Minimizing Finite Sums with the Stochastic Average Gradient

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Overview



Introduction

Proposed SAG Algorithm

Convergence Analysis

Implementation Issues

Results



▶ N: no of observations.



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- ▶ N: no of observations.
- P: dimension of each observation.
- ▶ **Objective:** To minimize the sum of finite set of **Smooth functions**. $\min_{x \in \mathbb{R}^P} g(x) := \frac{1}{N} \sum_{i=1}^N f_i(x)$
 - To efficiently solve when N or P is very large.
- Assumptions:
 - g is μ -Strongly convex. $g(y) \ge g(x) + g'(x)^T(y-x) + \frac{\mu}{2}||y-x||^2$
 - f_i Convex. $f_i(y) f_i(x) \ge f'_i(x)^T (y x)$
 - f_i' is L-Lipschitz continuous. $|f_i'(y) f_i'(x)| \le L||y x||$



- ► Deterministic gradient method:
 - $x_{t+1} = x_t \frac{\alpha_t}{N} \sum_{i=1}^N f_i'(x_t)$
 - Linear Convergence rate: $O(\rho^t)$
 - Iteration cost is linear in N



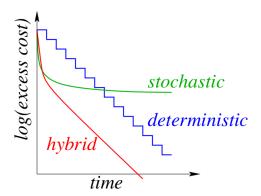
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- ► Stochastic gradient method:
 - Random selection of i(t) from $\{1, 2, ..., N\}$ $x_{t+1} = x_t \alpha_t f'_{i(t)}(x_t)$
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 - Sublinear convergence: $O(\frac{1}{t})$
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- ▶ Paper Objective: $O(\rho^t)$ rate with O(1) iteration cost with constant step-size.



- 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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- ▶ Needs storage of N gradient vectors. O(NP) storage.



$$C = \begin{pmatrix} I \\ \vdots \\ I \end{pmatrix} \in \mathbb{R}^{np \times p} \qquad f'(x) = \begin{pmatrix} f_{1}'(x) \\ \vdots \\ f_{n}'(x) \end{pmatrix} \in \mathbb{R}^{np} \qquad b^{k} = \begin{pmatrix} g_{1}^{k} \\ \vdots \\ g_{n}^{k} \\ \chi^{k} \end{pmatrix} \in \mathbb{R}^{\binom{n+1}{p}} \begin{pmatrix} f_{1}(\chi^{k}) \\ \vdots \\ f_{n}(\chi^{k}) \\ \chi^{k} \end{pmatrix}$$

$$b^{*} \in \mathbb{R}^{(n+1)p}$$

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then
$$(\theta^{k} - \theta^{k})^{T}$$
 $\begin{pmatrix} A & b \\ b^{T} & c \end{pmatrix}$ $\begin{pmatrix} \theta^{k} - \theta^{k} \end{pmatrix}$

$$= \begin{pmatrix} y^{k} - f(x^{k}) \end{pmatrix}^{T} A \begin{pmatrix} y^{k} - f'(x^{k}) \end{pmatrix} + 2 \begin{pmatrix} y^{k} - f'(x^{k}) \end{pmatrix}^{T} b \begin{pmatrix} x^{k} - x^{k} \end{pmatrix} + \begin{pmatrix} x^{k} - x^{k} \end{pmatrix}^{T} c \begin{pmatrix} x^{k} - x^{k} \end{pmatrix}$$

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$$(1-\frac{1}{n})$$
 $y_1^{\kappa-1} + \frac{1}{n}$ $f_i'(\alpha^{\kappa-1}) + z_i^{\kappa} [f_i'(\alpha^{\kappa-1}) - y_i^{\kappa-1}] - \mathbb{D}$

where z_i^{κ} is a R.V., takes nalue $(1-\frac{1}{n})$ with probability $\frac{1}{n}$
 $(-\frac{1}{n})$ with probability $(1-\frac{1}{n})$

REASON: f_{κ} (sampled $i_{\kappa}=i$) = $\frac{1}{n}$ & when $i_{\kappa}=i$, we want $y_i^{\kappa}=f_i'(\alpha^{\kappa-1})$

Tr (sampled $i_k=i$) = $\frac{1}{n}$ 4 when $i_k=i$, we want $y_i^*=f_i(x^{k-1})$ ① says that with probability $\frac{1}{n}$; z_i^* takes $\binom{1-1}{n}$ making $y_i^*=f_i'(x^{k-1})$

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$$x^{k+1} = x^k - \tfrac{\alpha_k}{N} \sum_{i=1}^N y_i^k$$



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• Similarly,
$$x^{k} = x^{k-1} - \frac{\alpha}{n} \sum_{i=1}^{n} \left[\left(1 - \frac{1}{n} \right) y^{k-1} + \frac{1}{n} f_{i}'(x^{k-1}) + z^{k} \left[f_{i}(x^{k-1}) - y^{k-1} \right] \right]$$

Matrix form = $x^{k-1} - \frac{\alpha}{n} \left[\left(1 - \frac{1}{n} \right) e^{T} y^{k-1} + g'(x^{k-1}) + (z^{k})^{T} \left[f(x^{k-1}) - y^{k-1} \right] \right]$

where $z^{k} = \left(z^{k} \cdot I \right) \in \mathbb{R}^{np\times p}$
 $z^{k} \cdot I = \sum_{i=1}^{n} f_{i}(x) = e^{T} f'(x)$

we used the equality $g'(x) = \sum_{i=1}^{n} f_{i}(x) = e^{T} f'(x)$

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- ► x*: unique minimizer of g. g is Strongly Convex so Strictly Convex also.
- $ightharpoonup \mathcal{F}_{k-1}$: σ-field of information generated by $z^1, z^2, ..., z^{k-1}$.



To Prove:

With a constant step size of $\alpha_k = \frac{1}{2nL}$, the SAG iterations satisfy for $k \geq 1$:

$$\mathbb{E}\left[\|x^k - x^*\|^2\right] \leqslant \left(1 - \frac{\mu}{8Ln}\right)^k \left[3\|x_0 - x^*\|^2 + \frac{9\sigma^2}{4L^2}\right].$$



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Outline of Proof:

- 1. Find a Lyapunov function Q from $\mathbb{R}^{(n+1)p}$ to \mathbb{R} such that the sequence $\mathbb{E}[Q^k]$ decreases at a linear rate.
- 2. Prove $Q(\theta^k)$ dominates $||x^k x^*||^2$



Step 1: Linear Convergence of Lyapunov Function A quadratic $Q(\theta^k) = (\theta^k - \theta^*)^T P(\theta^k - \theta^*)$ is chosen as Lyapunov Function, where

$$P = \begin{pmatrix} A & b \\ b^T & c \end{pmatrix}$$



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$$A = 3n\alpha^{2}I + \frac{\alpha^{2}}{n}(\frac{1}{n} - 2)ee^{\top}$$

$$b = -\alpha(1 - \frac{1}{n})e$$

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To show that: $\mathbb{E}[Q(\theta^k)|\mathcal{F}_{k-1}] - (1-\delta)Q(\theta^{k-1})$ is negative for some $\delta > 0$.

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Expanding the first term

$$\mathbb{E}\left[\left.(\theta^{k} - \theta^{*})^{\top} \begin{pmatrix} A & b \\ b^{\top} & c \end{pmatrix} (\theta^{k} - \theta^{*}) \middle| \mathcal{F}_{k-1}\right] \right]$$

$$= E\left[\left.(y^{k} - f'(x^{*}))^{\top} A(y^{k} - f'(x^{*})) + 2(y^{k} - f'(x^{*}))^{\top} b(x^{k} - x^{*}) + (x^{k} - x^{*})^{\top} c(x^{k} - x^{*}) \middle| \mathcal{F}_{k-1}\right]$$



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$$y_i^k = (1 - \frac{1}{n})y_i^{k-1} + \frac{1}{n}f_i'(x_i^{k-1}) + z_i^k[f_i'(x_i^{k-1}) - y_i^{k-1}]$$



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- $y_i^k = (1 \frac{1}{n})y_i^{k-1} + \frac{1}{n}f_i'(x_i^{k-1}) + z_i^k[f_i'(x_i^{k-1}) y_i^{k-1}]$
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- z_i^k : Random variable that takes value $(1-\frac{1}{n})$ with probability $\frac{1}{n}$ and take value $-\frac{1}{n}$ otherwise.



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$$\mathbb{E}[(z_i^k)^2] = (1 - \frac{1}{n})^2 (\frac{1}{n}) + (-\frac{1}{n})^2 (1 - \frac{1}{n}) = \frac{1}{n} (1 - \frac{1}{n})$$



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•
$$\mathbb{E}[z_i^k z_j^k] = 2(1 - \frac{1}{n})(\frac{-1}{n})(\frac{1}{n}) + (\frac{-1}{n})(\frac{-1}{n})\frac{n-2}{n} = -\frac{1}{n^2}$$



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Recall that:

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The randomness in $Q(\theta^k)$ comes only because of z^k

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After substituting the expectation of z^k & re-arranging, $\mathbb{E}[Q(\theta^k)|\mathcal{F}_{k-1}]$

$$= \left(1 - \frac{1}{n}\right) 3n\alpha^{2} (y^{k-1} - f'(x^{*}))^{\top} (y^{k-1} - f'(x^{*}))$$

$$+ (x^{k-1} - x^{*})^{\top} (x^{k-1} - x^{*}) - 2\alpha (x^{k-1} - x^{*})^{\top} g'(x^{k-1})$$

$$+ 3\alpha^{2} (f'(x^{k-1}) - f'(x^{*}))^{\top} (f'(x^{k-1}) - f'(x^{*}))$$

$$- 2\alpha \left(1 - \frac{1}{n}\right) (y^{k-1} - f'(x^{*}))^{\top} e(x^{k-1} - x^{*})$$



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► The goal is to bound $\mathbb{E}[Q(\theta^k)|\mathcal{F}_{k-1}] - (1-\delta)Q(\theta^{k-1})$ by $g'(x^{k-1})^T(x^{k-1}-x^*)$ positive due to Convexity.

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- ▶ The 3^{rd} term contains $(f'(x^{k-1}) f'(x^*))^T (f'(x^{k-1}) f'(x^*)) = \sum_{i=1}^n ||(f'_i(x^{k-1}) f'_i(x^*))||^2$



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- ► The goal is to bound $\mathbb{E}[Q(\theta^k)|\mathcal{F}_{k-1}] (1-\delta)Q(\theta^{k-1})$ by $g'(x^{k-1})^T(x^{k-1}-x^*)$ positive due to Convexity.
- ► The 3rd term contains $(f'(x^{k-1}) f'(x^*))^T (f'(x^{k-1}) f'(x^*)) = \sum_{i=1}^n ||(f_i'(x^{k-1}) f_i'(x^*))||^2 \le \sum_{i=1}^n (f_i'(x^{k-1}) f_i'(x^*))^T L(x^{k-1} x^*) = nLg'(x^{k-1})^T (x^{k-1} x^*)$ gradients' L-Lipschitz continuity & g'(x*)=0.



$$\begin{split} \mathbb{E}[Q(\theta^k)|\mathcal{F}_{k-1}] - (1-\delta)Q(\theta^{k-1}) &\leq \\ (y^{k-1} - f'(x^*))^T [3n\alpha^2(\delta - \frac{1}{n})I + (1-\delta)\frac{\alpha^2}{n}(2 - \frac{1}{n})ee^T](y^{k-1} - f'(x^*)) + \delta(x^{k-1} - x^*)^T (x^{k-1} - x^*) - (2\alpha - 3\alpha^2nL)(x^{k-1} - x^*)^T g'(x^{k-1}) + (y^{k-1} - f'(x^*))^T (-2\alpha(1 - \frac{1}{n})e)(x^{k-1} - x^*) \end{split}$$

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 - For $M \prec 0$, $s^T M s + s^T t = -\lambda ||s||^2 + s^T t + \left(-\frac{1}{4\lambda} ||t||^2\right) = -||2\lambda s t||^2 \le 0$



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 - Sufficient condition for $M \prec 0$ is $\delta \leq \frac{1}{3n}$

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Using this,

$$\mathbb{E}[Q(\theta^{k})|\mathcal{F}_{k-1}] - (1-\delta)Q(\theta^{k-1}) \leqslant -(2\alpha - 3\alpha^{2}nL)(x^{k-1} - x^{*})^{\top}g'(x^{k-1}) + \left(\delta - \frac{\delta^{2}\left(1 - \frac{1}{n}\right)^{2}}{\left[3n\delta - 1 - 2\delta + \frac{\delta - 1}{n}\right]}n\right) \|x^{k-1} - x^{*}\|^{2}$$



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Using this,

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Step 1(Linear Convergence of Lyapunov Function) finished.



Step 2: $Q(\theta^k)$ dominates $||x^k - x^*||^2$

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► Recall that $Q(\theta^k) = (\theta^k - \theta^*)^T P(\theta^k - \theta^*)$, where $P = \begin{pmatrix} A & b \\ b^T & c \end{pmatrix}$; A was positive definite.



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- ▶ $\mathbb{E}||x^k x^*||^2 \le 3\mathbb{E}[\theta^k]$. With all $y_i^0 = 0$, $\mathbb{E}||x^k x^*||^2 \le (1 \frac{\mu}{8NL})^k (\frac{9\sigma^2}{4L^2} + 3||x^k x^*||^2)$



▶ Theorem for faster rate: With $\alpha_t = \frac{1}{16L}$ SAG iteration satisfy $\mathbb{E}[g(x^k) - g(x^*)] \le (1 - \min\{\frac{\mu}{16L}, \frac{1}{8N}\})^k C$



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 - Accelerated: $O(\sqrt{\frac{L}{\mu}}(\frac{1}{\epsilon}))$
 - **SAG**: O(max{ $N, \frac{L}{\mu}$ } log($\frac{1}{\epsilon}$))



Algorithm 1 Basic SAG method for minimizing $\frac{1}{n} \sum_{i=1}^{n} f_i(x)$ with step size α

```
d = 0, y_i = 0 \text{ for } i = 1, 2, \dots, n

for k = 0, 1, \dots do

Sample i from \{1, 2, \dots, n\}

d = d - y_i + f_i'(x)

y_i = f_i'(x)

x = x - \frac{\alpha}{n}d

end for
```



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$$d = 0, y_i = 0 \text{ for } i = 1, 2, ..., n$$

for $k = 0, 1, ...$ do
Sample i from $\{1, 2, ..., n\}$
 $d = d - y_i + f'_i(x)$
 $y_i = f'_i(x)$
 $x = x - \frac{\alpha}{n}d$
end for

Termination criteria: When $||\frac{d}{N}|| = ||\frac{\sum_{i=1}^{N} y_i}{N}||$ becomes small.

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 - Double L if $f_{i_k}(x^k-\frac{1}{L^k}f'_{i_k}(x^k)) \le f_{i_k}(x^k)-\frac{1}{2L^k}||f'_{i_k}(x^k)||^2$ not satisfied. Smoothness



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- **4. Mini-batches** Batch-size of k leads to k-fold reduction in storage cost. L can be chosen to be one of max eigenvalue $\frac{1}{|\mathcal{B}|} \sum_{i \in \mathcal{B}} L_i \leq \max_{i \in \mathcal{B}} \{L_i\}$



- Non-uniform example selection: Convergence rate depends on $\frac{\mu}{L}$. One way to improve convergence rate by decreasing L. (For a sum of functions L is usually the max of all Lipschitz constants)
 - We can replace f_n by f_{n1} & f_{n2} st. $f_{n1}(x) = f_{n2}(x) = \frac{f_n(x)}{2}$, making $g(x) = \frac{1}{n} (\sum_{i=1}^{n-1} f_i(x) + f_{n1}(x) + f_{n2}(x))$ which can be written as $g(x) = \frac{1}{n+1} (\sum_{i=1}^{n-1} \frac{n+1}{n} f_i(x) + \frac{n+1}{n} f_{n1}(x) + \frac{n+1}{n} f_{n2}(x))$



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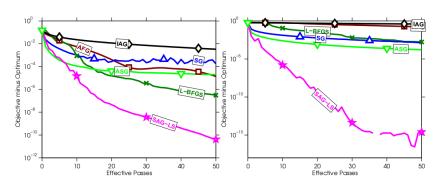
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 - ▶ Also increased probability of f_n being sampled from $\frac{1}{n}$ to $\frac{2}{(n+1)}$
 - Duplicate each function f_i a no. of times equal to it's Lipschitz constant of their gradient.
 - ▶ $g(x) = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{l} i \frac{f_i(x)}{l_i}$ which can be written as $g(x) = \frac{1}{\sum_k l_k} \sum_{i=1}^{n} \sum_{j=1}^{L} i \frac{\sum_k l_k}{l_i} \frac{f_i(x)}{l_i}$. Now L is equivalent to taking average of Lipschitz constants across f_i' instead of taking max.

Results-Comparison with FG & SG methods



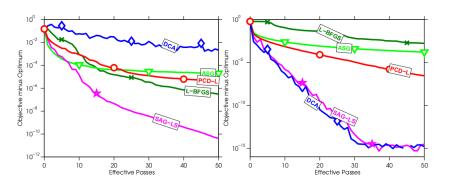
• quantum (n = 50000, p = 78) and rcv1 (n = 697641, p = 47236)



Results-Comparison with CD methods



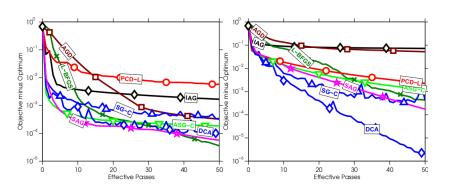
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Effect of non-uniform sampling



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



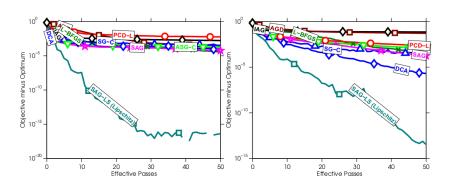
Datasets where SAG had the worst relative performance.

Before non-uniform sampling.

Effect of non-uniform sampling



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



• Lipschitz sampling helps a lot.

After non-uniform sampling.