

Stochastic Composite Optimization: Variance Reduction, Acceleration, and Robustness to Noise

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Inria Grenoble

ML in the real world, Criteo





Andrei Kulunchakov

- A. Kulunchakov and J. Mairal. Estimate Sequences for Variance-Reduced Stochastic Composite Optimization. International Conference on Machine Learning (ICML). 2019.
- A. Kulunchakov and J. Mairal. Estimate Sequences for Stochastic Composite Optimization: Variance Reduction, Acceleration, and Robustness to Noise. preprint arXiv:1901.08788. 2019.

Context

Many subspace identification approaches require solving a **composite** optimization problem

$$\min_{x \in \mathbb{R}^p} \{F(x) := f(x) + \psi(x)\},$$

where f is L -smooth and convex, and ψ is convex.

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Two settings of interest

Particularly interesting structures in machine learning are

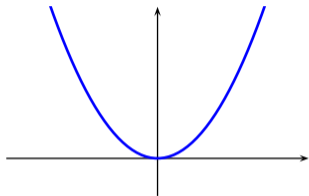
$$f(x) = \frac{1}{n} \sum_{i=1}^n f_i(x) \quad \text{or} \quad f(x) = \mathbb{E}[\tilde{f}(x, \xi)].$$

Those can typically be addressed with

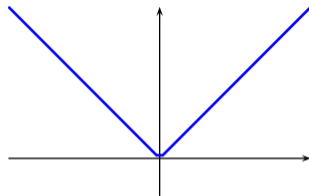
- variants of SGD for the general stochastic case.
- variance-reduced algorithms such as SVRG, SAGA, MISO, SARAH, SDCA, Katyusha. . .

Basics of gradient-based optimization

Smooth vs non-smooth



(a) smooth



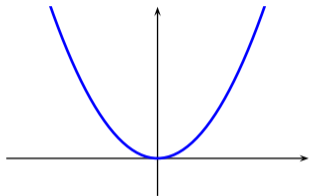
(b) non-smooth

An important quantity to quantify smoothness is the **Lipschitz constant** of the gradient:

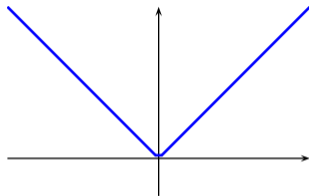
$$\|\nabla f(x) - \nabla f(y)\| \leq L\|x - y\|.$$

Basics of gradient-based optimization

Smooth vs non-smooth



(a) smooth



(b) non-smooth

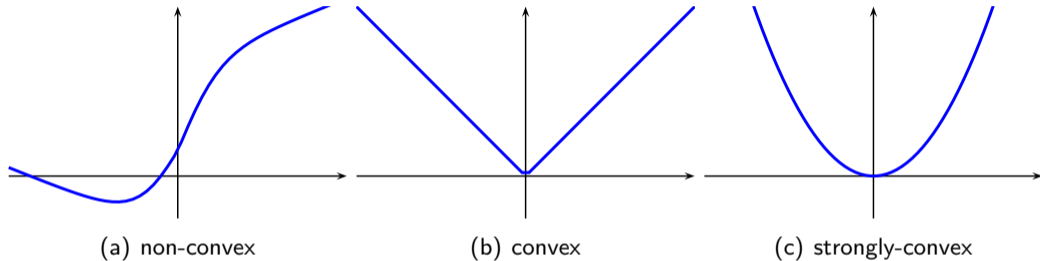
An important quantity to quantify smoothness is the **Lipschitz constant** of the gradient:

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If f is twice differentiable, L may be chosen as the **largest eigenvalue** of the Hessian $\nabla^2 f$. This is an upper-bound on the function curvature.

Basics of gradient-based optimization

Convex vs non-convex

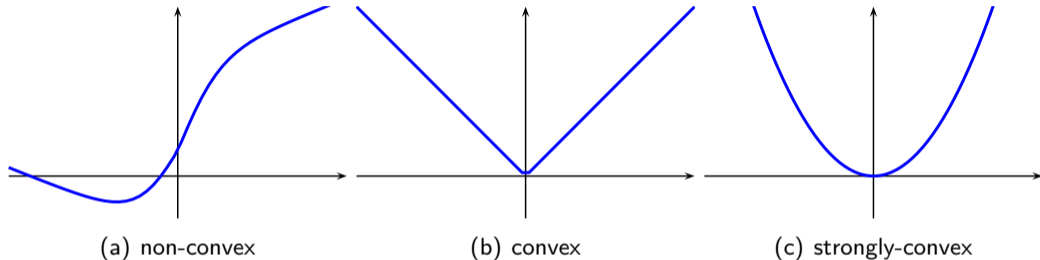


An important quantity to quantify convexity is the **strong-convexity** constant

$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) + \frac{\mu}{2} \|x - y\|^2,$$

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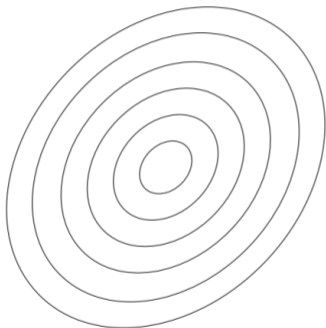
$$f(x) \geq f(y) + \nabla f(y)^\top (x - y) + \frac{\mu}{2} \|x - y\|^2,$$

If f is twice differentiable, μ may be chosen as the **smallest eigenvalue** of the Hessian $\nabla^2 f$. This is a lower-bound on the function curvature.

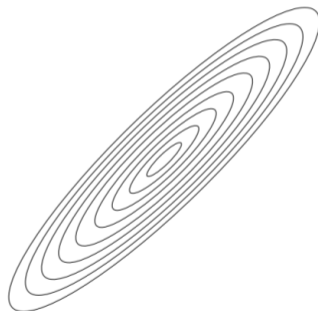
Basics of gradient-based optimization

Picture from F. Bach

Why is the condition number L/μ important?



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

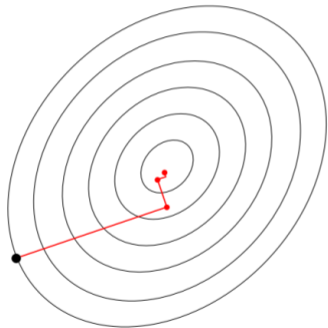


(large $\kappa = L/\mu$)

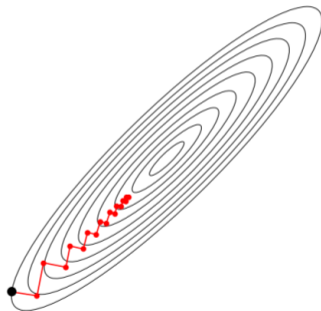
Basics of gradient-based optimization

Picture from F. Bach

Trajectory of gradient descent with optimal step size.



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



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

Variance reduction (1/2)

Variance reduction

Consider two random variables X, Y and define

$$Z = X - Y + \mathbb{E}[Y].$$

Then,

- $\mathbb{E}[Z] = \mathbb{E}[X]$
- $\text{Var}(Z) = \text{Var}(X) + \text{Var}(Y) - 2\text{cov}(X, Y)$.

The variance of Z may be smaller if X and Y are positively correlated.

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Why is it useful for stochastic optimization?

- step-sizes for SGD have to decrease to ensure convergence.
- with variance reduction, one may use **larger constant** step-sizes.

Variance reduction for smooth functions (2/2)

SVRG

$$x_t = x_{t-1} - \gamma (\nabla f_{i_t}(x_{t-1}) - \nabla f_{i_t}(y) + \nabla f(y)),$$

where y is updated every epoch and $\mathbb{E}[\nabla f_{i_t}(y) | \mathcal{F}_{t-1}] = \nabla f(y)$.

SAGA

$$x_t = x_{t-1} - \gamma (\nabla f_{i_t}(x_{t-1}) - y_{i_t}^{t-1} + \frac{1}{n} \sum_{i=1}^n y_i^{t-1}),$$

where $\mathbb{E}[y_{i_t}^{t-1} | \mathcal{F}_{t-1}] = \frac{1}{n} \sum_{i=1}^n y_i^{t-1}$ and $y_i^t = \begin{cases} \nabla f_i(x_{t-1}) & \text{if } i = i_t \\ y_i^{t-1} & \text{otherwise.} \end{cases}$

MISO/Finito: for $n \geq L/\mu$, same form as SAGA but

$$\frac{1}{n} \sum_{i=1}^n y_i^{t-1} = -\mu x_{t-1} \quad \text{and} \quad y_i^t = \begin{cases} \nabla f_i(x_{t-1}) - \mu x_{t-1} & \text{if } i = i_t \\ y_i^{t-1} & \text{otherwise.} \end{cases}$$

Complexity of SGD variants

We consider the worst-case complexity for finding a point \bar{x} such that $\mathbb{E}[F(\bar{x}) - F^*] \leq \varepsilon$ for

$$\min_{x \in \mathbb{R}^p} \{F(x) := \mathbb{E}[\tilde{f}(x, \xi)] + \psi(x)\},$$

In this talk, we consider the μ -strongly convex case only.

Complexity of SGD with iterate averaging

$$O\left(\frac{L}{\mu} \log\left(\frac{C_0}{\varepsilon}\right)\right) + O\left(\frac{\sigma^2}{\mu\varepsilon}\right),$$

under the (strong) assumption that the gradient estimates have **bounded variance** σ^2 .

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Complexity of accelerated SGD [Ghadimi and Lan, 2013]

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Complexity of SAGA/SVRG/SDCA/MISO/S2GD

$$O\left(\left(n + \frac{\bar{L}}{\mu}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right) \quad \text{with} \quad \bar{L} = \frac{1}{n} \sum_{i=1}^n L_i.$$

Complexity of GD and acc-GD

$$O\left(\left(n \frac{L}{\mu}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right) \quad \text{vs.} \quad O\left(\left(n \sqrt{\frac{L}{\mu}}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right).$$

see also SDCA [Shalev-Shwartz and Zhang, 2014] and Catalyst [Lin et al., 2018].

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Complexity of Katyusha [Allen-Zhu, 2017]

$$O\left(\left(n + \sqrt{\frac{n\bar{L}}{\mu}}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right).$$

see also SDCA [Shalev-Shwartz and Zhang, 2014] and Catalyst [Lin et al., 2018].

Contributions without acceleration

We extend and generalize the concept of **estimate sequences** introduced by Nesterov to

- provide a **unified proof of convergence** for SAGA/random-SVRG/MISO.
- provide them **adaptivity for unknown μ** (known before for SAGA only).
- make them **robust to stochastic noise**, e.g., for solving

$$f(x) = \frac{1}{n} \sum_{i=1}^n f_i(x) \quad \text{with} \quad f_i(x) = \mathbb{E}[\tilde{f}_i(x, \xi)].$$

with complexity

$$O\left(\left(n + \frac{\bar{L}}{\mu}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right) + O\left(\frac{\tilde{\sigma}^2}{\mu\varepsilon}\right) \quad \text{with} \quad \tilde{\sigma}^2 \ll \sigma^2,$$

where $\tilde{\sigma}^2$ is the variance due to small perturbations.

- obtain **new variants** of the above algorithms with the same guarantees.

The stochastic finite sum problem

$$\min_{x \in \mathbb{R}^p} \left\{ F(x) := \frac{1}{n} \sum_{i=1}^n f_i(x) + \psi(x) \right\} \quad \text{with} \quad f_i(x) = \mathbb{E}[\tilde{f}_i(x, \xi)],$$



The colorful Norwegian city of Bergen is also a gateway to majestic fjords. Bryggen Hanseatic Wharf will give you a sense of the local culture – take some time to snap photos of the Hanseatic commercial buildings, which look like scenery from a movie set.



The colorful of gateway to fjords. Hanseatic Wharf will sense the culture – take some to snap photos the commercial buildings, which look scenery a

Data augmentation on digits (left); Dropout on text (right).

Contributions with acceleration

- we propose a **new accelerated SGD algorithm** for composite optimization with optimal complexity

$$O\left(\sqrt{\frac{L}{\mu}} \log\left(\frac{C_0}{\varepsilon}\right)\right) + O\left(\frac{\sigma^2}{\mu\varepsilon}\right),$$

- we propose an **accelerated variant** of SVRG for the stochastic finite-sum problem with complexity

$$O\left(\left(n + \sqrt{\frac{n\bar{L}}{\mu}}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right) + O\left(\frac{\tilde{\sigma}^2}{\mu\varepsilon}\right) \quad \text{with} \quad \tilde{\sigma}^2 \ll \sigma^2.$$

When $\tilde{\sigma} = 0$, the complexity matches that of Katyusha.

A classical iteration

$$x_k \leftarrow \text{Prox}_{\eta_k \psi} [x_{k-1} - \eta_k g_k] \quad \text{with} \quad \mathbb{E}[g_k | \mathcal{F}_k] = \nabla f(x_{k-1}),$$

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Interpretation

x_k minimizes the quadratic function d_k , defined as

$$d_k(x) = (1 - \delta_k)d_{k-1}(x) + \delta_k \left(f(x_{k-1}) + g_k^\top (x - x_{k-1}) + \frac{\mu}{2} \|x - x_{k-1}\|^2 \right. \\ \left. \dots + \psi(x_k) + \psi'(x_k)^\top (x - x_k) \right),$$

where $\delta_k = \mu\eta_k$, $\psi'(x_k)$ is a subgradient in $\partial\psi(x_k)$, and $d_0(x) = d_0^* + \frac{\mu}{2} \|x - x_0\|^2$.

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This is similar to the construction of **estimate sequences** by Nesterov.

see also [Devolder, 2011, Lin et al., 2014] for stochastic problems.

A less classical iteration

$$x_k = \text{Prox}_{\psi/\mu} [\bar{x}_k] \quad \text{with} \quad \bar{x}_k \leftarrow (1 - \delta_k)\bar{x}_{k-1} + \delta_k x_k - \eta_k g_k \quad \text{and} \quad \mathbb{E}[g_k | \mathcal{F}_k] = \nabla f(x_{k-1}),$$

covers MISO/Finito/primal SDCA with $\delta_k = \mu\eta_k$.

Interpretation

x_k minimizes the function d_k , defined as

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With estimate sequences, convergence proofs for both types of iterations are identical.

Convergence results

General convergence result

if $\eta_t \leq 1/L$ for all $t \geq 0$, then for all $k \geq 1$,

$$\mathbb{E} \left[F(\hat{x}_k) - F^* + \frac{\mu}{2} \|x_k - x^*\|^2 \right] \leq \Gamma_k \left(F(x_0) - F^* + \frac{\mu}{2} \|x_0 - x^*\|^2 + \sum_{t=1}^k \frac{\delta_t \eta_t \sigma_t^2}{\Gamma_t} \right).$$

where $\Gamma_k = \prod_{t=1}^k (1 - \delta_t)$, $\hat{x}_k = (1 - \delta_k) \hat{x}_{k-1} + \delta_k x_k$, and $\sigma_t^2 = \mathbb{E}[\|g_t - \nabla f(x_{t-1})\|^2]$.

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Corollary: SGD with constant step size $\eta_k = 1/L$

$$\mathbb{E} \left[F(\hat{x}_k) - F^* + \frac{\mu}{2} \|x_k - x^*\|^2 \right] \leq 2 \left(1 - \frac{\mu}{L} \right)^k (F(x_0) - F^*) + \frac{\sigma^2}{L}.$$

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$$\# \text{Comp} = O \left(\frac{L}{\mu} \log \left(\frac{C_0}{\varepsilon} \right) \right) \quad \text{with} \quad \text{Bias} = \frac{\sigma^2}{L}.$$

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Corollary: two-stage SGD with (i) constant step size; then (ii) decreasing step sizes

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An accelerated SGD algorithm

An algorithm derived from the estimate sequence method.

$$\begin{aligned}x_k &= \text{Prox}_{\eta_k \psi} [y_{k-1} - \eta_k g_k] \quad \text{with} \quad \mathbb{E}[g_k | \mathcal{F}_{k-1}] = \nabla f(y_{k-1}) \\y_k &= x_k + \beta_k (x_k - x_{k-1}) \quad \text{with} \quad \beta_k = \frac{\delta_k (1 - \delta_k) \eta_{k+1}}{\eta_k \delta_{k+1} + \eta_{k+1} \delta_k^2},\end{aligned}$$

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Complexity: acc-SGD with constant step size $\eta_k = 1/L$

$$\mathbb{E}[F(x_k) - F^*] \leq 2 \left(1 - \sqrt{\frac{\mu}{L}}\right)^k (F(x_0) - F^*) + \frac{\sigma^2}{\sqrt{\mu L}}.$$

Note that the bias is larger than regular SGD by $\sqrt{L/\mu}$.

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An accelerated SVRG algorithm for stochastic finite-sum problems

- Choose the extrapolation point

$$y_{k-1} = \theta_k v_{k-1} + (1 - \theta_k) \tilde{x}_{k-1};$$

- Compute the noisy gradient estimator

$$g_k = \tilde{\nabla} f_{i_k}(y_{k-1}) - \tilde{\nabla} f_{i_k}(\tilde{x}_{k-1}) + \tilde{\nabla} f(\tilde{x}_{k-1});$$

- Obtain the new iterate

$$x_k \leftarrow \text{Prox}_{\eta_k \psi} [y_{k-1} - \eta_k g_k];$$

- Find the minimizer v_k of the estimate sequence:

$$v_k = (1 - \delta_k) v_{k-1} + \delta_k y_{k-1} + \frac{\delta_k}{\gamma_k \eta_k} (x_k - y_{k-1});$$

- Update the anchor point \tilde{x}_k with prob $1/n$.
- Output x_k (**no averaging needed**).

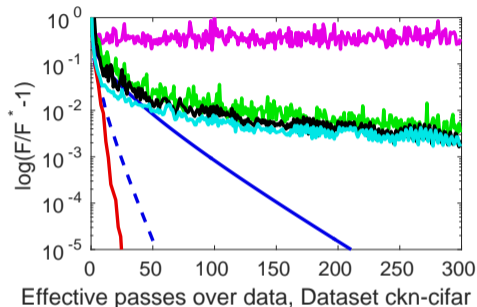
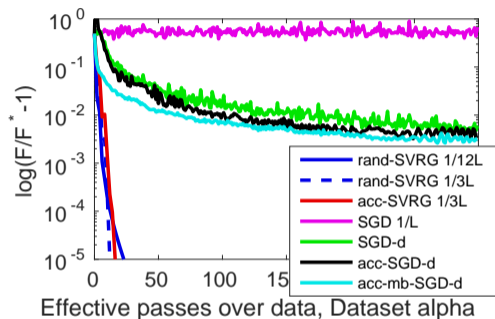
An accelerated SVRG algorithm for stochastic finite-sum problems

Remarks

- design of the algorithm and convergence proofs are based on estimate sequences.
- with two stages, the algorithm achieves the optimal complexity

$$O\left(\left(n + \sqrt{\frac{n\bar{L}}{\mu}}\right) \log\left(\frac{C_0}{\varepsilon}\right)\right) + O\left(\frac{\tilde{\sigma}^2}{\mu\varepsilon}\right) \quad \text{with} \quad \tilde{\sigma}^2 \ll \sigma^2.$$

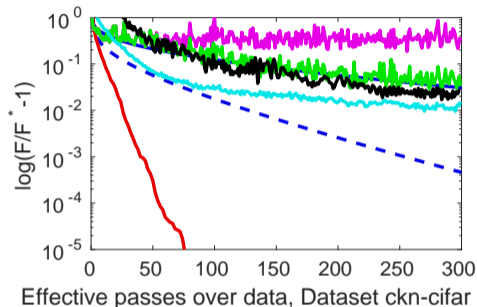
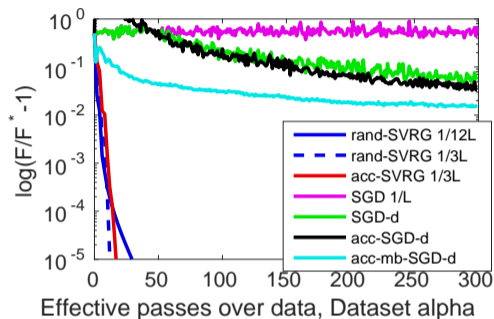
A few experiments



ℓ_2 -logistic regression on two datasets, with $\mu = 1/10n$.

- no big difference between the variants of SGD with decreasing step sizes;
- variance reduction makes a huge difference.
- acceleration helps on ckn-cifar.

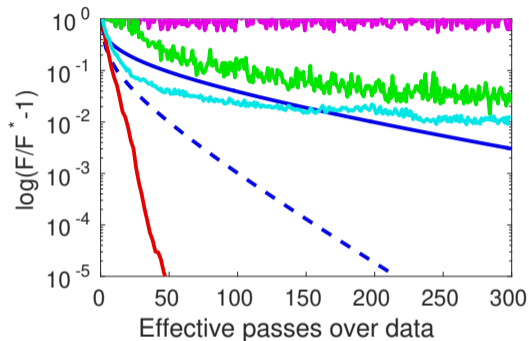
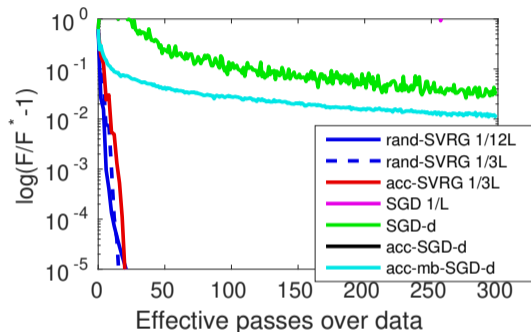
A few experiments



ℓ_2 -logistic regression on two datasets, with $\mu = 1/100n$.

- as conditioning worsens, the benefits of acceleration are larger.
- accelerated SGD with mini-batches take the lead among SGD methods.

A few experiments



SVM with squared hinge loss on two datasets, with $\mu = 1/10n$.

- here, gradients are potentially unbounded and accelerated SGD diverges!
- accelerated SGD with mini-batches is stable and faster than SGD.

Remark about accelerated SGD

It does not always work. Why?

- the bounded noise variance assumption is not safe.
- the accelerated algorithm with constant step size (which is used to forget the initial condition) has much worse dependency in σ^2 (see next slide).

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Convergence of SGD with $\eta_t = 1/L$

$$\mathbb{E}[f(\hat{x}_t) - f^*] \leq 2 \left(1 - \frac{\mu}{L}\right)^t (f(x_0) - f^*) + \frac{\sigma^2}{L}.$$

Convergence of accelerated SGD with $\eta_t = 1/L$

$$\mathbb{E}[f(\hat{x}_t) - f^*] \leq 2 \left(1 - \sqrt{\frac{\mu}{L}}\right)^t (f(x_0) - f^*) + \frac{\sigma^2}{\sqrt{\mu L}}.$$

Remark about accelerated SGD

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Is it worthless?

- **removing the need for averaging** is great for sparse problems.
- with a **mini-batch** of size $\sqrt{L/\mu}$, we obtain the same complexity as the unaccelerated algorithm and the same stability w.r.t. σ^2 , and we can parallelize for free!

References from this talk

The botany of incremental methods

- SAG [Schmidt et al., 2017].
- SAGA [Defazio et al., 2014a].
- SVRG [Xiao and Zhang, 2014].
- SDCA [Shalev-Shwartz and Zhang, 2014].
- Finito [Defazio et al., 2014b].
- MISO [Mairal, 2015].
- S2GD [Konečný and Richtárik, 2017].
- SARAH [Nguyen et al., 2017].
- MiG [Zhou et al., 2018].
- Katyusha [Allen-Zhu, 2017].
- Catalyst [Lin et al., 2018].
- ...

Conclusion

- The estimate sequence method is a **generic tool**, which can be applied to stochastic optimization problems, including finite-sums.
- We use it to develop and analyze algorithms **without and with** acceleration.
- We discuss empirical findings regarding the **stability** of accelerated stochastic algorithms.
- ...but stability issues can be fixed with mini-batching.

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