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 2013 - Site officiel de la célèbre course cycliste Le Tour de France.
Contient les itinéraires, coureurs, équipes et les infos des Tours passés.

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 L’Auto.
Histoire · Médiation du ... · Équipes et participation
Visual object recognition
Context

Machine learning for large-scale data

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  – \( d \) : 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**: large $d$, 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. 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*
  – 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 $(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}, \ i = 1, \ldots, n$

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

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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

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 $\theta \in \mathbb{R}^d$

(Regularized) empirical risk minimization: find $\hat{\theta}$ solution of

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

data fitting term + regularizer
Usual losses

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

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  – quadratic loss \( \ell(y, h(x, \theta)) = \frac{1}{2}(y - h(x, \theta))^2 \)

• **Classification:** \( y \in \{-1, 1\} \)
  
  – Logistic loss \( \ell(y, h(x, \theta)) = \log(1 + \exp(-yh(x, \theta))) \)
Usual losses

- **Regression**: \( y \in \mathbb{R} \)
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- **Classification**: \( y \in \{-1, 1\} \)
  - Logistic loss \( \ell(y, h(x, \theta)) = \log(1 + \exp(-yh(x, \theta))) \)

- **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)
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 $\theta \in \mathbb{R}^d$

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

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\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \left\{ \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta) \right\} = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)
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data fitting term + regularizer
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  data fitting term + regularizer

- **Optimization**: optimization of regularized risk training cost
Supervised machine learning

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

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

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

  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

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

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

- 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

\[
\forall \theta \in \mathbb{R}^d, \text{ eigenvalues}[g''(\theta)] \succeq 0
\]
Smoothness and (strong) convexity

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

$$\forall \theta \in \mathbb{R}^d, \text{ eigenvalues} \left[ g''(\theta) \right] \geq \mu$$
Smoothness and (strong) convexity

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

(small $\kappa = L/\mu$)  \hspace{3cm} (large $\kappa = L/\mu$)
Smoothness and (strong) convexity

- A twice differentiable function $g : \mathbb{R}^d \to \mathbb{R}$ is $\mu$-strongly convex if and only if
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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 $h(x, \theta) = \theta^\top \Phi(x)$
Smoothness and (strong) convexity

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

- **Strong convexity in machine learning**
  - With $g(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i, \theta))$
  - Strongly convex loss and linear predictions $h(x, \theta) = \theta^\top \Phi(x)$
Smoothness and (strong) convexity

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• **Strong convexity in machine learning**
  
  – With $g(\theta) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, h(x_i, \theta))$
  
  – Strongly convex loss and linear predictions $h(x, \theta) = \theta^\top \Phi(x)$
  
  – 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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- **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!

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

(small $\kappa = L/\mu$) (large $\kappa = L/\mu$)
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- **Gradient descent**: $\theta_t = \theta_{t-1} - \gamma_t g'(\theta_{t-1})$

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

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

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

(large $\kappa = L/\mu$)
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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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  - \( O(e^{-t/\kappa}) \) linear if strongly-convex \( \iff \) complexity = \( O(nd \cdot \kappa \log \frac{1}{\epsilon}) \)

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  - \( O(e^{-\rho^2 t}) \) quadratic rate \( \iff \) complexity = \( O((nd^2 + d^3) \cdot \log \log \frac{1}{\epsilon}) \)
Iterative methods for minimizing smooth functions

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

- **Gradient descent**: \( \theta_t = \theta_{t-1} - \gamma_t \nabla g(\theta_{t-1}) \)
  - \( O(1/t) \) convergence rate for convex functions
  - \( O(e^{-t/\kappa}) \) *linear* if strongly-convex \( \Leftrightarrow \) complexity \( = O(nd \cdot \kappa \log \frac{1}{\varepsilon}) \)

- **Newton method**: \( \theta_t = \theta_{t-1} - (\nabla^2 g(\theta_{t-1}))^{-1} \nabla g(\theta_{t-1}) \)
  - \( O(e^{-\rho^2 t}) \) *quadratic* rate \( \Leftrightarrow \) complexity \( = O((nd^2 + d^3) \cdot \log \log \frac{1}{\varepsilon}) \)

- **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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- **Key insights for machine learning** (Bottou and Bousquet, 2008)
  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 \( \{1, \ldots, n\} \)
  - 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
  - Adaptivity with self-concordance assumption (Bach, 2014)
  - Running-time complexity: \( O(d \cdot \kappa/\varepsilon) \)
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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 $f_i(\theta) = \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta)$

• 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 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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  - 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 decrease in log(excess cost) over time for both stochastic and deterministic methods](attachment:image)
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)

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

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

- Good choice of momentum term \( \delta_t \in [0, 1) \)
  \[ g(\theta_t) - g(\theta^*) \leq O\left(1/t^2\right) \]
  \[ g(\theta_t) - g(\theta^*) \leq O\left(e^{-t\sqrt{\mu/L}}\right) = O\left(e^{-t/\sqrt{\kappa}}\right) \text{ if } \mu\text{-strongly convex} \]
- Optimal rates after \( t = O(d) \) iterations (Nesterov, 2004)
**Accelerating gradient methods - Related work**

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

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

  - Good choice of momentum term \( \delta_t \in [0, 1) \)
  
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  \[ g(\theta_t) - g(\theta_*) \leq O(e^{-t\sqrt{\mu/L}}) = O(e^{-t/\sqrt{\kappa}}) \text{ if } \mu\text{-strongly convex} \]

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

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

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- **Stochastic methods in the dual (SDCA)**
  - Shalev-Shwartz and Zhang (2013)
  - Similar linear rate but limited choice for the $f_i$'s
  - Extensions without duality: see Shalev-Shwartz (2016)
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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 $f_i$, $i = 1, \ldots, n$
  - Random selection $i(t) \in \{1, \ldots, n\}$ with replacement
  - Iteration: $\theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^{n} y_i^t$ with $y_i^t = \begin{cases} 
  f_i'(\theta_{t-1}) & \text{if } i = i(t) \\
  y_{i}^{t-1} & \text{otherwise}
\end{cases}$
Stochastic average gradient
(Le Roux, Schmidt, and Bach, 2012)

- **Stochastic average gradient** (SAG) iteration
  - Keep in memory the gradients of all functions \( f_i, i = 1, \ldots, n \)
  - 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 \( y^t_i = \begin{cases} f'_i(\theta_{t-1}) & \text{if } i = i(t) \\ y^t_{i-1} & \text{otherwise} \end{cases} \)

functions \( g = \frac{1}{n} \sum_{i=1}^{n} f_i \) \( f_1 \quad f_2 \quad f_3 \quad f_4 \quad \cdots \quad f_{n-1} \quad f_n \)

gradients \( \in \mathbb{R}^d \) \( \frac{1}{n} \sum_{i=1}^{n} y^t_i \) \( y^t_1 \quad y^t_2 \quad y^t_3 \quad y^t_4 \quad \cdots \quad y^t_{n-1} \quad y^t_n \)
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    $$\theta_t = \theta_{t-1} - \frac{\gamma_t}{n} \sum_{i=1}^{n} y_i^t$$  
    with  
    $$y_i^t = \begin{cases} 
    f'_i(\theta_{t-1}) & \text{if } i = i(t) \\
    y_i^{t-1} & \text{otherwise}
    \end{cases}$$

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

gradients  
$$\in \mathbb{R}^d$$  
$$\frac{1}{n} \sum_{i=1}^{n} y_i^t$$  
$$y_1^t, y_2^t, y_3^t, y_4^t \ldots y_{n-1}^t, y_n^t$$
**Stochastic average gradient**
*(Le Roux, Schmidt, and Bach, 2012)*

- **Stochastic average gradient** (SAG) iteration
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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 $\mu$
Stochastic average gradient - Convergence analysis

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  - constant step size $\gamma_t = 1/(16L)$ - no need to know $\mu$

• 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

<table>
<thead>
<tr>
<th>Method</th>
<th>Running Time</th>
</tr>
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<tbody>
<tr>
<td>Stochastic gradient descent</td>
<td>( d \times \frac{L}{\mu} \times \frac{1}{\varepsilon} )</td>
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<tr>
<td>Gradient descent</td>
<td>( d \times n\frac{L}{\mu} \times \log \frac{1}{\varepsilon} )</td>
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<tr>
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<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>
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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: \( g(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta) \)

  – Each \( f_i \) convex \( L \)-smooth and \( g \) \( \mu \)-strongly convex

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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 ⇒ 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

Experimental results (logistic regression)

**quantum dataset**

\((n = 50,000, \quad d = 78)\)

**rcv1 dataset**

\((n = 697,641, \quad d = 47,236)\)
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
$(n = 145\,751, \; d = 74)$

sido dataset
$(n = 12\,678, \; d = 4\,932)$
After non-uniform sampling

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

sido dataset
(n = 12,678, d = 4,932)
Linearly convergent stochastic gradient algorithms

• Many related algorithms
  – SAG (Le Roux et al., 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
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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

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

- $EZ_\alpha = \alpha EX + (1 - \alpha) EY$
- $\text{var}(Z_\alpha) = \alpha^2 [\text{var}(X) + \text{var}(Y) - 2 \text{cov}(X, Y)]$
- $\alpha = 1$: no bias, $\alpha < 1$: potential bias (but reduced variance)
- 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
- $EY = \frac{1}{n} \sum_{i=1}^{n} f'_i(\tilde{\theta})$ 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
    \[
    \theta_t = \theta_{t-1} - \gamma \left[ g'(\tilde{\theta}) + (f'_i(\theta_{t-1}) - f'_i(\tilde{\theta})) \right]
    \]
  - Update $\tilde{\theta} = \theta_t$
- Output: $\tilde{\theta}$

- No need to store gradients - two gradient evaluations per inner step
- Two parameters: lengths of epoch + step-size
- 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 \( y_i^t = \begin{cases} f'_i(\theta_{t-1}) & \text{if } i = i(t) \\ y_{i}^{t-1} & \text{otherwise} \end{cases} \)

- Interpretation as lazy gradient evaluations
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  - Interpretation as lazy gradient evaluations

- SAG update: $\theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} y_i^{t-1} + \frac{1}{n} (f_i'(t)(\theta_{t-1}) - y_i^{t-1}) \right]$

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

  - Unbiased update
Interpretation of SAG as variance reduction

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

  - Interpretation as lazy gradient evaluations

- **SAG update**: $\theta_t = \theta_{t-1} - \gamma \left[ \frac{1}{n} \sum_{i=1}^{n} y^t_i - 1 + \frac{1}{n} (f'_i(\theta_{t-1}) - y^t_{i(t)}) \right]$  

  - Biased update (expectation w.r.t. to $i(t)$ not equal to full gradient)

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

  - Unbiased update

- **SAGA update**: $\theta_t = \theta_{t-1} - \gamma_t \left[ \frac{1}{n} \sum_{i=1}^{n} y^t_i + (f'_i(\theta_{t-1}) - y^t_{i(t)}) \right]$

  - Defazio, Bach, and Lacoste-Julien (2014a)

  - Unbiased update without epochs
SVRG vs. SAGA

- SAGA update: $\theta_t = \theta_{t-1} - \gamma_t \left[ \frac{1}{n} \sum_{i=1}^{n} y_i^{t-1} + (f'_i(t) - y_i^{t-1}) \right]$

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

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

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<td>$d n \frac{L}{\mu} \times \log \frac{1}{\varepsilon}$</td>
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<td>$d n \sqrt{\frac{L}{\mu}} \times \log \frac{1}{\varepsilon}$</td>
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<td>SAG(A), SVRG, SDCA, MISO</td>
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<tr>
<td>Accelerated versions</td>
<td>$d(n + \sqrt{n\frac{L}{\mu}}) \times \log \frac{1}{\varepsilon}$</td>
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- **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

Training cost

![Graph showing training cost with effective passes and objective minus optimum values.](image)
From training to testing errors

- rcv1 dataset \((n = 697\,641, d = 47\,236)\)
  - NB: IAG, SG-C, ASG with optimal step-sizes in hindsight
 SGD minimizes the testing cost!

- **Goal**: minimize $f(\theta) = \mathbb{E}_{p(x,y)} \ell(y, \theta^\top \Phi(x))$
  
  - Given $n$ independent samples $(x_i, y_i), i = 1, \ldots, n$ 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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- **Optimal convergence rates**: $O(1/\sqrt{n})$ and $O(1/(n\mu))$
  - Optimal for non-smooth losses (Nemirovski and Yudin, 1983)
  - Attained by averaged SGD with decaying step-sizes
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  - Attained by averaged SGD with decaying step-sizes

- **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 $\mu$
  - Simple choice of step-size (equal to $1/L$)
Robust averaged stochastic gradient  
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- Convergence in $O(1/n)$ for smooth losses with $O(d)$ online Newton step
Conclusions - Convex optimization

- Linearly-convergent stochastic gradient methods
  - Provable and precise rates
  - Improves on two known lower-bounds (by using structure)
  - Several extensions / interpretations / accelerations
Conclusions - Convex optimization

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  – Provable and precise rates
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• Extensions and future work
  – Extension to saddle-point problems (Balamurugan and Bach, 2016)
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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)
References


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