Advances in the Minimization of Finite Sums

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Context: Minimizing Finite Sums

- We want to minimize the sum of a finite set of smooth functions:

$$\min_{x \in \mathbb{R}^d} f(x) := \frac{1}{n} \sum_{i=1}^{n} f_i(x).$$

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- We will focus on strongly-convex functions g:
  - Any convex function plus L2-regularization.
- Simplest example is ℓ_2-regularized least-squares,

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

- Common framework in machine learning:
  - 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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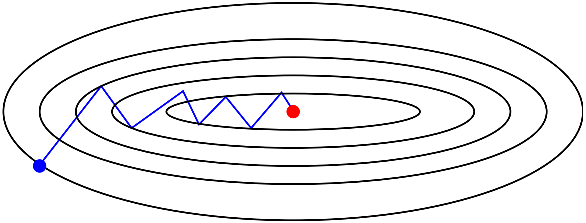

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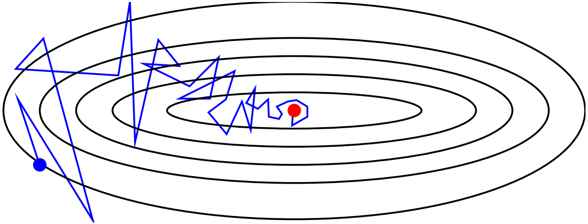
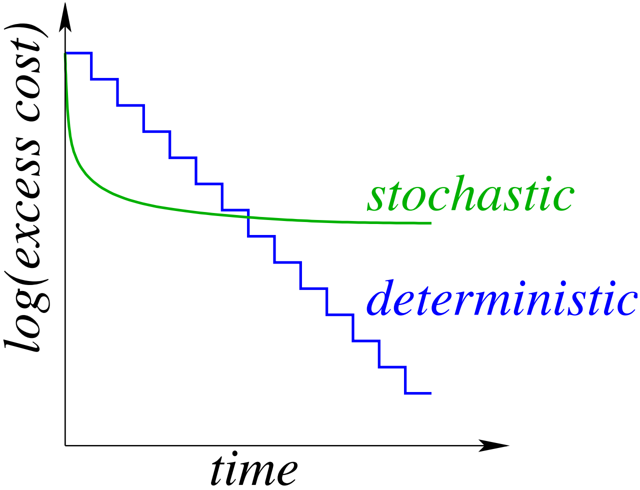


Motivation for New Methods

- 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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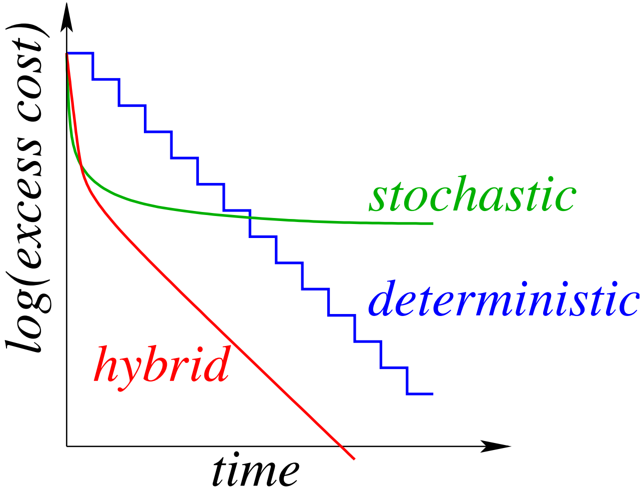

Stochastic Average Gradient (SAG)

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  - Randomly select i_t from $\{1, 2, \ldots, n\}$ and compute $f'_{i_t}(x_t)$,

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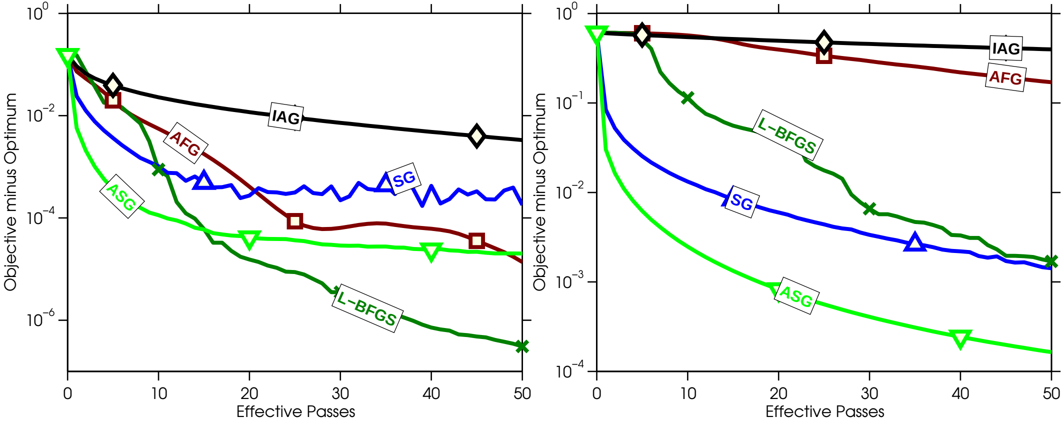
  where $y_i^t = f'_{i_s}$ from last iteration s where i was selected.
- **Achieves $O(\rho^t)$ convergence rate with $O(1)$ iteration cost**:
- Number of f'_i evaluations to reach accuracy of ϵ:
  - Stochastic gradient: $O(\kappa/\epsilon)$.
  - Deterministic gradient: $O(n\kappa \log(1/\epsilon))$.
  - Accelerated gradient: $O(n\sqrt{\kappa} \log(1/\epsilon))$.
  - Stochastic average gradient: $O((n+\kappa)\log(1/\epsilon))$.

Comparing FG and SG Methods

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



- Comparison of competitive deterministic and stochastic methods.

SAG Compared to FG and SG Methods

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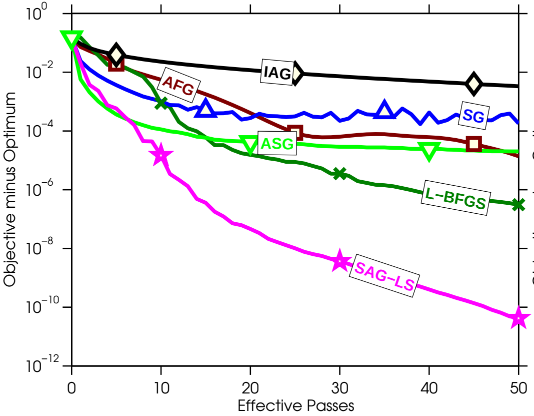

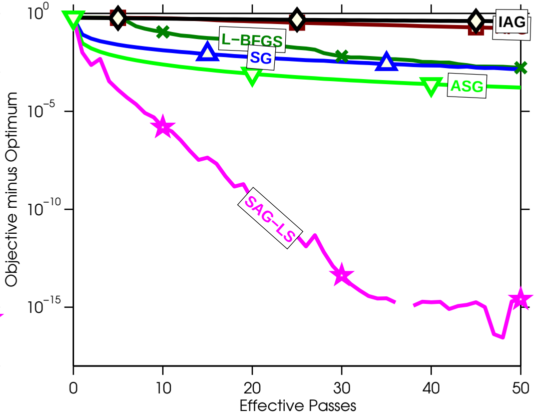

- SAG starts fast and stays fast.

Other Linearly-Convergent Methods

- Other methods subsequently shown to have this property:
  - SDCA [Shalev-Schwartz & Zhang, 2013].
  - MISO [Mairal, 2013].
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- Other methods subsequently shown to have this property:
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  - SAGA [Defazio et al., 2014].
- But, these all introduce memory requirements:
  - Require previous gradients f_i' or dual variables for each i.
  - Only $O(n)$ for some objectives, but $O(nd)$ in general.

Stochastic Variance-Reduced Gradient (SVRG)

- Recent methods with similar rates that avoid memory:
  - Mixed Gradient [Mahdavi & Jin, 2013, Zhang et al., 2013]
  - Stochastic variance-reduced gradient (SVRG) [Johnson & Zhang, 2013]
  - Semi-stochastic gradient [Konecny & Richtarik, 2013]

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- Memory is $O(d)$, but they require extra gradient calculations:
  - Two gradients on each iteration.
  - Occasional calculation of all n gradients.

Extra calculations make them slower than SAG and friends.

Outline

1. Deterministic, stochastic, and finite-sum methods.
2. Wasting fewer gradients in SVRG.
3. Making things go fast.

Stochastic Variance-Reduced Gradient

SVRG algorithm (SG method with *control variate*):

- Start with x_0
- for $s = 0, 1, 2 \ldots$ (outer loop)
  - $d_s = \frac{1}{N} \sum_{i=1}^{N} f_i'(x_s)$ (full gradient calculation)

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  - $x^0 = x_s$
  - for $t = 1, 2, \ldots m$ (inner loop)
    - Randomly pick $i_t \in \{1, 2, \ldots, n\}$
    - $x^t = x^{t-1} - \alpha_t (f_{i_t}'(x^{t-1}) - f_{i_t}'(x_s) + d_s)$ (two gradients per iteration)

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  - $x_{s+1} = x^t$ for random $t \in \{1, 2, \ldots, m\}$ (initialize next outer loop)

Only need to store x_s and d_s.

Convergence Analysis of SVRG

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$$\mathbb{E}[f(x^{s+1}) - f(x^*)] \leq \rho(L, L)[f(x^s) - f(x^*)],$$

  where

$$\rho(a, b) = \frac{1}{1 - 2\alpha a}\left(2b\alpha + \frac{1}{m\mu\alpha}\right).$$

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- In practice:
  - $m = n$ (alternate between computing gradient and stochastic pass).
  - $\alpha = 1/L$ (slightly larger than allowed by theory).
  - $x^{s+1} = x_m$ (rather than random).

Convergence Analysis of SVRG with Error

- We first give a result for SVRG with error:
- Assume:
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- Implications:
  - Same convergence rate if $\max\{\mathbb{E}\|e^s\|, \mathbb{E}\|e^s\|^2\} = O(\tilde{\rho}^s)$ for $\tilde{\rho} < \rho$.
  - Tolerates large error when far from solution.

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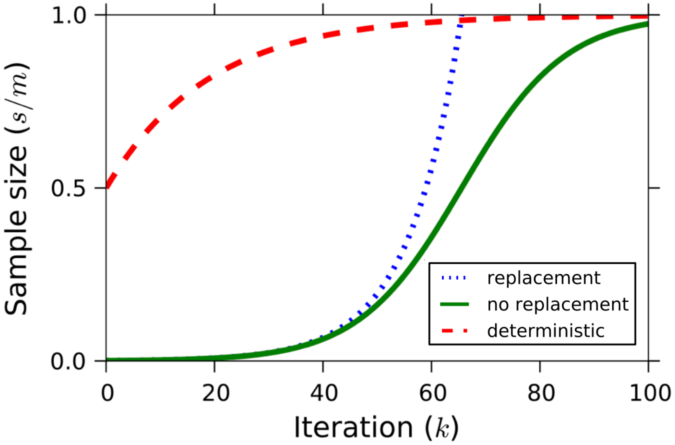
- Hard to do in practice, but w know shape of optimal batch schedule...

Batch Schedule Needed for Linear Rate



[Aravkin et al, 2012]

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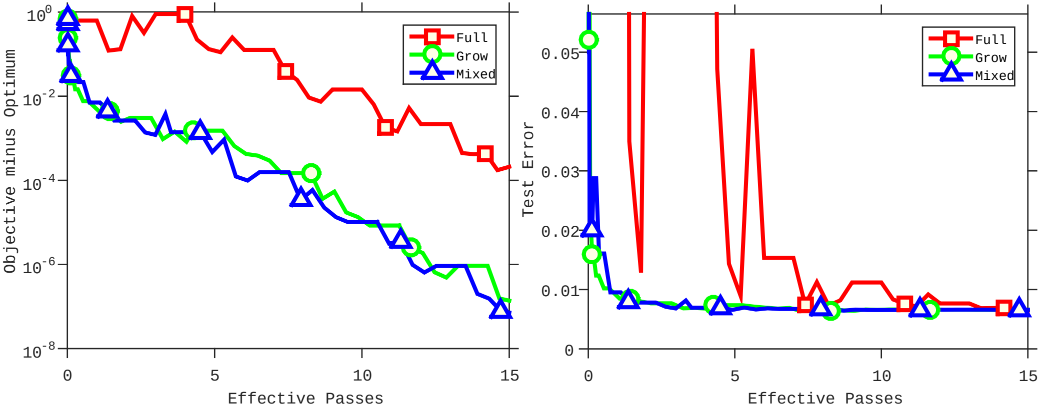
- Convergence rate:

$$\mathbb{E}[f(x^{s+1}) - f(x^*)] \leq \rho\left(L, \frac{|\mathcal{B}^s|}{n}L\right)[f(x^s) - f(x^*)] + \frac{\alpha\mathbb{E}\left[\|e^s\|^2\right] + Z\mathbb{E}\left[\|e^s\|\right]}{1 - 2\alpha L} + \frac{\alpha}{2}\frac{(1 - |\mathcal{B}^s|/n)\sigma^2}{(1 - 2\alpha L)}.$$

- Improves rate when far from solution.
- But dependence on variance σ^2.

Numerical Experiments with Batching

Training/testing loss for ℓ_2-regularized logistic on spam filtering data.



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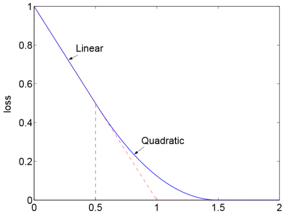
- For certain objectives, can improve close to solution.
- Consider Huberized hinge loss problem [Rosset & Zhu, 2006]:

$$\min_{x\in\mathbb{R}^d} \frac{1}{n}\sum_{i=1}^{n} f(b_i a_i^T x), \quad f(\tau) = \begin{cases} 0 & \text{if } \tau > 1+\epsilon, \\ 1-\tau & \text{if } \tau < 1-\epsilon, \\ \frac{(1+\epsilon-\tau)^2}{4\epsilon} & \text{if } |1-\tau| \leq \epsilon. \end{cases}$$



- The solution is sparse in the f_i' (has support vectors).

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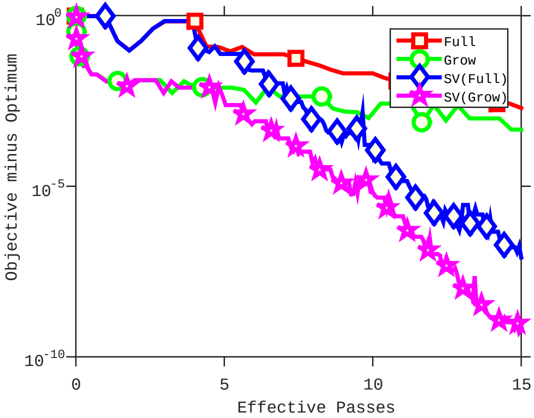
  - f it continues to be zero, skip its next 2 evaluations.
  - If it continues to be zero, skip its next 4 evaluations.
  - Can reduce number of gradients per iteration to 1 or 0.
- Related to shrinking heuristic in SVM solvers [Joachims, 1999, Usunier et al., 2010].

Numerical Experiments with Support Vectors

ℓ_2-regularized Huberized hinge on spam filtering data.



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Sparse Gradients and L2-Regularization

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$$x^t = x^{t-1} - \alpha_t((\lambda x^{t-1} + g_{i_t}'(x^{t-1})) - (\lambda x_s + g_{i_t}'(x_s)) + d_s),$$

which approximates $\sum_i g_i$ and uses exact regularizer gradient:

$$x^t = (1 - \alpha_t\lambda)x^{t-1} - \alpha_t(g_{i_t}'(x^{t-1}) - g_{i_t}'(x_s) + (d_g)_s),$$

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- This form is nice for sparse implementation (also used in SAG/SAGA codes).
- We show that regularized update satisfies:

$$\mathbb{E}[f(x^{s+1}) - f(x^*)] \leq \rho(L^m, L^m)[f(x^s) - f(x^*)],$$

  where $L^m = \max\{\lambda, L_g\}$.
- SVRG actually converges faster than expected.

Proximal-Gradient and ADMM

- A common non-smooth variation is solving problems of the form

$$\operatorname*{argmin}_{x \in \mathbb{R}^p} \frac{1}{n} \sum_{i=1}^{n} f_i(x) + r(x),$$

where the f_i are smooth but r is non-smooth.

- Examples: L1-regularization, bound constraints.
- Proximal-gradient methods use iterations of the form

$$x^{k+1} = \text{prox}_{\alpha_k} \left[x^k - \frac{\alpha_k}{n} \sum_{i=1}^{n} f_i'(x^k) \right],$$

and achieve the same rates as methods for smooth optimization.

- Proximal-gradient variants of SAG[A]/MISO/SDCA/SVRG have been developed:
  - Mairal [2013], Defazio et al. [2014], Xiao & Zhang [2014].
- There are also combinations of these methods with ADMM:
  - Suzuki [2014], Zhong & Kwok [2014].

Acceleration

- Several Nesterov-like accelerated variants have been developed:
  - SDCA [Shalev-Schwartz & Zhang, 2013, Shalev-Schwartz & Zhang, 2014].
  - SVRG [Nitanda, 2014].
  - Primal-Dual Coordinate Descent [Zhang & Xiao, 2014].
  - All methods [Lin et al., 2015].
  - RPDG [Lan, 2015].
  - Catalyst [Lin et al., 2016].
- Reduces complexity from $O((n+\kappa)\log(1/\epsilon))$ to $O(\sqrt{n\kappa}\log(1/\epsilon))$.

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  - SVRG [Nitanda, 2014].
  - Primal-Dual Coordinate Descent [Zhang & Xiao, 2014].
  - All methods [Lin et al., 2015].
  - RPDG [Lan, 2015].
  - Catalyst [Lin et al., 2016].
- Reduces complexity from $O((n+\kappa)\log(1/\epsilon))$ to $O(\sqrt{n\kappa}\log(1/\epsilon))$.
- There also exist coordinate-wise and Newton-like variants:
  - Konečný et al. [2014], Sohl-Dickstein et al. [2014].

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- In practice: combine with line-search for adaptive sampling.

(see paper/code for details)

SAG with Non-Uniform Sampling

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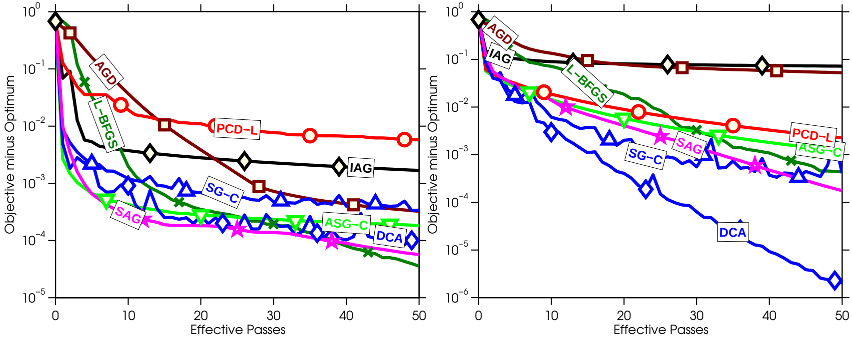

- Datasets where SAG had the worst relative performance.

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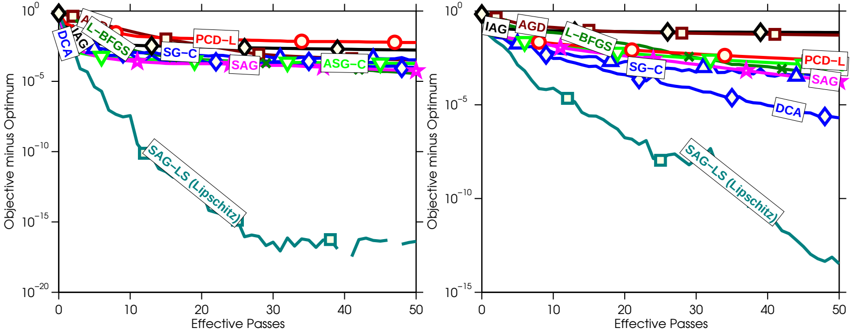
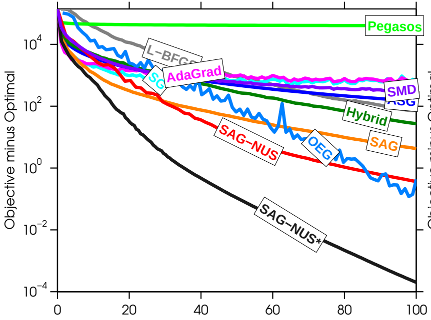
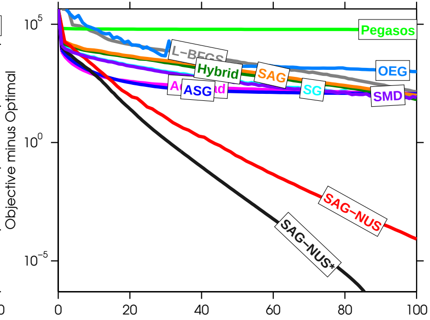


- Lipschitz sampling helps a lot.

SAG with Non-Uniform Sampling

CRF performance for optical-character and named-entity recognition.





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  - Growing batch sizes [Byrd et al., 2012].
  - Re-visiting examples with SVRG [Babanezhad et al., 2015].
  - Streaming SVRG [Frostig et al., 2015].

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- Strong-convexity can relaxed:
  - Gong & Ye [2014], Garber & Hazan [2016], Karimi et al. [2016], Reddi et al. [2016]
- Thank you for the invitation.