Converging on the Ultimate Algorithm for Minimizing Convex Sums

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Minimizing Convex Sums

- We consider the problem of minimizing a finite sum,

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x),$$

  of smooth and convex functions f_i.

- Classic problem frequently arising in machine learning (ML):
  - Basic models like Least squares, logistic regression:

$$f_i(x) = \frac{1}{2}(a_i^T x - b_i)^2, \quad f_i(x) = \log(1 + \exp(-b_i a_i^T x)),$$

    and more advanced models like conditional random fields:

$$f_i(x) = -w^T \phi(x_i, y_i) + \log \sum_{y'} \exp(w^T \phi(x_i, y')).$$

- Stochastic gradient methods are traditional approach for large n.

Modern Stochastic Gradient Methods

- Classic stochastic gradient have a sublinear convergence rate.
- Since 2012: new stochastic gradient method with linear rates.
  - Many papers on this topic (see our tutorial tomorrow).
- Algorithms from papers often work great in practice.
  - Sometimes better than existing highly-tuned libraries.
  - Now used in standard ML packages and commercial products
- But they could potential work much better in practice.
  - Worst-case analyses don't account for all structure in the data.
  - There are still a important practical tricks to be discovered.

This Talk: Tricks for Speeding Up SAG and SVRG

- This talk: tricks that could make SAG or SVRG much faster.
  - Same tricks could likely speed up other methods.
  - I'm mostly going to stay away from parallel/distributed issues.
- My goal: build the best "black box" implementation possible.
- What I want from you:
  - If you like to prove, some of these are good challenges.
  - If you like to implement, these could help.
  - If I'm missing tricks, let me know!

Stochastic Average Gradient (SAG) Algorithm

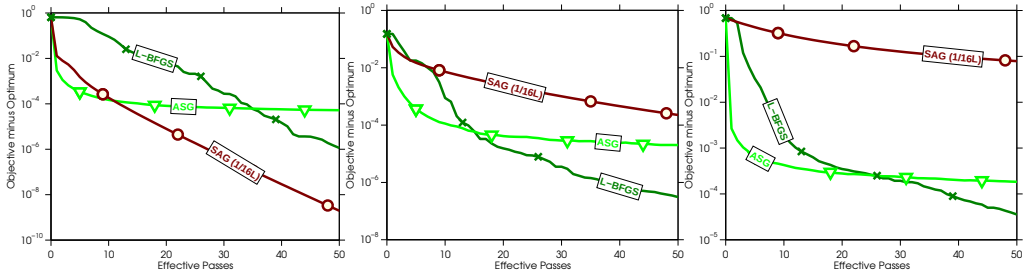
- The stochastic average gradient (SAG) algorithm has the form

$$x^{t+1} = x^t - \frac{\alpha_t}{n} \sum_{i=1}^{n} f_i'(x^{i_t}),$$

  a gradient descent step but with old gradient estimates.
- Each iteration evaluates $f_i'(x^t)$ for a random i.
  - We set $i_t = t$ for this example and $i_t = i_{t-1}$ for the others.
- Number of gradients to reach accuracy ϵ: $\tilde{O}((n + \kappa))$.
  - Gradient method requires $\tilde{O}(n\kappa)$.
  - Classic stochastic methods require $O(1/\epsilon)$.

Stochastic Average Gradient (SAG) Algorithm

- Comparing algorithm from theorem to best implementations:

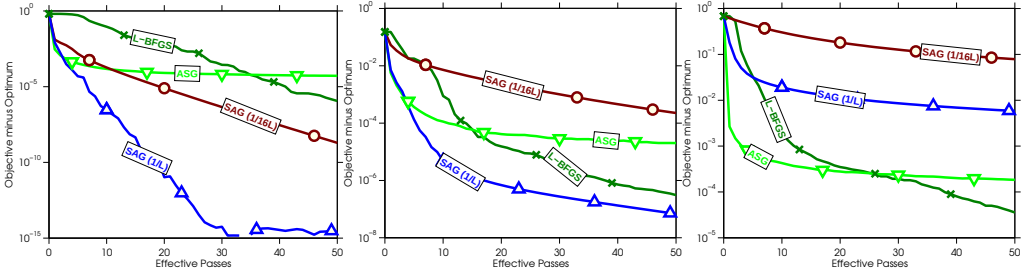


- Sometimes it does better but often it does worse...

Bigger Step Sizes for SAG

- Assumptions in the analysis:
  - Function f is strongly-convex.
  - Gradients f_i' are L-Lipschitz continuous.
  - Step-size α_t is set to $1/16L$.

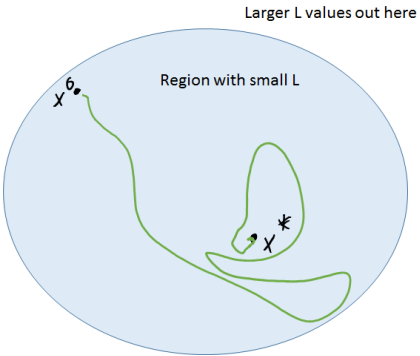
- Algorithm works better in practice with $\alpha_t = 1/L$.



Even-Bigger Step Sizes for SAG

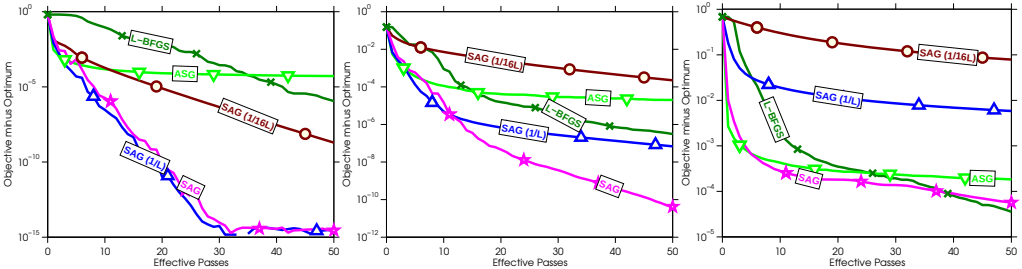
- In general SAG does not work with $\alpha_t = 10/L$ (or even $1/L$).
  - But for some problems it works way better with this choice.
- Why???

- For some problems: local L is much smaller than global L.



Even-Bigger Step Sizes for SAG

- Using global L vs. trying to estimate local L:

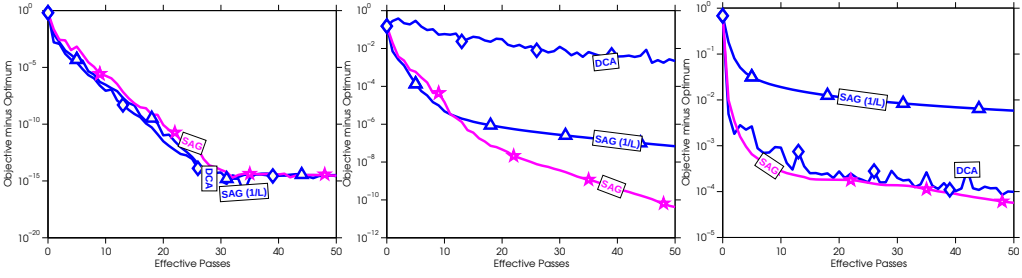


- See Section 4 of Le Roux et al. [2012] and also Vainsencher et al. [2015].

Algorithms Depending on μ

- What about step-sizes depending on μ?
  - Should we use $\alpha_t = \frac{2}{L+n\mu}$?.

- Watch out for local μ vs. global μ.
  - SDCA uses global μ so sometimes does really bad:



Better Step-Sizes?

- What about just trying to figure out step-size that works the best?
- Mairal [2013] gives a simple line-search method:
  - Search for the best performance on a subset of the data (Bottou trick).
- Is there a better method to be discovered?

SAG vs. SVRG

- Disadvantage of SAG is that it has a huge memory requirement.
- For many problems, gradient structure allows us to reduce this.
  - Least squares, logistic regression, conditional random fields.
- For general problems, we can instead use SVRG.

Stochastic Variance-Reduced Gradient (SVRG)

SVRG algorithm:

- 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)
  - $x^0 = x_s$
  - 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)
  - $x_{s+1} = x^t$ (initialize next outer loop)
- Only need to store x_s and d_s.
- Choices that seem to work well are $\alpha_t = 1/L$ and $m = n$.
- Full gradient calculations are wasteful when far from the solution.

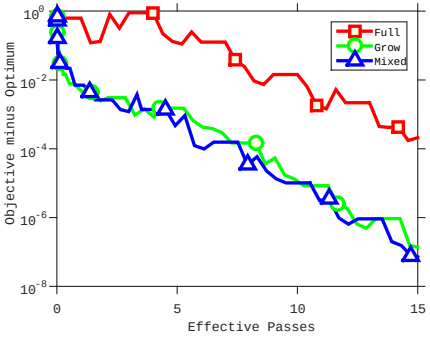
Stochastic Variance-Reduced Gradient (SVRG)

Practical SVRG algorithm:

- Start with x_0
- for $s = 0, 1, 2 \ldots$ (outer loop)
  - $d_s = \frac{1}{|\mathcal{B}_s|} \sum_{i \in \mathcal{B}_s} f_i'(x_s)$ (batch gradient calculation)
  - $x^0 = x_s$
  - 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)
  - $x_{s+1} = x^t$ (initialize next outer loop)
- Control variate d_s can be based on a subset of the examples.
- Preserve rate if $\mathcal{B}_s$ grows fast enough.
- For example, $\mathcal{B}_s = \min\{2^s, n\}$.

Practical SVRG

- SVRG with full-gradient d^s compared to growing batch:



- Is there a better way to grow d^s or choose $\mathcal{B}_s$?
- Recent work shows that maybe we should be updating d^s [Ngyuen et al., 2017].

Non-Uniform Sampling

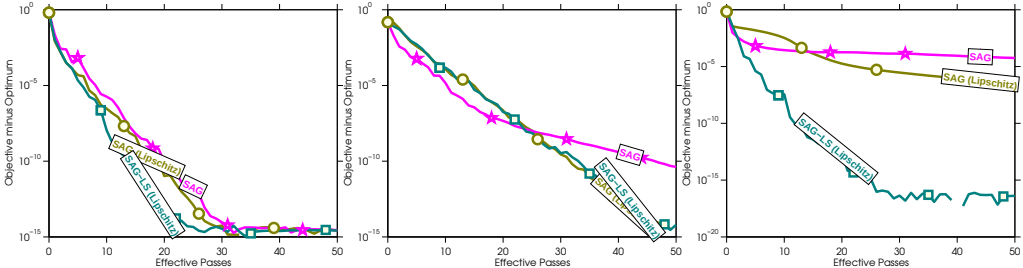
- Can we improve performance by non-uniform sampling?
- Consider case where each f_i' has Lipschitz constant L_i:
  - Improve the rate theoretically by sampling biasing towards L_i.

[Xiao & Zhang, 2014]

- Justification: frequently sample gradients that change quickly.
- In practice, a huge difference between local L_i and global L_i.

Non-Uniform Sampling

- Uniform vs. non-uniform (global L_i) vs. non-uniform (local L_i).



- Is this sampling proportional to L_i optimal across iterations?
- Work on stratified sampling and clustering examples.

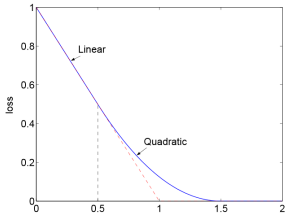
[Zhao & Zhang, 2014, Hoffman et al., 2015, Allen-Zhu et al., 2016]

Identifying Support Vectors

- A related idea: identifying support vectors.

- Consider a smoothed SVM problem [Rosset & Zhu, 2006]:

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

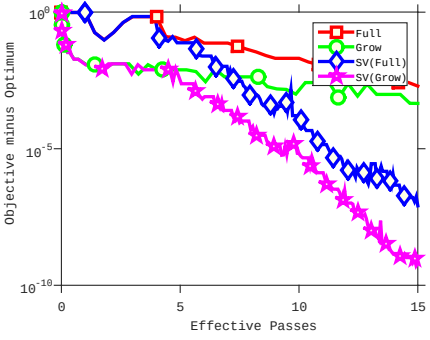


- The solution is sparse in the f_i' (has support vectors).

Identifying Support Vectors

- Keep track of number z of consecutive times $f_i'(x^t)$ was zero.
- If it's zero at least twice $(z \geq 2)$, skip the next 2^{z-2} evaluations.
  - May only evaluate non-support examples a logarithmic number of times.

[Babanezhad et al., 2015]



Choosing the Batch

- We can often evaluate several gradients in parallel.
- Logical way to pick the batch size: number of parallel gradients.
- Two possibilities ways to sample the batch:
  - Sample from a fixed set of data “blocks”.
  - Sample the original variables.
- For the original variables, Lipschitz sampling again helps.
- For constructing “blocks”, there may be better strategies.
  - Try to make the blocks have small or varied Lipschitz constants.

Acceleration

- Can we accelerate these methods as with gradient methods?
  - Is $\tilde{O}(n + \kappa)$ the best we can do?
- We can't reduce runtime to $\tilde{O}(n + \sqrt{\kappa})$.
- But several authors give algorithms achieving $\tilde{O}(n + \sqrt{n\kappa})$.

Acceleration

- Most common strategy: inexact proximal point methods use

$$x_{k+1} = \operatorname*{argmin}_x f(x) + \frac{\lambda_k}{2}\|x - x_k\|^2,$$

  and solve this up to accuracy ϵ_k using stochastic method.

[Shalev-Schwartz & Zhang, 2014]

- But needs sequence of parameters and termination criteria.
  - Although some nice tricks in Lin et al. [2015].

- Recent alternatives don't need the inner/outer setup.

[Lan & Zhou, 2015, Allen-Zhu, 2016, Defazio, 2016]

Newton-Like Methods

- Can we make Newton-like versions of these methods?

- If we use a matrix H and apply the update

$$x^{t+1} = x^t - \frac{\alpha_t}{n} H \sum_{i=1}^{n} f_i'(x^{i_t}),$$

  then we get the convergence for minimzing $f(H^{1/2}x)$ instead of $f(x)$.

- Can be much faster, but doesn't give superlinear for any H.
  - Superlinear not possible for random, but possible for cyclic [Rodomanov & Kropotov, 2016]
- Not clear how to choose a sequence of H_t matrices.
  - But many recent works on this topic.
- Non-diagonal H_t substantial increase runtime for sparse datasets.

Summary

- Methods are great in theory, but practical details need to be worked out too.
- How do we use/identify bigger step-sizes?
- Is sampling based on Lipschitz constants optimal?
  - Particularly for accelerated and Newton-like methods.
- Can we cleverly choose the batch or batch size?
- Can we make accelerated methods adaptive to μ?
- Can we design robust/efficient Newton-like method?