CONVERGENCE RATES FOR OPTIMIZATION ALGORITHMS

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CONVERGENCE RATES

CONVERGENCE RATE AND ASSUMPTIONS

A sequence $\{x^k\}$ is said to converge at the rate γ^k, if:

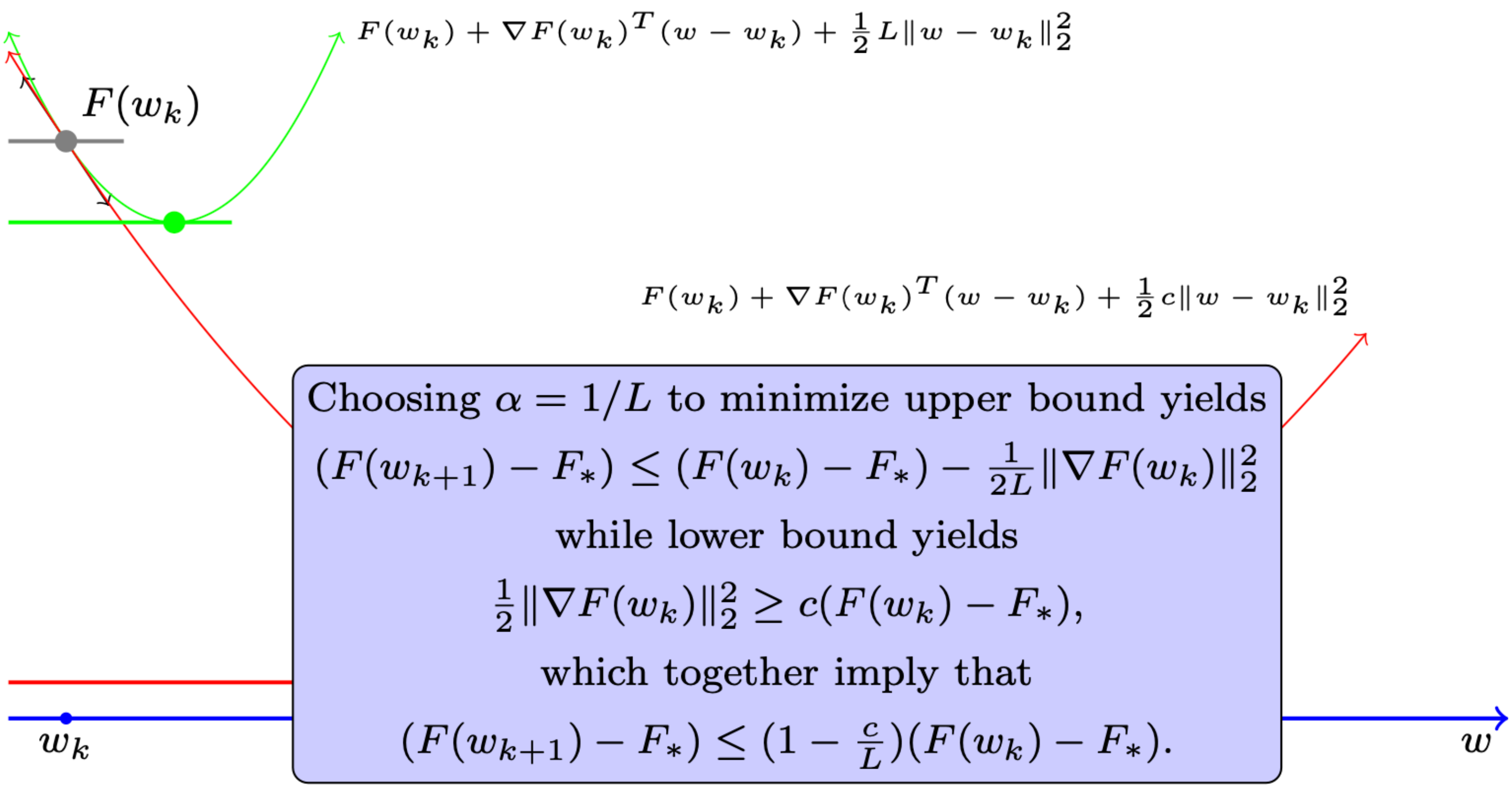
$$\|\mathbf{x}^{k+1} - \mathbf{x}^*\| \leq \gamma \|\mathbf{x}^k - \mathbf{x}^*\| \quad (\Rightarrow \|\mathbf{x}^k - \mathbf{x}^*\| \leq \gamma^k \|\mathbf{x}^0 - \mathbf{x}^*\|),$$

Assumption $\langle L/c \rangle$

The objective function $F : \mathbb{R}^d \to \mathbb{R}$ is

- *c-strongly convex ($\Rightarrow$ unique minimizer) and*
- *L-smooth (i.e., ∇F is Lipschitz continuous with constant L).*

GRADIENT DESCENT CONVERGENCE



Choosing $\alpha = 1/L$ to minimize upper bound yields

$$(F(w_{k+1}) - F_*) \leq (F(w_k) - F_*) - \frac{1}{2L} \|\nabla F(w_k)\|_2^2$$

while lower bound yields

$$\frac{1}{2} \|\nabla F(w_k)\|_2^2 \geq c(F(w_k) - F_*),$$

which together imply that

$$(F(w_{k+1}) - F_*) \leq (1 - \frac{c}{L})(F(w_k) - F_*).$$

L-SMOOTH OBJECTIVE FUNCTION

$$\left|\left|\nabla F(w) - \nabla F(\overline{w})\right|\right| \leq L||w - \overline{w}||$$

Proof of inequality:

$$\begin{aligned} F(w) &= F(\overline{w}) + \int_0^1 \frac{\partial F(\overline{w} + t(w - \overline{w}))}{\partial t}\, dt \\ &= F(\overline{w}) + \int_0^1 \nabla F(\overline{w} + t(w - \overline{w}))^T (w - \overline{w})\, dt \\ &= F(\overline{w}) + \nabla F(\overline{w})^T (w - \overline{w}) + \int_0^1 \left[\nabla F(\overline{w} + t(w - \overline{w})) - \nabla F(\overline{w})\right]^T (w - \overline{w})\, dt \\ &\leq F(\overline{w}) + \nabla F(\overline{w})^T (w - \overline{w}) + \int_0^1 L\|t(w - \overline{w})\|_2 \|w - \overline{w}\|_2\, dt, \end{aligned}$$

C-STRONG CONVEXITY

$$F(w) \geq F(w_k) + \nabla F(w_k)^T (w - w_k) + \frac{c}{2} ||w - w_k||^2$$

Minimizing the RHS w.r.t. w:

$$\tilde{w} = w_k - \frac{1}{c} \nabla F(w_k)$$

Lower bound on RHS: $F(w_k) - \frac{1}{2c} ||\nabla F(w_k)||^2$

Putting back in the first equation:

$$c\big(F(w_k) - F(w)\big) \leq 1/2 \; ||\nabla F(w_k)||^2$$

Convergence Rate and Computational Complexity

Overall Complexity (ϵ) = Convergence Rate$^{-1}(\epsilon)$ $*$ Complexity of each iteration

	Strongly Convex + Smooth			Convex + Smooth		
	Convergence Rate	Complexity of each iteration	Overall Complexity	Convergence Rate	Complexity of each iteration	Overall Complexity
GD	$O\left(\exp\left(-\frac{t}{Q}\right)\right)$	$O(n \cdot d)$	$O\left(nd \cdot Q \cdot \log\left(\frac{1}{\epsilon}\right)\right)$	$O\left(\frac{\beta}{t}\right)$	$O(n \cdot d)$	$O\left(nd \cdot \beta \cdot \left(\frac{1}{\epsilon}\right)\right)$
SGD	$O\left(\frac{1}{t}\right)$	$O(d)$	$O\left(\frac{d}{\epsilon}\right)$	$O\left(\frac{1}{\sqrt{t}}\right)$	$O(d)$	$O\left(\frac{d}{\epsilon^2}\right)$

SGD ANALYSIS

THEOREM 14.8 *Let* $B, \rho > 0$. *Let* f *be a convex function and let* $\mathbf{w}^\star \in \operatorname{argmin}_{\mathbf{w}:\|\mathbf{w}\| \le B} f(\mathbf{w})$. *Assume that SGD is run for* T *iterations with* $\eta = \sqrt{\frac{B^2}{\rho^2 T}}$. *Assume also that for all* t, $\|\mathbf{v}_t\| \le \rho$ *with probability* 1. *Then,*

$$\mathbb{E}[f(\bar{\mathbf{w}})] - f(\mathbf{w}^\star) \le \frac{B\,\rho}{\sqrt{T}}.$$

Therefore, for any $\epsilon > 0$, *to achieve* $\mathbb{E}[f(\bar{\mathbf{w}})] - f(\mathbf{w}^\star) \le \epsilon$, *it suffices to run the SGD algorithm for a number of iterations that satisfies*

$$T \ge \frac{B^2 \rho^2}{\epsilon^2}.$$

SGD ANALYSIS

LEMMA 14.1 *Let $\mathbf{v}_1, \ldots, \mathbf{v}_T$ be an arbitrary sequence of vectors. Any algorithm with an initialization $\mathbf{w}^{(1)} = 0$ and an update rule of the form*

$$\mathbf{w}^{(t+1)} = \mathbf{w}^{(t)} - \eta \mathbf{v}_t \tag{14.4}$$

satisfies

$$\sum_{t=1}^{T} \langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t \rangle \leq \frac{\|\mathbf{w}^\star\|^2}{2\eta} + \frac{\eta}{2} \sum_{t=1}^{T} \|\mathbf{v}_t\|^2. \tag{14.5}$$

In particular, for every $B, \rho > 0$, if for all t we have that $\|\mathbf{v}_t\| \leq \rho$ and if we set $\eta = \sqrt{\frac{B^2}{\rho^2 T}}$, then for every $\mathbf{w}^\star$ with $\|\mathbf{w}^\star\| \leq B$ we have

$$\frac{1}{T} \sum_{t=1}^{T} \langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t \rangle \leq \frac{B\,\rho}{\sqrt{T}}.$$

SGD ANALYSIS

Proof Using algebraic manipulations (completing the square), we obtain:

$$\begin{aligned}
\langle \mathbf{w}^{(t)} - \mathbf{w}^{\star}, \mathbf{v}_t \rangle &= \frac{1}{\eta} \langle \mathbf{w}^{(t)} - \mathbf{w}^{\star}, \eta \mathbf{v}_t \rangle \\
&= \frac{1}{2\eta} \left(-\|\mathbf{w}^{(t)} - \mathbf{w}^{\star} - \eta \mathbf{v}_t\|^2 + \|\mathbf{w}^{(t)} - \mathbf{w}^{\star}\|^2 + \eta^2 \|\mathbf{v}_t\|^2 \right) \\
&= \frac{1}{2\eta} \left(-\|\mathbf{w}^{(t+1)} - \mathbf{w}^{\star}\|^2 + \|\mathbf{w}^{(t)} - \mathbf{w}^{\star}\|^2 \right) + \frac{\eta}{2} \|\mathbf{v}_t\|^2,
\end{aligned}$$

SGD ANALYSIS

where the last equality follows from the definition of the update rule. Summing the equality over t, we have

$$\sum_{t=1}^{T} \langle \mathbf{w}^{(t)} - \mathbf{w}^{\star}, \mathbf{v}_t \rangle = \frac{1}{2\eta} \sum_{t=1}^{T} \left(-\|\mathbf{w}^{(t+1)} - \mathbf{w}^{\star}\|^2 + \|\mathbf{w}^{(t)} - \mathbf{w}^{\star}\|^2 \right) + \frac{\eta}{2} \sum_{t=1}^{T} \|\mathbf{v}_t\|^2. \tag{14.6}$$

The first sum on the right-hand side is a telescopic sum that collapses to

$$\|\mathbf{w}^{(1)} - \mathbf{w}^{\star}\|^2 - \|\mathbf{w}^{(T+1)} - \mathbf{w}^{\star}\|^2.$$

SGD ANALYSIS

Plugging this in Equation (14.6), we have

$$\begin{aligned}\sum_{t=1}^{T}\langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t\rangle &= \frac{1}{2\eta}(\|\mathbf{w}^{(1)} - \mathbf{w}^\star\|^2 - \|\mathbf{w}^{(T+1)} - \mathbf{w}^\star\|^2) + \frac{\eta}{2}\sum_{t=1}^{T}\|\mathbf{v}_t\|^2 \\ &\leq \frac{1}{2\eta}\|\mathbf{w}^{(1)} - \mathbf{w}^\star\|^2 + \frac{\eta}{2}\sum_{t=1}^{T}\|\mathbf{v}_t\|^2 \\ &= \frac{1}{2\eta}\|\mathbf{w}^\star\|^2 + \frac{\eta}{2}\sum_{t=1}^{T}\|\mathbf{v}_t\|^2,\end{aligned}$$

where the last equality is due to the definition $\mathbf{w}^{(1)} = 0$. This proves the first part of the lemma (Equation (14.5)). The second part follows by upper bounding $\|\mathbf{w}^\star\|$ by B, $\|\mathbf{v}_t\|$ by ρ, dividing by T, and plugging in the value of η. □

SGD ANALYSIS

$$\underset{\mathbf{v}_{1:T}}{\mathbb{E}}[f(\bar{\mathbf{w}}) - f(\mathbf{w}^\star)] \leq \underset{\mathbf{v}_{1:T}}{\mathbb{E}}\left[\frac{1}{T}\sum_{t=1}^{T}(f(\mathbf{w}^{(t)}) - f(\mathbf{w}^\star))\right].$$

Since Lemma 14.1 holds for any sequence $\mathbf{v}_1, \mathbf{v}_2, \ldots \mathbf{v}_T$, it applies to SGD as well. By taking expectation of the bound in the lemma we have

$$\underset{\mathbf{v}_{1:T}}{\mathbb{E}}\left[\frac{1}{T}\sum_{t=1}^{T}\langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t\rangle\right] \leq \frac{B\,\rho}{\sqrt{T}}. \qquad (14.9)$$

It is left to show that

$$\underset{\mathbf{v}_{1:T}}{\mathbb{E}}\left[\frac{1}{T}\sum_{t=1}^{T}(f(\mathbf{w}^{(t)}) - f(\mathbf{w}^\star))\right] \leq \underset{\mathbf{v}_{1:T}}{\mathbb{E}}\left[\frac{1}{T}\sum_{t=1}^{T}\langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t\rangle\right], \qquad (14.10)$$

SGD ANALYSIS

Using the linearity of the expectation we have

$$\mathop{\mathbb{E}}_{\mathbf{v}_{1:T}}\left[\frac{1}{T}\sum_{t=1}^{T}\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle\right]=\frac{1}{T}\sum_{t=1}^{T}\mathop{\mathbb{E}}_{\mathbf{v}_{1:T}}[\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle].$$

Next, we recall the *law of total expectation*: For every two random variables α,β, and a function g, $\mathbb{E}_{\alpha}[g(\alpha)]=\mathbb{E}_{\beta}\,\mathbb{E}_{\alpha}[g(\alpha)|\beta]$. Setting $\alpha=\mathbf{v}_{1:t}$ and $\beta=\mathbf{v}_{1:t-1}$ we get that

$$\begin{aligned}\mathop{\mathbb{E}}_{\mathbf{v}_{1:T}}[\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle] &= \mathop{\mathbb{E}}_{\mathbf{v}_{1:t}}[\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle]\\ &= \mathop{\mathbb{E}}_{\mathbf{v}_{1:t-1}}\mathop{\mathbb{E}}_{\mathbf{v}_{1:t}}[\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle\,|\,\mathbf{v}_{1:t-1}]\,.\end{aligned}$$

Once we know $\mathbf{v}_{1:t-1}$, the value of $\mathbf{w}^{(t)}$ is not random any more and therefore

$$\mathop{\mathbb{E}}_{\mathbf{v}_{1:t-1}}\mathop{\mathbb{E}}_{\mathbf{v}_{1:t}}[\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathbf{v}_t\rangle\,|\,\mathbf{v}_{1:t-1}]=\mathop{\mathbb{E}}_{\mathbf{v}_{1:t-1}}\langle \mathbf{w}^{(t)}-\mathbf{w}^{\star},\mathop{\mathbb{E}}_{\mathbf{v}_t}[\mathbf{v}_t\,|\,\mathbf{v}_{1:t-1}]\rangle\,.$$

SGD ANALYSIS

Since $\mathbf{w}^{(t)}$ only depends on $\mathbf{v}_{1:t-1}$ and SGD requires that $\mathbb{E}_{\mathbf{v}_t}[\mathbf{v}_t \mid \mathbf{w}^{(t)}] \in \partial f(\mathbf{w}^{(t)})$ we obtain that $\mathbb{E}_{\mathbf{v}_t}[\mathbf{v}_t \mid \mathbf{v}_{1:t-1}] \in \partial f(\mathbf{w}^{(t)})$. Thus,

$$\mathop{\mathbb{E}}_{\mathbf{v}_{1:\,t-1}} \langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathop{\mathbb{E}}_{\mathbf{v}_t}[\mathbf{v}_t \mid \mathbf{v}_{1:\,t-1}] \rangle \;\geq\; \mathop{\mathbb{E}}_{\mathbf{v}_{1:\,t-1}} [f(\mathbf{w}^{(t)}) - f(\mathbf{w}^\star)].$$

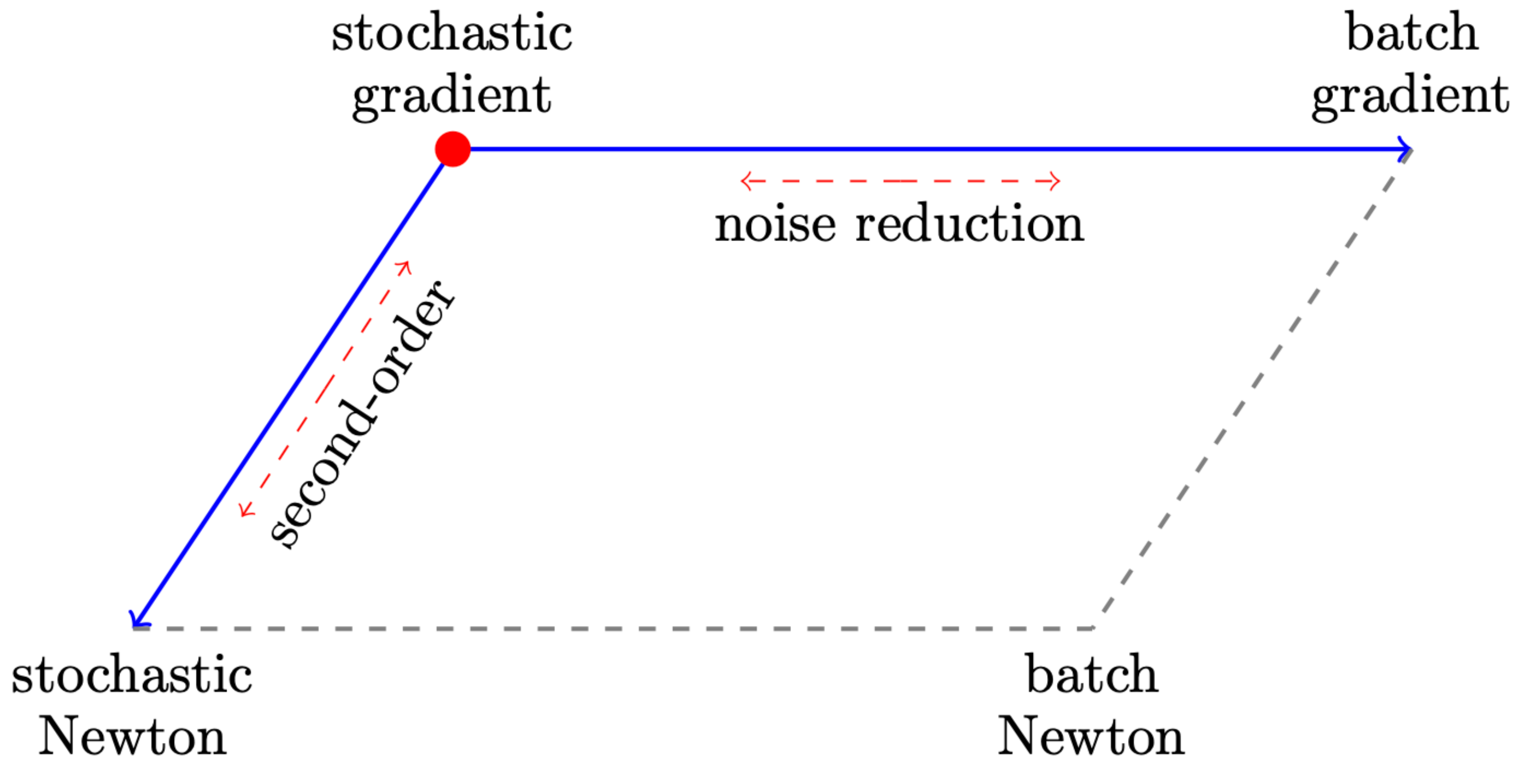
Overall, we have shown that

$$\begin{aligned} \mathop{\mathbb{E}}_{\mathbf{v}_{1:T}} [\langle \mathbf{w}^{(t)} - \mathbf{w}^\star, \mathbf{v}_t \rangle] &\geq \mathop{\mathbb{E}}_{\mathbf{v}_{1:t-1}} [f(\mathbf{w}^{(t)}) - f(\mathbf{w}^\star)] \\ &= \mathop{\mathbb{E}}_{\mathbf{v}_{1:T}} [f(\mathbf{w}^{(t)}) - f(\mathbf{w}^\star)] \,. \end{aligned}$$

Summing over t, dividing by T, and using the linearity of expectation, we get that Equation (14.10) holds, which concludes our proof. $\square$

LINEAR RATE METHODS

IMPROVING SGD



Slides taken from Jorge Nocedal

STOCHASTIC AVERAGED GRADIENT

- **Can we have a rate of $O(\rho^t)$ with only 1 gradient evaluation per iteration?**
  - YES! The stochastic average gradient (SAG) algorithm:
    - Randomly select i_t from $\{1, 2, \ldots, N\}$ and compute $f'_{i_t}(x^t)$.

$$x^{t+1} = x^t - \frac{\alpha^t}{N} \sum_{i=1}^{N} y_i^t$$

    - **Memory**: $y_i^t = \nabla f_i(x^t)$ from the last t where i was selected. [Le Roux et al., 2012]
  - Stochastic variant of increment average gradient (IAG). [Blatt et al., 2007]
  - Assumes gradients of non-selected examples don't change.
  - Assumption becomes accurate as $||x^{t+1} - x^t|| \to 0$.

Slides taken from Mark Schmidt

SAG CONVERGENCE RATE

- If each f_i' is $L-$continuous and f is strongly-convex, with $\alpha_t = 1/16L$ SAG has

$$\mathbb{E}[f(x^t) - f(x^*)] \leqslant \left(1 - \min\left\{\frac{\mu}{16L}, \frac{1}{8N}\right\}\right)^t C,$$

where

$$C = [f(x^0) - f(x^*)] + \frac{4L}{N}\|x^0 - x^*\|^2 + \frac{\sigma^2}{16L}.$$

- Linear convergence rate but only 1 gradient per iteration.
  - For well-conditioned problems, constant reduction per pass:

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

  - For ill-conditioned problems, almost same as deterministic method (but N times faster).

SAG CONVERGENCE RATE

- Assume that $N = 700000$, $L = 0.25$, $\mu = 1/N$:
  - Gradient method has rate $\left(\frac{L-\mu}{L+\mu}\right)^2 = 0.99998$.
  - Accelerated gradient method has rate $\left(1 - \sqrt{\frac{\mu}{L}}\right) = 0.99761$.
  - SAG (N iterations) has rate $\left(1 - \min\left\{\frac{\mu}{16L}, \frac{1}{8N}\right\}\right)^N = 0.88250$.
  - *Fastest possible* first-order method: $\left(\frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}\right)^2 = 0.99048$.
- SAG beats two lower bounds:
  - Stochastic gradient bound (of $O(1/t)$).
  - Deterministic gradient bound (for typical L, μ, and N).
- Number of f_i' evaluations to reach ϵ:
  - Stochastic: $O(\frac{L}{\mu}(1/\epsilon))$.
  - Gradient: $O(N\frac{L}{\mu}\log(1/\epsilon))$.
  - Accelerated: $O(N\sqrt{\frac{L}{\mu}}\log(1/\epsilon))$.
  - SAG: $O(\max\{N, \frac{L}{\mu}\}\log(1/\epsilon))$.

SAG IMPLEMENTATION

- Basic SAG algorithm:
  - while(1)
  - Sample i from $\{1, 2, \ldots, N\}$.
  - Compute $f_i'(x)$.
  - $d = d - y_i + f_i'(x)$.
  - $y_i = f_i'(x)$.
  - $x = x - \frac{\alpha}{N} d$.
- Practical variants of the basic algorithm allow:
  - Regularization.
  - Sparse gradients.
  - Automatic step-size selection.
    - Common to use adaptive step-size procedure to estimate L.
  - Termination criterion.
    - Can use $\|x^{t+1} - x^t\|/\alpha = \frac{1}{n} d \approx \|\nabla f(x^t)\|$ to decide when to stop.
  - Acceleration [Lin et al., 2015].
  - Adaptive non-uniform sampling [Schmidt et al., 2013].

SAG IMPLEMENTATION

- Does re-shuffling and doing full passes work better?
  - For classic SG: Maybe?
    - Noncommutative arithmetic-geometric mean inequality conjecture.

[Recht & Ré, 2012]

  - For SAG: NO.
  - Performance is intermediate between IAG and SAG.
- Can non-uniform sampling help?
  - For classic SG methods, can only improve constants.
  - For SAG, bias sampling towards Lipschitz constants L_i,

$$\|\nabla f_i(x) - \nabla f_i(y)\| \leq L_i \|x - y\|.$$

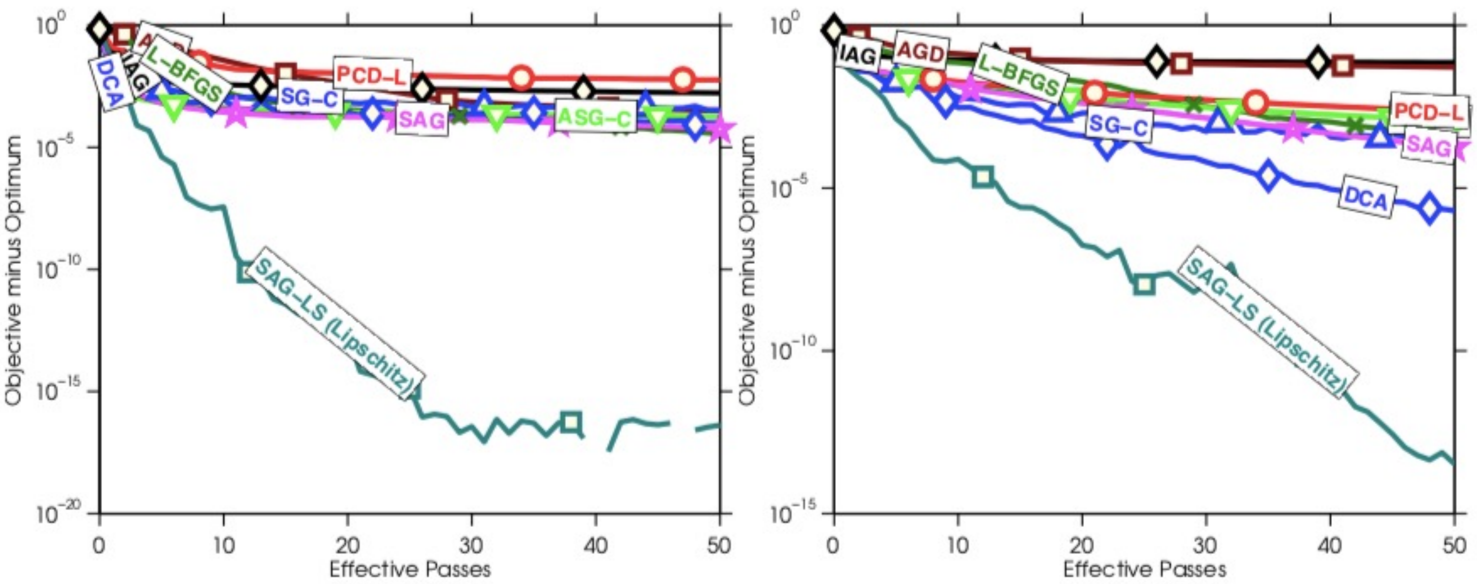
improves rate to depend on L_{mean} instead of L_{max}.

(with bigger step size)

  - Adaptively estimate L_i as you go. (see paper/code).
  - Slowly learns to ignore well-classified examples.

SAG with Non-Uniform Sampling

- protein ($n = 145751$, $p = 74$) and sido ($n = 12678$, $p = 4932$)



- Adaptive non-uniform sampling helps a lot.

STOCHASTIC VARIANCE REDUCED GD

SVRG algorithm:

- Start with x_0
- for $s = 0, 1, 2 \dots$
  - $d_s = \frac{1}{N} \sum_{i=1}^{N} f_i'(x_s)$
  - $x^0 = x_s$
  - for $t = 1, 2, \dots m$
    - Randomly pick $i_t \in \{1, 2, \dots, N\}$
    - $x^t = x^{t-1} - \alpha_t (f_{i_t}'(x^{t-1}) - f_{i_t}'(x_s) + d_s)$.
  - $x_{s+1} = x^t$ for random $t \in \{1, 2, \dots, m\}$.

Requires 2 gradients per iteration and occasional full passes, but only requires storing d_s and x_s.

Practical issues similar to SAG (acceleration versions, automatic step-size/termination, handles sparsity/regularization, non-uniform sampling, mini-batches).

References:

- Convergence rate analysis of GD and SGD:
  Understanding Machine Learning: Theory to Algorithms
  Shai Shalev Shwartz and Shai Ben David.

THANKS

QUESTIONS?

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