} \theta_u \)
Stochastic gradient descent (SGD) for finite sums

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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
  - Running-time complexity: \( O(d \cdot \kappa/\varepsilon) \)
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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

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- Batch gradient descent: $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1}) = \theta_{t-1} - \gamma_t \sum_{i=1}^{n} f'_i(\theta_{t-1})$
  
  - Linear (e.g., exponential) convergence rate in $O(e^{-t/\kappa})$
  - Iteration complexity is linear in $n$
Stochastic vs. deterministic methods

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

• Stochastic gradient descent: $\theta_t = \theta_{t-1} - \gamma_t f_{i(t)}'(\theta_{t-1})$
  
  – Sampling with replacement: $i(t)$ random element of $\{1, \ldots, n\}$
  – 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 $f_i(\theta) = \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta)$

- **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

![Graph showing log(excess cost) vs. time for stochastic and deterministic methods.](image-url)
**Stochastic vs. deterministic methods**

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

- **Generic acceleration** (Nesterov, 1983, 2004)

\[ \theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t (\theta_t - \theta_{t-1}) \]
Accelerating gradient methods - Related work

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\[ \theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t (\theta_t - \theta_{t-1}) \]

- Good choice of momentum term \( \delta_t \in [0, 1) \)

\[ g(\theta_t) - g(\theta_*) \leq O\left(\frac{1}{t^2}\right) \]

\[ g(\theta_t) - g(\theta_*) \leq O\left(e^{-t\sqrt{\frac{\mu}{L}}}\right) = O\left(e^{-t/\sqrt{\kappa}}\right) \text{ if } \mu-\text{strongly convex} \]

- **Optimal rates** after \( t = O(d) \) iterations (Nesterov, 2004)
**Accelerating gradient methods - Related work**

- **Generic acceleration** (Nesterov, 1983, 2004)

  \[ \theta_t = \eta_{t-1} - \gamma_t g'(\eta_{t-1}) \text{ and } \eta_t = \theta_t + \delta_t (\theta_t - \theta_{t-1}) \]

  - Good choice of momentum term \( \delta_t \in [0, 1) \)

  \[ g(\theta_t) - g(\theta_*) \leq O\left(\frac{1}{t^2}\right) \]

  \[ g(\theta_t) - g(\theta_*) \leq O\left(e^{-t\sqrt{\mu/L}}\right) = O\left(e^{-t/\sqrt{\kappa}}\right) \text{ if } \mu\text{-strongly convex} \]

  - **Optimal rates** after \( t = O(d) \) iterations (Nesterov, 2004)

  - Still \( O(nd) \) iteration cost: complexity \( = O(n d \cdot \sqrt{\kappa} \log \frac{1}{\varepsilon}) \)
Accelerating gradient methods - Related work

- Constant step-size stochastic gradient
  - Solodov (1998); Nedic and Bertsekas (2000)
  - Linear convergence, but only up to a fixed tolerance
Accelerating gradient methods - Related work

- **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 (SAG) iteration

- Keep in memory the gradients of all functions $f_i$, $i = 1, \ldots, n$
- Random selection $i(t) \in \{1, \ldots, n\}$ with replacement
- Iteration: $\theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^{n} y^t_i$ with $y^t_i = \begin{cases} f'_i(\theta_{t-1}) & \text{if } i = i(t) \\ y^t_{i-1} & \text{otherwise} \end{cases}$
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(Le Roux, Schmidt, and Bach, 2012)

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functions $g = \frac{1}{n} \sum_{i=1}^{n} f_i$ \hspace{1cm} f_1 \hspace{0.2cm} f_2 \hspace{0.2cm} f_3 \hspace{0.2cm} f_4 \hspace{0.5cm} \ldots \hspace{0.5cm} f_{n-1} \hspace{0.5cm} f_n$

gradients $\in \mathbb{R}^d$ $\frac{1}{n} \sum_{i=1}^{n} y_i^t$ \hspace{0.2cm} y_1^t \hspace{0.2cm} y_2^t \hspace{0.2cm} y_3^t \hspace{0.2cm} y_4^t \hspace{0.5cm} \ldots \hspace{0.5cm} y_{n-1}^t \hspace{0.5cm} y_n^t$
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functions $g = \frac{1}{n} \sum_{i=1}^{n} f_i$  
$f_1 \quad f_2 \quad f_3 \quad f_4 \quad \cdots \quad f_{n-1} \quad f_n$

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functions \( g = \frac{1}{n} \sum_{i=1}^{n} f_i \)

gradients \( \in \mathbb{R}^d \)

\[
\begin{align*}
\frac{1}{n} \sum_{i=1}^{n} y_i^t & \quad y_1^t & \quad y_2^t & \quad y_3^t & \quad y_4^t & \quad \ldots & \quad y_{n-1}^t & \quad y_n^t
\end{align*}
\]
Stochastic average gradient
(Le Roux, Schmidt, and Bach, 2012)

• **Stochastic average gradient** (SAG) iteration
  
  – Keep in memory the gradients of all functions \( f_i, i = 1, \ldots, n \)
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• Stochastic version of incremental average gradient (Blatt et al., 2008)
Stochastic average gradient
(Le Roux, Schmidt, and Bach, 2012)

• Stochastic average gradient (SAG) iteration
  – Keep in memory the gradients of all functions $f_i$, $i = 1, \ldots, n$
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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, $i = 1, \ldots, n$
  - $g = \frac{1}{n} \sum_{i=1}^{n} f_i$ is $\mu$-strongly convex
  - Constant step size $\gamma_t = 1/(16L)$ - no need to know $\mu$
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• Strongly convex case (Le Roux et al., 2012; Schmidt et al., 2016)

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

  – Linear (exponential) convergence rate with $O(d)$ iteration cost
**Stochastic average gradient - Convergence analysis**

- **Assumptions**
  - Each $f_i$ is $L$-smooth, $i = 1, \ldots, n$
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- **Strongly convex case** (Le Roux et al., 2012; Schmidt et al., 2016)
  \[
  \mathbb{E}[g(\theta_t) - g(\theta_*)] \leq \text{cst} \times \exp\left(-t \cdot \min\left\{\frac{1}{8n}, \frac{\mu}{16L}\right\}\right)
  \]
  - 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

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Running time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stochastic gradient descent</td>
<td>( d \times \frac{L}{\mu} \times \frac{1}{\varepsilon} )</td>
</tr>
<tr>
<td>Gradient descent</td>
<td>( d \times n \frac{L}{\mu} \times \log \frac{1}{\varepsilon} )</td>
</tr>
<tr>
<td>Accelerated gradient descent</td>
<td>( d \times n \sqrt{\frac{L}{\mu}} \times \log \frac{1}{\varepsilon} )</td>
</tr>
<tr>
<td>SAG</td>
<td>( d \times (n + \frac{L}{\mu}) \times \log \frac{1}{\varepsilon} )</td>
</tr>
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</table>

- 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)

- **Assumptions:** \( g(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) \)
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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 (\( \mu = 0 \))

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<tr>
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• 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
$(n = 697,641, d = 47,236)$
Experimental results (logistic regression)

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

rcv1 dataset
$(n = 697\,641, d = 47\,236)$
Before non-uniform sampling

protein dataset

\[(n = 145\,751, \quad d = 74)\]

sido dataset

\[(n = 12\,678, \quad d = 4\,932)\]
After non-uniform sampling

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

sido dataset
\((n = 12,678, d = 4,932)\)
From training to testing errors

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

Training cost
From training to testing errors

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

1. Introduction/motivation: Supervised machine learning
   - Optimization of finite sums
   - Existing optimization methods for finite sums

2. Stochastic average gradient (SAG)
   - Linearly-convergent stochastic gradient method
   - Precise convergence rates

3. Extensions
   - Link with variance reduction
   - Acceleration
   - Saddle-point problems
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)
  – ...

• Similar rates of convergence and iterations
Linearly convergent stochastic gradient algorithms

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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

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

- $\mathbb{E}Z_\alpha = \alpha\mathbb{E}X + (1 - \alpha)\mathbb{E}Y$
- $\text{var}(Z_\alpha) = \alpha^2\left[ \text{var}(X) + \text{var}(Y) - 2\text{cov}(X, Y) \right]$
- $\alpha = 1$: no bias, $\alpha < 1$: potential bias (but reduced variance)
- Useful if $Y$ positively correlated with $X$
**Variance reduction**

- **Principle**: reducing variance of sample of $X$ by using a sample from another random variable $Y$ with known expectation

$$Z_\alpha = \alpha(X - Y) + EY$$

- $EZ_\alpha = \alpha EX + (1 - \alpha) EY$
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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
  - $EY = \frac{1}{n} \sum_{i=1}^{n} f'_i(\tilde{\theta})$ 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
    $$\theta_t = \theta_{t-1} - \gamma \left[ g'(\tilde{\theta}) + (f'_{i(t)}(\theta_{t-1}) - f'_{i(t)}(\tilde{\theta})) \right]$$
  - Update $\tilde{\theta} = \theta_t$
- Output: $\tilde{\theta}$

- 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
Stochastic variance reduced gradient (SVRG) (Johnson and Zhang, 2013; Zhang et al., 2013)

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Interpretation of SAG as variance reduction

- **SAG update**: \( \theta_t = \theta_{t-1} - \frac{\gamma}{n} \sum_{i=1}^{n} y^t_i \) with \( y^t_i = \begin{cases} f'_i(\theta_{t-1}) & \text{if } i = i(t) \\ y^t_{i-1} & \text{otherwise} \end{cases} \)
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  - Interpretation as lazy gradient evaluations

- **SAG update:** \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} y_{i(t)}^{t-1} + \frac{1}{n} (f'_{i(t)}(\theta_{t-1}) - y_{i(t)}^{t-1}) \right] \)
  
  - Biased update (expectation w.r.t. to \( i(t) \) not equal to full gradient)
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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• SVRG update: \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} f_i'(\tilde{\theta}) + (f_i'(\theta_{t-1}) - f_i'(\tilde{\theta})) \right] \)
  
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- **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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- **SAG update**: \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} y_i^{t-1} + \frac{1}{n} (f'_i(t)(\theta_{t-1}) - y_{i(t)}^{t-1}) \right] \)

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- **SVRG update**: \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} f'_i(\tilde{\theta}) + (f'_i(t)(\theta_{t-1}) - f'_i(t)(\tilde{\theta})) \right] \)

  - Unbiased update

- **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**: \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} y_{i(t)}^{t-1} + \left( f_{i(t)}'(\theta_{t-1}) - y_{i(t)}^{t-1} \right) \right] \)

- **SVRG update**: \( \theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} f_{i}(\tilde{\theta}) + \left( f_{i(t)}'(\theta_{t-1}) - f_{i(t)}'(\tilde{\theta}) \right) \right] \)

<table>
<thead>
<tr>
<th></th>
<th>SAGA</th>
<th>SVRG</th>
</tr>
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<tbody>
<tr>
<td><strong>Storage of gradients</strong></td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td><strong>Epoch-based</strong></td>
<td>no</td>
<td>yes</td>
</tr>
<tr>
<td><strong>Parameters</strong></td>
<td>step-size</td>
<td>step-size &amp; epoch lengths</td>
</tr>
<tr>
<td><strong>Gradient evaluations per step</strong></td>
<td>1</td>
<td>at least 2</td>
</tr>
<tr>
<td><strong>Adaptivity to strong-convexity</strong></td>
<td>yes</td>
<td>no</td>
</tr>
<tr>
<td><strong>Robustness to ill-conditioning</strong></td>
<td>yes</td>
<td>no</td>
</tr>
</tbody>
</table>

– 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
  - $h$ convex, potentially non-smooth
Proximal extensions

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  - \( f_i \) smooth and convex
  - \( h \) convex, potentially non-smooth
  - Constrained optimization: \( h(\theta) = 0 \) if \( \theta \in K \), and \( +\infty \) otherwise
  - Sparsity-inducing norms, e.g., \( h(\theta) = \|\theta\|_1 \)
Proximal extensions

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  - Constrained optimization: \(h(\theta) = 0\) if \(\theta \in K\), and \(+\infty\) otherwise
  - Sparsity-inducing norms, e.g., \(h(\theta) = \|\theta\|_1\)

- **Proximal methods (a.k.a. splitting methods)**
  - Extra projection / soft thresholding step after gradient update
  - See, e.g., Combettes and Pesquet (2011); Bach, Jenatton, Mairal, and Obozinski (2012); Parikh and Boyd (2014)
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
  - \( h \) convex, potentially non-smooth
  - Constrained optimization: \( h(\theta) = 0 \) if \( \theta \in K \), and \(+\infty\) otherwise
  - Sparsity-inducing norms, e.g., \( h(\theta) = \|\theta\|_1 \)

- **Proximal methods** (a.k.a. splitting methods)
  - Extra projection / soft thresholding step after gradient update
  - See, e.g., Combettes and Pesquet (2011); Bach, Jenatton, Mairal, and Obozinski (2012); Parikh and Boyd (2014)

- **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)

<table>
<thead>
<tr>
<th>Method</th>
<th>Complexity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gradient descent</td>
<td>( d \times n \frac{L}{\mu} \times \log \frac{1}{\epsilon} )</td>
</tr>
<tr>
<td>Accelerated gradient descent</td>
<td>( d \times n \sqrt{\frac{L}{\mu}} \times \log \frac{1}{\epsilon} )</td>
</tr>
<tr>
<td>SAG(A), SVRG, SDCA, MISO</td>
<td>( d \times (n + \frac{L}{\mu}) \times \log \frac{1}{\epsilon} )</td>
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### Acceleration

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- **Catalyst** (Lin, Mairal, and Harchaoui, 2015)
  - Widely applicable generic acceleration scheme
Saddle-point problems
(Balamurugan and Bach, 2016)

• Lazy evaluation / variance reduction beyond gradient descent
  – As soon as an iterative algorithm uses a large finite sum
Saddle-point problems
(Balamurugan and Bach, 2016)

• **Goal:** Solve
\[
\min_{\theta \in \mathbb{R}^d} \max_{\alpha \in \mathbb{R}^m} L(\theta, \alpha) = \frac{1}{n} \sum_{i=1}^{n} K_i(\alpha, \theta)
\]

  – \( L \) convex/concave
  – **Example:**
\[
\min_{\theta \in \mathbb{R}^d} \max_{\alpha \in \mathbb{R}^m} h(\theta) - f^*(\alpha) + \alpha^\top K \theta = \min_{\theta \in \mathbb{R}^d} h(\theta) + f(K\theta)
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• **Forward method:**
  \[
  \begin{align*}
  \theta_t &= \theta_{t-1} - \gamma \frac{\partial L}{\partial \theta}(\theta_{t-1}, \alpha_{t-1}) \\
  \alpha_t &= \alpha_{t-1} + \gamma \frac{\partial L}{\partial \alpha}(\theta_{t-1}, \alpha_{t-1})
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• **SAG(A) / SVRG** can be straightforwardly applied

  - Convergence proof applies to all **monotone operators**
  
  - Strongly convex/concave problems with proximal operators
  
  - No need for convex/concavity of each \( K_i \)
  
  - Catalyst acceleration is particularly simple
Saddle-point problems  
(Balamurugan and Bach, 2016)

• sido dataset \( (n = 12,678, \, d = 4,932) \)
  - Convex surrogate to area under the ROC curve (AUC)
Conclusions

- **Linearly-convergent stochastic gradient methods**
  - Provable and precise rates
  - Improves on two known lower-bounds (by using structure)
  - Several extensions / interpretations / accelerations
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  – Bounds on testing errors for incremental methods
  – Parallelization (Leblond et al., 2016)
  – Non-convex problems (Reddi et al., 2016)
  – Other forms of acceleration (Scieur, d’Aspremont, and Bach, 2016)
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References


