# ADAM, SARAH

Variance Reduction

Alex Salce SIE 596 | 04/18/2024

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## Introduction

In general, we are solving an optimization problem of the form…

We have covered techniques to reduce variance of the randomized gradient steps in a minibatch or stochastic gradient descent algorithm, but can we improve upon these (SVRG, SAG/SAGA, etc)?

#### **ADAM** (orig. 2015)

[7] D. P. KINGMA AND J. BA, Adam: A method for stochastic optimization, 2017.

#### **SARAH** (2017)

[8] L. M. NGUYEN, J. LIU, K. SCHEINBERG, AND M. TAKÁČ, Sarah: A novel method for machine learning problems using stochastic recursive gradient, 2017.

Each has a unique approach to address variance reduction. Both utilize recursive gradient information.

$$
\min_{x \in \mathbb{R}^d} \left\{ P(x) = \frac{1}{n} \sum_{i=1}^n f_i(x) \right\}
$$

### **ADAM ADA**ptive **M**oment estimation

*Variant of minibatch GD, Momentum, RMSProp*

### **SARAH S**toch**A**stic **R**ecursive gr**A**dient algorit**H**m *Variant of SVRG*

## Why is it important?

We are highly motivated to improve gradient descent optimization methods. Why? Computational efficiency when optimizing model parameters for large datasets.

ADAM is a popular optimizer

➔ Very popular in training of neural networks (nonconvex objectives), NLP tasks, GANs, Reinforcement Learning

SARAH offers improved convergence over SVRG

 $\rightarrow$  Can replace GD methods in practice for convex optimization like we have seen in this course

Applications for convex and nonconvex objectives (though we will only focus upon convex)

### Assumptions (for reference)

•  $[{\sf CONVEX}] f_i$  is convex

 $f_i(y) \ge f_i(x) + \nabla f_i(x)^T (y - x)$ 

• **[SCONVEX]** Each  $f_i$  is  $\mu$ -strongly convex,  $\exists \mu > 0$  *s.t.*  $f_i(y) \ge f_i(x) + \nabla f_i(x)^T (y - x) +$  $\mu$ 2  $y - x$ 2 ,  $\forall x, y \in \mathbb{R}$ 

Note, a function is mu-strongly convex if  $\lambda_{min}\left(\nabla^2 f(x)\right) \geq \mu, \mu > 0 \; \forall x \in \mathbb{R}$  $\mathbb{R}^d$ , where  $\lambda_{min} (*)$  operator returns the smallest eigenvalue of \*.So,  $\mu$ **should be less than or equal to the smallest eigenvalue of the Hessian of the objective function.**



## Assumptions (for reference)

• **[LSMOOTH]** Each  $f_i$  is convex,  $L$ -smooth (Lipschitz continuous gradient), ∃  $L > 0$   $s.$   $t.$  $|f_i(x) - f_i(y)| \leq L ||x - y||, \forall x, y \in \mathbb{R}$ 

#### •  $[LOL1S]$  ( $L_0, L_1$ ) smoothness

**Assumption 1** (( $L_0, L_1$ ) Smoothness). All of  $\{f_i\}_{i=0}^{n-1}$  satisfy ( $L_0, L_1$ ) smoothness, i.e., there exist positive constants  $(L_0, L_1)$ , such that,  $\forall w_1, w_2 \in \mathbb{R}^d$  satisfying  $\|w_1 - w_2\| \leq \frac{1}{L_1}$ ,

$$
\|\nabla f_i(\boldsymbol{w}_1) - \nabla f_i(\boldsymbol{w}_2)\| \le (L_0 + L_1 \|\nabla f_i(\boldsymbol{w}_1)\|) \|\boldsymbol{w}_1 - \boldsymbol{w}_2\|,
$$
\n(3)

and  $f_i(\boldsymbol{w})$  is lower bounded,  $\forall i \in [0, n-1]$ .

Eq. (3) generalizes the classical bounded smoothness condition (i.e.,  $L_1 = 0$  in Assumption 3), and allows for a wide range of simple and important functions such as the polynomials and even the exponential functions. Moreover, empirical observation [36, 34] suggests that Eq. (3) is a preciser characterization of the loss landscape of neural networks than the classical bounded smoothness condition in tasks where Adam outperforms SGD.

[9] B. WANG, Y. ZHANG, H. ZHANG, Q. MENG, Z.-M. MA, T.-Y. LIU, AND W. CHEN, Provable *adaptivity in adam, 2022.* 

## ADAM - Summary

- Combines Momentum and RMSProp techniques for accelerating/reducing variance
- Constant learning rate hyperparameters, but adaptive steps (bias corrected)
- Recursive batch gradient information
- No gradient table
- Converges  $\boldsymbol{0}\left(\frac{1}{\sqrt{2}}\right)$  $\frac{1}{\overline{T}}$  for  $T$ iterations



## ADAM Algorithm

#### Initialization

- Objective function  $f \in \mathbb{R}^{n \times 1}$
- Constant learning rate  $\eta$
- Exponential decay rates  $\beta_1, \beta_2$
- Epsilon  $\varepsilon$
- Vectors  $w_0 \in \mathbb{R}^{1 \times m}$ ,  $m_0 \in \mathbb{R}^{1 \times m}$ ,  $v_0 \in \mathbb{R}^{1 \times m}$ **Loop**:
- Stochastic (**batch**) Gradient step
- **Gradient 1st moment estimate (mean of past grads), moving average param & bias correction**
- **Gradient 2nd moment estimate (ssqares of past grads), moving average param & bias correction**
- Parameter update

#### Algorithm 1 ADAM

- (0) **Require:** stochastic objective function  $f_i(w)$
- (1) **Require:** learning rate  $\eta$ , exponential decay rates  $\beta_1, \beta_2 \in [0, 1)$ , tolerance  $\epsilon$
- (2) Initialize: initial parameter vector  $w_0$ , initial 1<sup>st</sup> moment vector  $m_0 \leftarrow 0$ , initial 2<sup>nd</sup> moment vector  $v_0 \leftarrow 0$ , initial timestep  $t \leftarrow 0$
- while  $w_t$  is not converged do  $(3)$

#### $t \leftarrow t + 1$

- $g_t \leftarrow \nabla_w f_t(w_{t-1})$  (batch gradient at iteration t)
- (*udpate baised first moment estimate*)  $m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot q_t$
- $v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 \beta_2) \cdot g_t^2$  (udpate baised second raw moment estimate)
- $\hat{m}_t \leftarrow m_t/(1-\beta_1^t)$  (bias-corrected first moment estimate)  $\hat{v}_t \leftarrow v_t/(1-\beta_2^t)$  (bias-corrected second raw moment estimate)
	- $w_t \leftarrow w_{t-1} \eta \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$  $(update\ parameters)$

end while

return  $w_t$ 

Typical choice:  $\eta = 0.001$ ,  $\beta_1 = 0.9$ ,  $\beta_2 = 0.999$ ,  $\varepsilon = 1e - 8$ 

## ADAM Algorithm – Momentum

- $m_t$  exponential moving average based on previous aggregate batch gradient information
- This step is analogous to **Momentum** (same general idea as Acceleration)
- Estimate is biased toward initialization (zero), so an additional **bias-correction step** is employed



## ADAM Algorithm – RMSProp

- $v_t$  exponential moving average of sum of squares of past gradients
- This step is **RMSProp**
- Estimate is biased toward initialization (zero), so an additional **bias-correction step** is employed



## ADAM Algorithm – ADAM update

- **Parameter update** like descent, subtracting learning rate  $\eta$  times bias-corrected Momentum  $\hat{m}_t$ combined with bias-corrected RMSProp  $1/(\sqrt{\hat{v}_t} + \varepsilon)$ .
- Variance reduction -> RMSProp



 $\widehat{m}_t$  $\frac{\partial t}{\partial \widehat{v_{t}}}$  - Signal to Noise Ratio (SNR)

### ADAM



Momentum uses average past gradient information to reduce variance, RMSProp adaptively scales learning rate by magnitude of current and average of past gradients

https://wiki.cloudfactory.com/docs/mp-wiki/solvers-optimizers/rmsprop



## ADAM Convergence Summary

### For [CONVEX] and [L0L1S] objective

Under basic convexity assumptions for the objective,

ADAM is guaranteed convergence at rate  $\bm{0}(\frac{1}{\sqrt{2}})$  $\frac{1}{T}$ 

NOTE: There are known flaws in the original proof of Kingma and Ba that are addressed with  $(L_0, L_1)$ smoothness condition



B. WANG, Y. ZHANG, H. ZHANG, Q. MENG, Z.-M. MA, T.-Y. LIU, AND W. CHEN, Provable adaptivity in adam, 2022.

$$
R(T) = \sum_{t=1}^{T} [f_t(\theta_t) - f_t(\theta^*)]
$$

**Theorem 4.1.** Assume that the function  $f_t$  has bounded gradients,  $\|\nabla f_t(\theta)\|_2 \leq G$ ,  $\|\nabla f_t(\theta)\|_{\infty} \leq$  $G_{\infty}$  for all  $\theta \in R^d$  and distance between any  $\theta_t$  generated by Adam is bounded,  $\|\theta_n - \theta_m\|_2 \le D$ ,  $\|\theta_m - \theta_n\|_{\infty} \leq D_{\infty}$  for any  $m, n \in \{1, ..., T\}$ , and  $\beta_1, \beta_2 \in [0, 1)$  satisfy  $\frac{\beta_1^2}{\sqrt{\beta_2}} < 1$ . Let  $\alpha_t = \frac{\alpha}{\sqrt{t}}$ and  $\beta_{1,t} = \beta_1 \lambda^{t-1}$ ,  $\lambda \in (0,1)$ . Adam achieves the following guarantee, for all  $T \ge 1$ 

$$
R(T) \le \frac{D^2}{2\alpha(1-\beta_1)} \sum_{i=1}^d \sqrt{T\hat{v}_{T,i}} + \frac{\alpha(1+\beta_1)G_{\infty}}{(1-\beta_1)\sqrt{1-\beta_2}(1-\gamma)^2} \sum_{i=1}^d ||g_{1:T,i}||_2 + \sum_{i=1}^d \frac{D_{\infty}^2 G_{\infty} \sqrt{1-\beta_2}}{2\alpha(1-\beta_1)(1-\lambda)^2}
$$

**Corollary 4.2.** Assume that the function f<sub>t</sub> has bounded gradients,  $\|\nabla f_t(\theta)\|_2 \leq G$ ,  $\|\nabla f_t(\theta)\|_{\infty} \leq$  $G_{\infty}$  for all  $\theta \in \mathbb{R}^d$  and distance between any  $\theta_t$  generated by Adam is bounded,  $\|\theta_n - \theta_m\|_2 \leq D$ ,  $\|\hat{\theta}_m - \theta_n\|_{\infty} \leq D_{\infty}$  for any  $m, n \in \{1, ..., T\}$ . Adam achieves the following guarantee, for all  $T\geq 1$ .  $\frac{R(T)}{T} = O(\frac{1}{\sqrt{T}})$ 

## SARAH - Summary

- Very similar to SVRG (same hyperparameter choices)
- Modifies inner loop, uses recursive gradient info rather than only outer loop gradient
	- Biased inner loop computations, but total expectation is unbiased
- Constant learning rate
- No gradient table
- Similar performance to SVRG, some advantages in strong convex cases

#### **Algorithm 1 SARAH**

**Parameters:** the learning rate  $\eta > 0$  and the inner loop size m. **Initialize:**  $\tilde{w}_0$ **Iterate:** for  $s = 1, 2, ...$  do  $w_0 = \tilde{w}_{s-1}$  $v_0 = \frac{1}{n} \sum_{i=1}^n \nabla f_i(w_0)$  $w_1 = w_0 - \eta v_0$ **Iterate:** for  $t = 1, ..., m - 1$  do Sample  $i_t$  uniformly at random from  $[n]$  $v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_{t-1}) + v_{t-1}$  $w_{t+1} = w_t - \eta v_t$ end for Set  $\tilde{w}_s = w_t$  with t chosen uniformly at random from  $\{0,1,\ldots,m\}$ end for

## SARAH Algorithm

*Italics are same steps as SVRG*

#### Initialization

- *Constant learning rate*
- *Objective function*
- *Inner loop steps*
- *Initial parameters*  $\widetilde{w}_0$

#### **Outer Loop**

- *Full gradient descent update ("snapshot point")* **Inner Loop (Variance Reduction)**
- **Recursive Stochastic Gradient (one sample) estimate step ("SARAH" update)**
- *Parameter update*

#### **Stochastic Re -initialization**

• Initialize random weight for outer loop  $\widetilde{w}_{s-1}$ 



#### **Algorithm 1 SARAH**

**Parameters:** the learning rate  $\eta > 0$  and the inner loop  $size m$ **Initialize:**  $\tilde{w}_0$ **Iterate:** for  $s = 1, 2, ...$  do  $w_0 = \tilde{w}_{s-1}$  $v_0 = \frac{1}{n} \sum_{i=1}^n \nabla f_i(w_0)$  $w_1 = w_0 - \eta v_0$ **Outer Loop Iterate:** for  $t = 1, ..., m - 1$  do Sample  $i_t$  uniformly at random from  $[n]$ **Inner loop**  $v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_{t-1}) + v_{t-1}$  $w_{t+1} = w_t - \eta v_t$ end for Set  $\tilde{w}_s = w_t$  with t chosen uniformly at random from  $\{0,1,\ldots,m\}$ end for

## SARAH Algorithm

#### **Variance Reduction**

The SARAH Algorithm first calculates a full gradient in the outer loop (like SVRG), then uses recursive stochastic gradient information  $v_t$  at each iteration of the inner loop, rather than stochastic updates relative to outer loop full gradient calculation.

The key step of the algorithm is a recursive update of the stochastic gradient estimate (SARAH update)

$$
v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_{t-1}) + v_{t-1},
$$
 (2)

followed by the iterate update:

$$
w_{t+1} = w_t - \eta v_t. \tag{3}
$$

For comparison, SVRG update can be written in a similar way as

$$
v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_0) + v_0.
$$
 (4)



## SARAH Algorithm

#### **Bias**

For SVRG,  $v_t$  is an unbiased estimator for the gradient,  $E_{it}[v_t] = \nabla P(\widetilde{w}_t)$  \* Expectation of inner loop iterate is not equal to the full gradient "snapshot", but the total expectation of the full loop is.

> $E_{it}[v_t] \neq \nabla P(\widetilde{w}_t)$  \*  $E[v_t] = \nabla P(\widetilde{w}_t)$

The key step of the algorithm is a recursive update of the stochastic gradient estimate (SARAH update)

$$
v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_{t-1}) + v_{t-1}, \tag{2}
$$

followed by the iterate update:

$$
w_{t+1} = w_t - \eta v_t. \tag{3}
$$

 $*$ 

For comparison, SVRG update can be written in a similar way as

$$
v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_0) + v_0.
$$
 (4)





## SARAH Convergence Summary

### For [CONVEX], [LSMOOTH] objective

For functions satisfying [CONVEX] and [LSMOOTH], we can guarantee convergence  $\bm{O}(\left(n+\frac{1}{\epsilon}\right))$  $\left(\frac{1}{\varepsilon}\right)log(\frac{1}{\varepsilon})$  $\frac{1}{\epsilon})$ 

### $\mathbb{E}[\|\nabla P(w_{\mathcal{T}})\|^2] \leq \epsilon.$  (7)

### SARAH SVRG

 $\sigma_m \stackrel{\text{def}}{=} \frac{1}{\mu n(m+1)} + \frac{\eta L}{2 - nL} < 1.$   $\alpha_m = \frac{1}{\mu n(1 - 2Ln)m} + \frac{2\eta L}{1 - 2nL} < 1.$ 

 $\min_{0 < n < 1/L} \sigma_m$  $\min_{0 \leq n \leq 1/4} \alpha_m,$ 





### For [CONVEX], [LSMOOTH], [SCONVEX] objective

If our objective has [SCONVEX], SARAH guarantees convergence  $\bm{O}(\bm{n} + \frac{L}{n})$  $\left(\frac{L}{\mu}\right)log(\frac{1}{\varepsilon})$  $(\frac{1}{\varepsilon})$ ). Same order as SVRG, but uniformly better due to variance bound



Figure 3: Theoretical comparisons of learning rates (left) and convergence rates (middle and right) with  $n = 1,000,000$  for SVRG and SARAH in one inner loop.



## SARAH Convergence Summary

Table 1: Comparisons between different algorithms for strongly convex functions.  $\kappa = L/\mu$  is the condition number.



Table 2: Comparisons between different algorithms for convex functions.



[5] L. M. NGUYEN, J. LIU, K. SCHEINBERG, AND M. TAKÁČ, Sarah: A novel method for machine learning problems using stochastic recursive gradient, 2017.

#### Convergence comparisons

SARAH converges at comparable rates to SVRG/SAG/SAGA for convex functions, but has significant advantages for strong convexity of the objective function.

#### Computational advantages

Recursive update does not require storage of past information, less computationally expensive that similar methods like SAG/SAGA

## SARAH – Nguyen, Liu, Scheinberg, Takac

Variance of inner loops approaches zero as  $m$  increases for SARAH, does not for SVRG



## Conclusions

- Used in practice for fast convergence
- Adaptive unlike SGD methods, locally smooth
	- Minimizes oscillations near optimal solution
- Batch descent can reduce noise

- SARAH doesn't seem to be used as widely in practice, but has some nonconvex applications in use/research
- Ongoing research on modifications to algorithm, like random reshuffling, mini-batch, etc.

#### ADAM SARAH Comparisons

ADAM – Adaptive learning rate (with bias-correction)

SARAH – SGD constant learning rate (generally a "step in the right direction" from SVRG)

## Numerical Experiment – GD, SARAH ADAM

#### **Data**

- 500 features
- 10000 samples
- 3170 weight updates per algorithm

**SARAH/SVRG** – ~3.5s **ADAM** – ~4.5s **GD** – 95s



#### Extensions/Further Research la post



For those interested…

### ADAM

- → **AdaMax:** Variant of ADAM that utilizes infinity norm for update in lieu of RMSProp
- ➔ **Ada-class algorithms**: AdaMax, Adadelta, Nadam (Nesterov momentum)

### SARAH

- ➔ **SARAH+:** Variant of ADAM that utilizes infinity norm for update in lieu of RMSProp
- → **Random-Reshuffled SARAH:** Does not need full gradient computations [1]

### References

- [1] A. BEZNOSIKOV AND M. TAKÁČ, Random-reshuffled sarah does not need full gradient computations, Optimization Letters,  $18$  (2023), p.  $727-749$ .
- [2] S. BOCK, J. GOPPOLD, AND M. WEISS, An improvement of the convergence proof of the  $adam\text{-}ontimizer$ , 04 2018.
- [3] V. K. CHAUHAN, A. SHARMA, AND K. DAHIYA, Saags: Biased stochastic variance reduction methods for large-scale learning, Applied Intelligence, 49 (2019), p. 3331-3361.
- [4] J. CHEN, R. ZHANG, AND Y. LIU, An adam-enhanced particle swarm optimizer for latent factor analysis, 2023.
- [5] A. DÉFOSSEZ, L. BOTTOU, F. BACH, AND N. USUNIER, A simple convergence proof of adam and adaqrad, 2022.
- [6] M. GÜRBÜZBALABAN, A. OZDAGLAR, AND P. A. PARRILO, Why random reshuffling beats stochastic gradient descent, Mathematical Programming, 186 (2019), p. 49–84.
- [7] D. P. KINGMA AND J. BA, Adam: A method for stochastic optimization, 2017.
- [8] L. M. NGUYEN, J. LIU, K. SCHEINBERG, AND M. TAKÁČ, Sarah: A novel method for machine learning problems using stochastic recursive gradient, 2017.
- [9] B. WANG, Y. ZHANG, H. ZHANG, Q. MENG, Z.-M. MA, T.-Y. LIU, AND W. CHEN, Provable adaptivity in adam, 2022.

### Additional Resources

- Momentum:<https://distill.pub/2017/momentum/?ref=blog.paperspace.com>
- [https://medium.com/analytics-vidhya/a-complete-guide-to-adam-and-rmsprop-optimizer-](https://medium.com/analytics-vidhya/a-complete-guide-to-adam-and-rmsprop-optimizer-75f4502d83be)[75f4502d83be](https://medium.com/analytics-vidhya/a-complete-guide-to-adam-and-rmsprop-optimizer-75f4502d83be)
- <https://optimization.cbe.cornell.edu/index.php?title=Adam>
- [https://medium.com/geekculture/a-2021-guide-to-improving-cnns-optimizers-adam-vs-sgd-](https://medium.com/geekculture/a-2021-guide-to-improving-cnns-optimizers-adam-vs-sgd-495848ac6008)[495848ac6008](https://medium.com/geekculture/a-2021-guide-to-improving-cnns-optimizers-adam-vs-sgd-495848ac6008)

### SARAH SVRG delta from numerical experiment slide



## SARAH+ Algorithm

#### Initialization

- Constant learning rate\*\*
- **Objective function**
- Initial parameters  $\widetilde{w}_0$

#### **Outer Loop**

- Full gradient descent update ("snapshot point") **Inner Loop (Variance Reduction)**
- **Recursive Stochastic Gradient (single sample) estimate step ("SARAH" update)**
- Parameter update

#### **Stochastic Re -initialization**

- Initialize random weight for outer loop  $\widetilde{w}_{s-1}$ Break inner loop when  $||v_t||$  is small enough
- Specify hyperparameter  $\gamma \in (0,1]$

