Minimizing Finite Sums with the Stochastic Average Gradient Algorithm

Mark Schmidt

Joint work with Nicolas Le Roux and Francis Bach

University of British Columbia

Context: Machine Learning for "Big Data"

- **Large-scale machine learning**: large N, large P
  - N: number of observations (inputs)
  - P: dimension of each observation
- **Regularized empirical risk minimization**: find x^* solution of

$$\min_{x \in \mathbb{R}^P} \frac{1}{N} \sum_{i=1}^{N} \ell(x^T a_i) \quad + \quad \lambda r(x)$$

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- Applications to any data-oriented field:
  - Vision, bioinformatics, speech, natural language, web.
- Main practical challenges:
  - Choosing regularizer r and data-fitting term ℓ.
  - Designing/learning good features a_i.
  - Efficiently solving the problem when N or P are very large.

This talk: Big-N Problems

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- We are interested in cases where N is very large.
- We will focus on strongly-convex functions g.
- Simplest example is ℓ_2-regularized least-squares,

$$f_i(x) := (a_i^T x - b_i)^2 + \frac{\lambda}{2}\|x\|^2.$$

- Other examples include any ℓ_2-regularized convex loss:
  - logistic regression, Huber regression, smooth SVMs, CRFs, etc.

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- Stochastic gradient method [Robbins & Monro, 1951]:
  - Random selection of $i(t)$ from $\{1, 2, \ldots, N\}$,

$$x_{t+1} = x_t - \alpha_t f_{i(t)}'(x_t).$$

  - Iteration cost is independent of N.
  - Sublinear convergence rate: $O(1/t)$.

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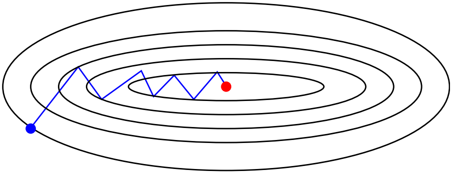

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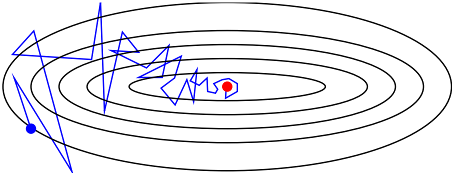

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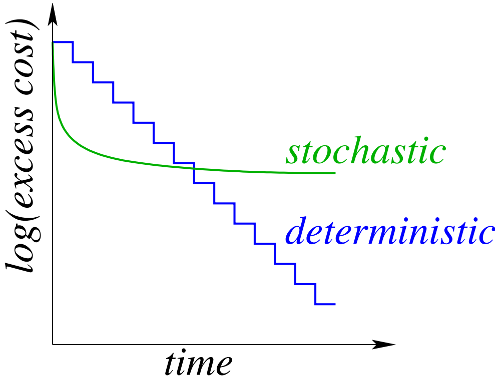
- FG method has $O(N)$ cost with $O(\rho^t)$ rate.
- SG method has $O(1)$ cost with $O(1/t)$ rate.



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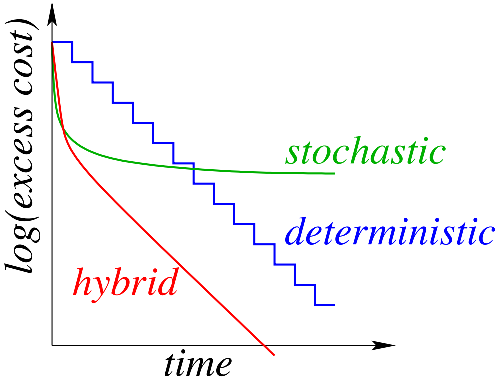

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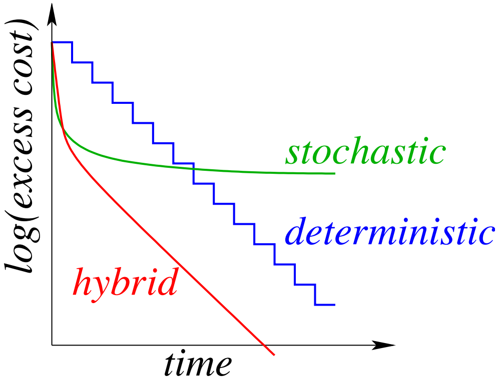

- Goal is $O(1)$ cost with $O(\rho^k)$ rate.

Prior Work on Speeding up SG Methods

A variety of methods have been proposed to speed up SG methods:

- **Step-size strategies, momentum, gradient/iterate averaging**
  - Polyak & Juditsky (1992), Tseng (1998), Kushner & Yin (2003) Nesterov (2009), Xiao (2010), Hazan & Kale (2011), Rakhlin et al. (2012)
- **Stochastic version of accelerated and Newton-like methods**
  - Bordes et al. (2009), Sunehag et al. (2009), Ghadimi and Lan (2010), Martens (2010), Xiao (2010), Duchi et al. (2011)

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- None of these methods improve on the $O(1/t)$ rate

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Existing linear convergence results:

- **Constant step-size SG, accelerated SG**
  - Kesten (1958), Delyon and Juditsky (1993), Nedic and Bertsekas (2000)
  - Linear convergence up to a fixed tolerance: $O(\rho^t) + O(\alpha)$.
- **Hybrid methods, incremental average gradient**
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- **Special Problems Classes**
  - Collins et al. (2008), Strohmer & Vershynin (2009), Schmidt and Le Roux (2012), Shalev-Shwartz and Zhang (2012)
  - Linear rate but limited choice for the f_i's

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    - Randomly select $i(t)$ from $\{1, 2, \ldots, N\}$ and compute $f'_{i(t)}(x^t)$.

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  - Assumes that gradients of other examples don't change.
  - This assumption becomes accurate as $||x^{t+1} - x^t|| \to 0$.
  - Stochastic variant of increment aggregated gradient (IAG). [Blatt et al. 2007]

Convergence Rate of SAG: Attempt 1

Proposition 1. *With* $\alpha_t = \frac{1}{2NL}$ *the SAG iterations satisfy*

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- **Convergence rate of $O(\rho^t)$ with cost of $O(1)$.**
- Is this useful?!?
- This rate is very slow: performance similar to cyclic method.

Convergence Rate of SAG: Attempt 2

***Proposition 2**. With $\alpha_t \in [\frac{1}{2N\mu}, \frac{1}{16L}]$ and $N \geq 8\frac{L}{\mu}$, the SAG iterations satisfy*

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- Much bigger step-sizes: $\mu << L$ and $L << NL$ (causes cyclic algorithm to diverge)
- Gives constant non-trivial reduction per pass:

$$\left(1 - \frac{1}{8N}\right)^N \leq \exp\left(-\frac{1}{8}\right) = 0.8825.$$

- $N \geq O(\frac{L}{\mu})$ has been called 'big data' condition.

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- Still get linear rate for any $\alpha_t \leq \frac{1}{16L}$.

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  - SAG: $O(\max\{N, \frac{L}{\mu}\}\log(1/\epsilon))$.

Proof Technique: Lyapunov Function

- We define a Lyapunov function of the form

$$\mathcal{L}(\theta^t) = 2h[g(x^t + de^\top y^t) - g(x^*)] + (\theta^t - \theta^*)^\top \begin{bmatrix} A & B \\ B^\top & C \end{bmatrix} (\theta^t - \theta^*),$$

with

$$\theta^t = \begin{bmatrix} y_1^t \\ \vdots \\ y_t^N \\ x^t \end{bmatrix}, \quad \theta^* = \begin{bmatrix} f_i'(x^*) \\ \vdots \\ f_N'(x^*) \\ x^* \end{bmatrix}, \quad e = \begin{bmatrix} I \\ \vdots \\ I \end{bmatrix}, \quad \begin{aligned} A &= a_1 ee^\top + a_2 I, \\ B &= be, \\ C &= cI. \end{aligned}$$

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- Proof involves finding $\{\alpha, a_1, a_2, b, c, d, h, \delta, \gamma\}$ such that

$$\mathbb{E}(\mathcal{L}(\theta^t)|\mathcal{F}_{t-1}) \leqslant (1-\delta)\mathcal{L}(\theta^{t-1}), \quad \mathcal{L}(\theta^t) \geqslant \gamma[g(x^t) - g(x^*)].$$

- Apply recursively and initial Lyapunov function gives constant.

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  - If we initialize with $y_i^0 = f_i'(x^0) - g'(x^0)$ we have

$$C = \frac{3}{2}[g(x^0) - g(x^*)] + \frac{4L}{N}\|x^0 - x^*\|^2.$$

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$$C = \frac{3}{2}[g(x^0) - g(x^*)] + \frac{4L}{N}\|x^0 - x^*\|^2.$$
  - If we initialize with N stochastic gradient iterations,
$$[g(x^0) - g(x^*)] = O(1/N), \quad \|x^0 - x^*\|^2 = O(1/N).$$

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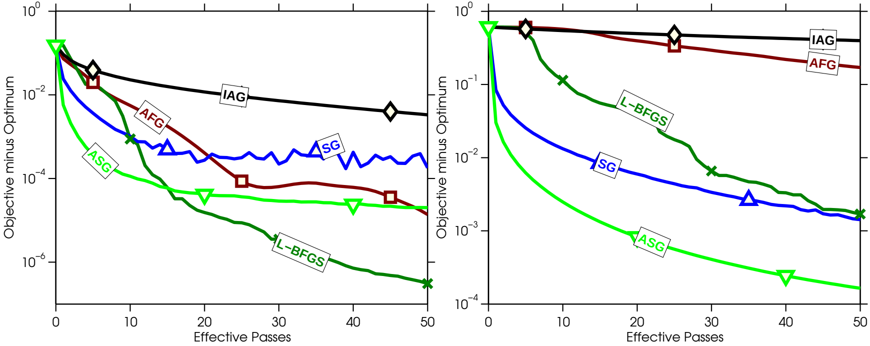
- Same algorithm could be used in non-convex case.
- Contrast with stochastic dual coordinate ascent:
  - Requires explicit strongly-convex regularizer.
  - Not adaptive to μ, does not allow $\mu = 0$.

Comparing FG and SG Methods

- quantum ($n = 50000$, $p = 78$) and rcv1 ($n = 697641$, $p = 47236$)



- Comparison of competitive deterministic and stochastic methods.

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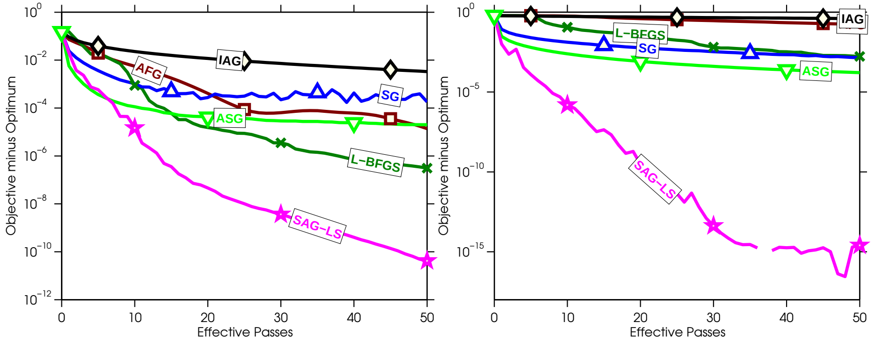

- SAG starts fast and stays fast.

SAG Compared to Coordinate-Based Methods

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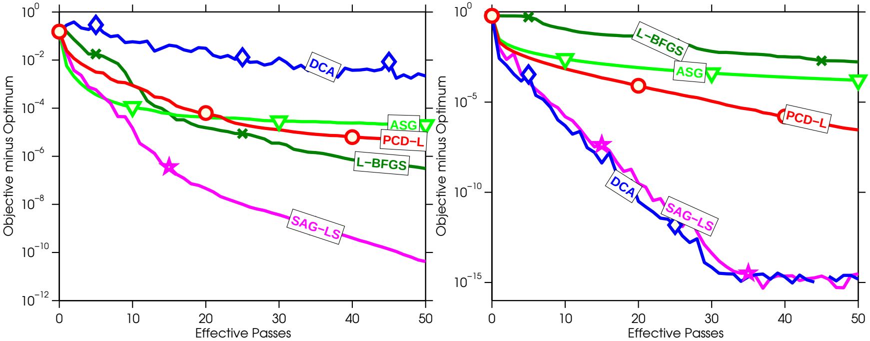

- PCD/DCA are similar on some problems, much worse on others.

SAG Implementation Issues

- while(1)
  - Sample i from $\{1, 2, \dots, N\}$.
  - Compute $f_i'(x)$.
  - $d = d - y_i + f_i'(x)$.
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  - Should we shuffle the data?

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Implementation Issues: Normalization

- Should we normalize by N in the early iterations?
- The parameter update:
  - $x = x - \frac{\alpha}{M} d.$
- We normalize by number of examples seen (M).
- Better performance on early iterations.
- Similar to doing one pass of SG.

Implementation Issues: Memory Requirements

- Can we reduce the memory?
- The memory update for $f_i(a_i^T x)$:
  - Compute $f_i'(a_i^T x)$.
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- Use that $f_i'(a_i^T x) = a_i f_i'(\delta)$.
- Only store the scalars $f_i'(\delta)$.
- Reduces the memory from $O(NP)$ to $O(N)$.

Implementation Issues: Memory Requirements

- Can we reduce the memory in general?
- We can re-write the SAG iteration as:

$$x^{t+1} = x^t - \frac{\alpha_t}{N}\left(f_i'(x^t) - f_i'(x^i) + \sum_{j=1}^{N} f_j'(x^j)\right).$$

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where we occasionally update $\tilde{x}$.

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- Gets rid of memory for two f_i' evaluations per iteration.

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- Apply previous k updates when it changes.
- Reduces the iteration cost from $O(P)$ to $O(\|f_i'(x)\|_0)$.
- Standard tricks allow ℓ_2-regularization and ℓ_1-regularization.

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  - Increase L until we satisfy:

$$f_i(x - \frac{1}{L} f_i'(x)) \leq f_i'(x) - \frac{1}{2L} \|f_i'(x)\|^2.$$

    (assuming $\|f_i'(x)\|^2 \geq \epsilon$)
  - Decrease L between iterations.

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  (Lipschitz approximation procedure from FISTA)
- For $f_i(a_i^T x)$, this costs $O(1)$ in N and P:

$$f_i(a_i^T x - \frac{f_i'(\delta)}{L} \|a_i\|^2).$$

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- And SAG has $y_i \to f_i'(x)$.
- We can check the size of $\|\frac{1}{N}d\| = \|\frac{1}{N}\sum_{i=1}^{N} y_i\| \to \|f'(x)\|$

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  - In practice, Lipschitz approximation procedure on to determine $L_{\mathcal{B}}$.

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- If f_i are non-smooth, could smooth them or use dual methods.

[Nesterov, 2005, Lacoste-Julien et al., 2013, Shalev-Schwartz and Zhang, 2013]

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  - Combine with the line-search for adaptive sampling.

    (see paper/code for details)

SAG with Non-Uniform Sampling

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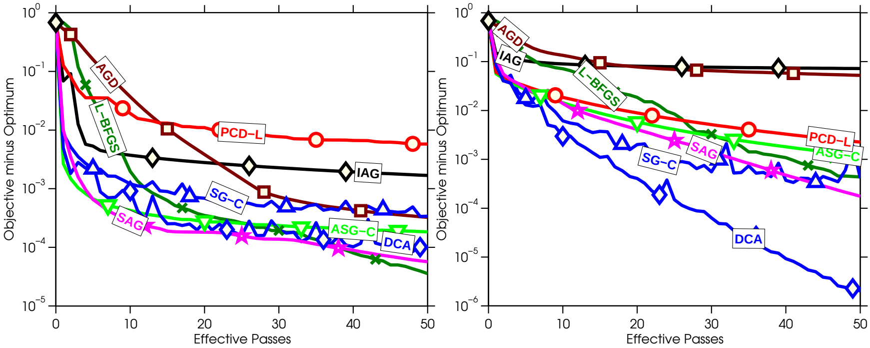

- Datasets where SAG had the worst relative performance.

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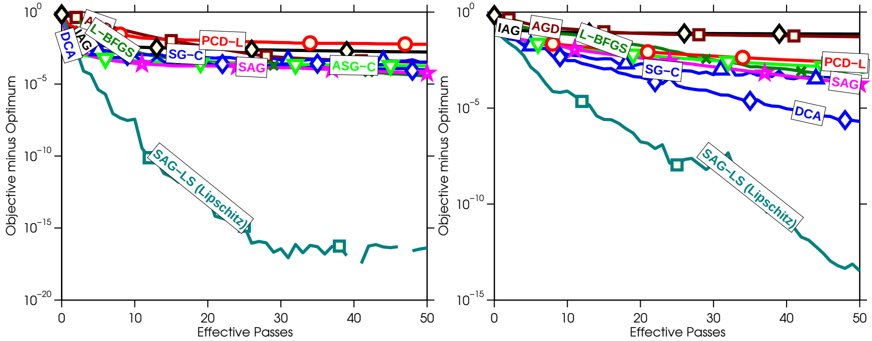

- Lipschitz sampling helps a lot.

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- Quasi-Newton method proposed that has empirically-faster convergence, but much overhead.

  [Sohl-Dickstein et al., 2014]

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- Thank you for the invitation.