# Variance Reduction Techniques: SARAH and ADAM

Alex Salce
Department of Mathematics,
The University of Arizona,
asalce@arizona.edu

SIE 596, Spring 2024

**Abstract**

## 1 Introduction

Technological advancements in recent history have delivered capabilities to both capture and process huge amounts of data, and accessibility to such data is not prohibitive even to the general public. Machine Learning (ML) frameworks are utilizing increasingly large datasets for training, serving as motivation to develop computationally efficient algorithms that optimize model parameters. Many of the parameter optimization problems in ML frameworks can be approached utilizing a continuously differentiable convex objective function, for which a generalized first-order gradient descent algorithm (GD) can be sensibly applied. However, gradient computations can become prohibitive in terms of computational performance when training using large datasets, as a gradient computation of the full dataset at each step is impractical.

One effective approach to addressing this prohibitive computation is to compute subsets of the full gradient at each step rather than the full gradient. First-order GD algorithms utilizing stochastic gradients (individual gradient selected uniformly at random) or minibatch gradients (set of more than one gradient each selected uniformly at random), have consequently become core staples in ML frameworks due to their advantageous computational efficiency for applications to datasets of both large sample size and dimensionality.

Generally, these approaches in the context of convex optimization are optimizing model parameters $x \in \mathbb{R}^d$ by solving the following problem.

$$min_{x\in\mathbb{R}^d}\left\{P(x) \;=\; \frac{1}{b}\sum_{i=1}^{b} f_i(x)\right\},\; I_k \subset 1,...,n,\; |I_k| = b \tag{1}$$

1: $b = 1$ stochastic, $n > b > 1$ minibatch

A drawback of a stochastic or minibatch approach is the inherent variance in gradient updates due to the decreased fidelity and inherent randomness of the gradient computations and subsequent

parameter updates over each timestep. For algorithms utilizing these approaches, controlling variance can be critical to guarantee convergence, which has motivated variance reduction techniques in the development new algorithms.

The subjects of this paper, ADAM and SARAH, are stochastic optimizers that utilize stochastic/minibatch gradients with variance reduction techniques. Although the two algorithms are fundamentally different in their approaches, they both utilize recursive accumulated gradient information for variance reduction. ADAM has an adaptive learning rate and is the overall more popular of the two in ML frameworks due to its optimal convergence properties for stochastic methods. SARAH is a direct modulation of the well known stochastic method SVRG, which will allow us to draw some direct comparisons to something well-established.

### 1.1 Applications

The ADAM optimizer is one of the most popular optimizers in a variety of ML frameworks including deep learning, neural networks, natural language processing, and generative adversarial networks, to name a few. These applications benefit from ADAM's strengths against other optimizers; it is fast, requires little hyperparameter tuning, performs well with sparse gradients, and can be applied to stochastic objective functions. Further, it has proven convergence for convex objective functions, as well as demonstrated convergence for nonconvex [heconvergence ]**CITE both of these convex/nonconvex**. The success of ADAM in practice has motivated variants like AdaMax, which has also become popular in sparse dataset applications. **CITE?**. ADAM, AdaMax, and other ADAM methods are built-in to the TensorFlow Keras package [1]

SARAH is a direct modification of SVRG, however does not seem to be used as widely in practice as SVRG. While speculation as to why is not worthwhile, it is noteworthy that SARAH's variance reduction technique utilizes a biased methodology, where SVRG is unbiased. Still, there is a fair amount of research available for futher modifications of SARAH, notably for nonconvex objectives **CITE**. For applications, SARAH can be a direct substitute for SVRG with only some updated parameter tuning considerations, so it can be utilized for a very large variety of applications as a SVRG replacement.

### 1.2 Literature review

ADAM, "ADAptive Moment estimation", was initially proposed in the paper *Adam: A method for stochastic optimization* by D.P. Kingma and J. Ba originally submitted in 2014, and most recently updated in 2017 [5]. This paper was scrutinized for its proofs of convergence for ADAM and whether ADAM was really advantageous over stochastic gradient descent (SGD). In 2022, *Provable Adaptivity In ADAM* by B. Wang, Y. Zhang, H. Zhang, Q. Meng, Z.-M. Ma, T.-Y. Liu, and W. Chen [8] proposed a "relaxed" smoothness condition that addressed some shortcomings of the original theoreticall anlaysis. Another paper, *An improvement of the convergence proof of the ADAM-Optimizer* by S. Bock, J. Goppold, and M. Weiß in 2018 [3] corrected some errors in the original proof, adding to the scrutiny of the original paper's proof. Still, ADAM remains very popular despite the original paper's theoretical shortcomings.

SARAH, "StochAstic Recursive grAdient algoritHm", was initially proposed in the paper *Sarah: A novel method for machine learning problems using stochastic recursive gradient* by L.M. Nguyen, J.Liu, K. Scheinberg, and M. Takáč published in 2017 [6]. A follow on paper including one of the original authors, *Random-reshuffled sarah does not need full gradient computations* by A.

Beznosikov and M. Takáč in 2022 [2] demonstrates that, utilizing a random reshuffling technique, SARAH can be modified to eliminate full gradient computations entirely. *SARAH-M*, published this year by Z. Yang [9], explores the incorporation of momentum with the SARAH algorithm, similar to ADAM. Examples like this, among others, indicate an interest in the algorithm despite not being a clearly preferred optimizer over SVRG or similar methods.

The subsequent coverage of each algorithm will draw primarily from their respective original publications. While we will not go into detail about variants of either algorithm, these are references suggested for further research.

# 2 Methodology/Algorithm description

## 2.1 ADAM (ADAptive Moment estimation) [5], see 1

The ADAM algorithm combines the concepts of momentum and RMSProp ("Root Mean Squared Propogation") using minibatch or stochastic gradient information to iteratively udpate parameters. The key feature of stochastic optimization method is an *adaptive* learning rate that is modulated by recursive accumulated gradient information.

In basic terms, the steps that are similar to momentum utilize an exponential weighted average of previous gradient information to calculate the gradient term at each descent step from previous gradient averages, having the effect of reducing variance in steps and moving more accurately in the direction of the optimum. The steps similar to RMSProp have the effect of adaptively scaling the learning rate based on an exponential weighted average of the magnitude of recent gradients. Both of these terms are biased toward the initialized weights, and ADAM employs bias-correction udpates to both the momentum and RMSProp terms.

### 2.1.1 Bias

The bias-correction differentiates ADAM from RMSProp and can be attributed to it's advantageous performance with sparse data. Kingma and Ba derive the bias term using for the second moment estimate $v_t$ by selecting $v_0 = \mathbf{0}$ and taking the expectation of the term at time $t$. With intermediate calculations omitted, they show the following.

$$\mathbb{E}[v_t] = \mathbb{E}[g_t^2] \cdot (1 - \beta_2^t) + \zeta$$

Where $\zeta$ is assumed to be small since $\beta_2$ should be selected to assign very small weights to gradients far enough in the past. The proof given in the paper also applies to the first moment estimate. Hence, the first and second moment bias correction terms are incorporated by dividing the respective estimates by this term in Algorithm 1, and giving $\mathbb{E}[\hat{m}_t] = \mathbb{E}[g_t]$ and $\mathbb{E}[\hat{v}_t] = \mathbb{E}[g_t^2]$. [5]

### 2.1.2 Convergence

The convergence proof given by Kingma and Ba imposes the following requirements for $f$. First, $f$ is convex, defined by the following.

**Definition 1.** *A function $f : \mathbb{R}^d \to \mathbb{R}$ is convex if for all $x, y \in \mathbb{R}^d$, for all $\lambda \in (0, 1)$*

$$\lambda f(x) + (1 - \lambda) f(y) \geq f(\lambda x + (1 - \lambda) y)$$

Additionally, we note that the following property holds for convex functions.

**Lemma 1.** *If a function $f : \mathbb{R}^d \to \mathbb{R}$ is convex, then for all $x, y \in \mathbb{R}^d$*

$$f(y) \geq f(x) + \nabla f(x)^T (y - x)$$

Omitting details of the proof, Kingma and Ba use Lemma 1 to establish an upper bound on the regret function $R(T) = \sum_{t=1}^{T} f_t(x_t) - f_t(x^*)$, where $x^*$ is the optimal parameters for minimizing $f$.

**Theorem 1.** *Assume that the function $f_t$ has bounded gradients, $||\nabla f_t(x)||_2 \leq G$, $||\nabla f_t(x)||_\infty \leq G_\infty$ for all $x \in \mathbb{R}^d$ and distance between any $x_t$ generated by ADAM is bounded, $||x_n - x_m||_2 \leq D$, $||x_n - x_m||_\infty \leq D_\infty$ 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 $T \geq 1$.*

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

In simple terms, the proximity of $f_t(x_t$ to the optimum is bounded by tunable parameters and constant bounds based on the data. Under the assumptions of $f_t$ from Theorem 1, the following convergence follows.

$$\frac{R(T)}{T} = \mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$$

$\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ is the best theoretical convergence of regular SGD, however there has been some criticism of the theory regarding the advantages of ADAM over SGD despite observed advantages in emperical performance. Further, some shortcomings have been pointed out in Kingma and Ba's proof, and even some examples of ADAM diverging under its stated assumptions have been identified [7]. In 2022, *Provable Adaptivity in ADAM* [8] proposed the $(L_0, L_1)$ smoothness assumption, which slightly relaxes the $L$-smooth condition for bounding gradients, and in conjunction with a growth condition bounding sum of square gradients, can prove the $\mathcal{O}\left(\frac{1}{\sqrt{T}}\right)$ convergence of ADAM.

## 2.2 SARAH (StochAstic Recursive grAdient algoritHm) [6]

The SARAH algorithm is a stochastic optimizer that converges for convex L-smooth objectives $f_i$ with some theoretical advantages over similar methods like SAG, SAGA, and SVRG. It is most similar to SVRG, using an identical outer loop step and a modified inner loop calculation of the gradient estimate, using recursive gradient information rather than using only the outer loop gradient at each inner loop iterate.

### 2.2.1 Bias

Reference Algorithm 2. SVRG and SARAH employ the same outer/inner loop structure, with the inner loop reducing variance in the steps. We first observe the inner loop update for SVRG.

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

**Algorithm 1** The ADAM algorithm computes a batch stochastic gradient. UPDATE

**Require:** parameters $w$, stochastic objective function $f_i(w)$
**Require:** learning rate $\eta$, exponential decay rates $\beta_1, \beta_2 \in [0, 1)$, tolerance $\epsilon$
**Initialize:** initial parameter vector $w_0$, initial $1^{st}$ moment vector $m_0 \leftarrow 0$, initial $2^{nd}$ moment vector $v_0 \leftarrow 0$, initial timestep $t \leftarrow 0$
**while** $w_t$ is not converged **do**
$t \leftarrow t + 1$
$g_t \leftarrow \nabla_w f_t(w_{t-1})$ (*batch gradient at iteration t*)
$m_t \leftarrow \beta_1 \cdot m_{t-1} + (1 - \beta_1) \cdot g_t$ (*[Monentum] udpate baised first moment estimate*)
$v_t \leftarrow \beta_2 \cdot v_{t-1} + (1 - \beta_2) \cdot g_t^2$ (*[RMSProp] udpate baised second raw moment estimate*)
$\hat{m}_t \leftarrow m_t / (1 - \beta_1^t)$ (*[Monentum] bias-corrected first moment estimate*)
$\hat{v}_t \leftarrow v_t / (1 - \beta_2^t)$ (*[RMSProp] bias-corrected second raw moment estimate*)
$w_t \leftarrow w_{t-1} - \eta \cdot \hat{m}_t / (\sqrt{\hat{v}_t} + \epsilon)$ (*[Momentum + RMSProp] update parameters*)
**end while**
**return** $w_t$

**Algorithm 2** The SARAH algorithm is identical to SVRG except for the *SARAH update*, which modifies the stochastic gradient estimate to use recursive gradient estimate information rather than the initialized gradient to update the gradient estimate in the inner loop.

**Require:** objective function $f(w)$
**Require:** learning rate $\eta > 0$, inner loop size $m$, outer loop size $s$
**Initialize:** initial parameter vector $\tilde{w}_0$
**Iterate:**
**for** $s = 1, 2, ...$ **do**
$w_0 = \tilde{w}_{s-1}$
$v_0 = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w_0)$ (*outer loop full gradient computation*)
$w_1 = w_0 - \eta v_0$ (*outer loop parameter update*)
**for** $t = 1, ..., m - 1$ **do**
Sample $i_t$ uniformly at random from $[n]$
$v_t = \nabla f_{i_t}(w_t) - \nabla f_{i_t}(w_{t-1}) + v_{t-1}$ (*SARAH update*)
$w_{t+1} = w_t - \eta v_t$ (*inner loop parameter update*)
**end for**
Set $\tilde{w}_s = w_t$ with $t$ chosen uniformly at random from $\{0, 1, ..., m\}$
**end for**

Where $w_0$ is computed in the outer loop step feeding into the inner loop. The SARAH update replaces the outer loop gradient with a recursive gradient update framework.

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

As it holds in statistical theory, there is a bias-variance tradeoff with the SARAH update. The use of recursive gradient information in SARAH actually reduces the variance of the inner loop steps to zero as inner loops iterates increase, whereas this is not the case for SVRG. However, while the inner loops of SVRG are unbaised, individual inner loop iterates for SARAH are biased. As shown in [6] the expectation of the innter loop after $t$ iterations is as follows,

$$\mathbb{E}[v_t|F_t] = \nabla P(w_t) - \nabla P(w_{t-1}) + v_{t-1} \neq \nabla P(w_t)$$

where $F_t = \sigma(w_0, i_1, i_2, ..., it-1$ is the sigma algebra generated by the sequence of updates from $w_0$ (we will use $P$ as in Equation 1). However, the total expectation holds $\mathbb{E}[v_t] = [\mathbb{E}\nabla P(w_t)]$, which distinguishes SARAH from SAG/SAGA.

### 2.2.2 Convergence

In general, we aim to bound the expected norm of the gradient for stochastic algorithms as follows.

$$\mathbb{E}[||\nabla P(w_\tau)||^2] \leq \epsilon \tag{2}$$

The general convergence result imposes the same convexity assumption for $f_i$s as Definition 1. Additionally, we require $f_i$s to be $L-$smooth (Lipschitz continuous gradient) as follows.

**Definition 2.** *Each $f_i : \mathbb{R}^d \to \mathbb{R}$, $i \in [n]$, is L-smooth if and only if there exists a constant $L > 0$ such that*

$$||\nabla f_i(w) - \nabla f_i(w')|| \leq L||w - w'||, \forall w, w' \in \mathbb{R}^d$$

Under these assumptions, SARAH shows a sublinear convergence rate.

**Corollary 1.** *Suppose that each $f_i$ conforms with definitions 1 and 2. For Algorithm 2 within a single outer iteration with the learning rate $\eta = \sqrt{\frac{2}{L(m+1)}}$ where $m \geq 2L - 1$ is the total number of iterations, then $||\nabla P(w_t)||^2$ converges sublinearly in expectation with a rate of $\sqrt{\frac{2L}{m+1}}$, and therefore, the total complexity to achieve an $\epsilon$-accurate solution defined by Equation 2 is $\mathcal{O}(n + 1/\epsilon^2)$.*

Reference [6], for the general convex case, it can be shown that with appropriate choice of learning and rate and inner loops based on the data, the total complexity to achieve an $\epsilon$-accuracy solution for Equation 2 is $\mathcal{O}((n + (1/\epsilon)) \log 1/\epsilon)$.

A further assumption of strong convexity imposed on $f_i$s can improve convergence of SARAH.

**Definition 3.** *The function $P : \mathbb{R}^d \to \mathbb{R}$, is $\mu$-strongly convex if and only if there exists a constant $\mu > 0$ such that $\forall w, w' \in \mathbb{R}^d$,*

$$P(w) \geq P(w') + \nabla P(w')^T(w - w') + \frac{\mu}{2}||w - w'||^2$$

Assuming $f_i$s are strongly convex in addition to regular convexity assumption and $L$-smooth, we have the following.

**Theorem 2.** *For $f_i$s convex, $L$-smooth, and $\mu$-strongly convex, choosing $\eta$ and $\mu$ such that*

$$\sigma_m \overset{def}{=} \frac{1}{\mu\eta(m+1)} + \frac{\eta L}{2-\eta L} < 1$$

*we have*

$$\mathbb{E}[||\nabla P(\tilde{w}_s||^2||] \leq (\sigma_m)^s ||\nabla P(\tilde{w}_0)||^2$$

This result implies that the variance bound $\sigma_m^s$ on the expectation of the norm squared gradient after $s$ outer loops is smaller than the equivalent variance bound after $s$ loops $\alpha_m$ for SVRG.

$$\sigma_m \overset{def}{=} \frac{1}{\mu\eta(m+1)} + \frac{\eta L}{2-\eta L} < \frac{1}{\mu\eta(1-2L\eta)m} + \frac{1}{\frac{1}{2\eta L}-1} = \alpha_m$$

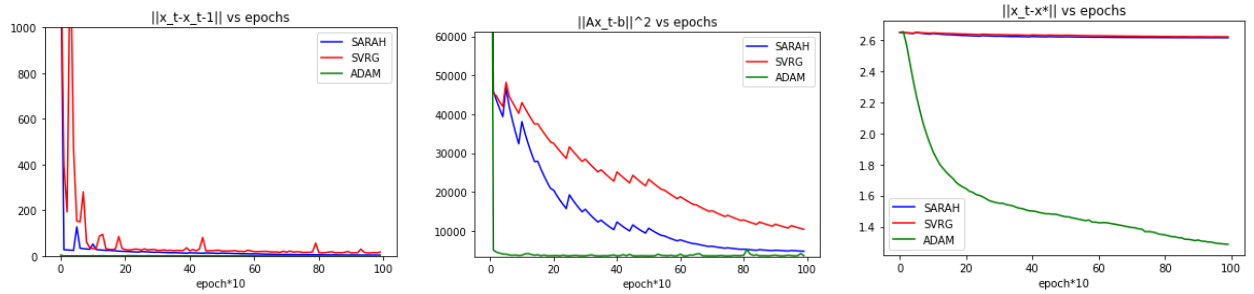
Both methods converge with rate $\mathcal{O}((n + L/\mu)\log(1/\epsilon))$, however SARAH's best theoretical convergence rate can use a higher learning rate than SVRG.

## 3 Numerical Experiments

The purpose of the numerical experiment will be to evaluate general performance of ADAM and SARAH on real data and to illustrate a bias-variance tradeoff between SVRG and SARAH. We use the "Wine Quality" [4] dataset from the UC Irvine Machine Learning Repository. The data are measurements of wine characteristics (features) used to predict wine quality scores. There are $n = 6497$ instances and $m = 11$ features. The experiements will use a simple least squares linear regression objective, assuming a system with data $A$ and response $b$ is of the form $Ax = b$.

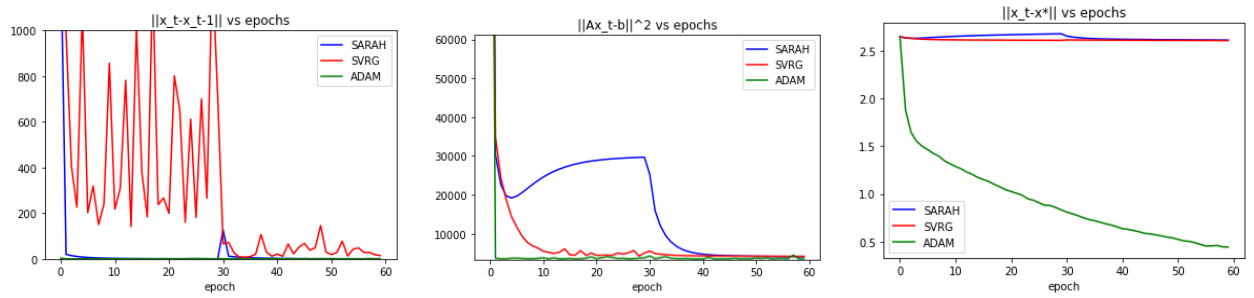
$$\min_x ||Ax - b||^2$$

The least squares objective was chosen because it is strongly convex to attempt to differentiate SARAH and SVRG. $x^*$ was computed separately using `scipy.optimize.lsq_linear` with tolerance set to $1e-10$.




| ADAM | | SARAH | | SVRG | |
|---|---|---|---|---|---|
| Parameters | time | Parameters | time | Parameters | time |
| $\beta_1 = 0.9, \beta_2 = 0.999, \alpha = 0.001$, $batch = 10$ | 6.37s | $\eta = \frac{1}{2.1 \cdot L}, m = 3248, s = 20$ | 6.51s | $\eta = \frac{1}{5 \cdot L}, m = 3248, s = 20$ | 6.49s |

Figure 1: Exp. A — 64970 total iterations




| ADAM | | SARAH | | SVRG | |
|---|---|---|---|---|---|
| Parameters | time | Parameters | time | Parameters | time |
| $\beta_1 = 0.9, \beta_2 = 0.999, \alpha = 0.001$, $batch = 10$ | 38.6s | $\eta = \frac{1}{2.1 \cdot L}, m = 194910, s = 2$ | 38.8s | $\eta = \frac{1}{5 \cdot L}, m = 194910, s = 2$ | 38.5s |

Figure 2: Exp. B — 389820 total iterations

The two examples chosen illustrate some high level takeaways. In terms of computational performance, both ADAM and SARAH are virtually identical to SVRG, though ADAM can become slightly slower for increased batch sizes. See Figures 1 and 2 for settings and computation time. Convergence for SARAH and SVRG are limited in flexibility for learning rate for this data with $L$ large, and we can see benefit of the adaptive learning rate of ADAM for both Exp A and B. SARAH and SVRG both descend (SARAH able to use larger learning rate than SVRG), but are moving extremely slowly toward $x^*$, whereas ADAM is moving toward it much faster and it continues to descend as iterations increase ($||x_t - x^*||$ vs. epochs).

Comparing SARAH and SVRG, we run the inner loop for half an epoch in Exp. A and for 30 epochs in Exp. B. The spirit of this approach, specifically Exp. B, was to demonstrate where SARAH has advantages SVRG in variance reduction, attempting to emulate a section in [6] which details a "Single Inner Loop" case. In both Exp. A and B, and much more clearly in Exp. B, $||x_t - x_{t-1}||$ is significantly smoother for SARAH than SVRG, however we observe that the number of effective passes over the data in the inner loop can matter. In both the $||Ax_t - b||$ and $||x_t - x^*||$ plots, SARAH will stray away from the optimal solution due to bias after around 4 epochs. It is ultimately corrected by breaking the inner loop, but we can see how the biased steps of the inner loop can break SARAH whereas SVRG continues to descend. As is the reality of statistics, we are trading variance for bias.

## 4 Conclusion and Future Direction

Summarize the results and state the gap(s) and possible future directions.

## A Algorithms

## References

[1] *TensorFlow Keras Optimizers Method tf.keras.optimizers.* `https://www.tensorflow.org/api_docs/python/tf/keras/optimizers/Adam`. Accessed: 2024-04-20.

[2] A. Beznosikov and M. Takáč, *Random-reshuffled sarah does not need full gradient computations*, Optimization Letters, 18 (2023), p. 727–749.

[3] S. Bock, J. Goppold, and M. Weiss, *An improvement of the convergence proof of the adam-optimizer*, 04 2018.

[4] P. Cortez, A. Cerdeira, F. Almeida, T. Matos, and J. Reis, *Wine Quality.* UCI Machine Learning Repository, 2009. DOI: https://doi.org/10.24432/C56S3T.

[5] D. P. Kingma and J. Ba, *Adam: A method for stochastic optimization*, 2017.

[6] L. M. Nguyen, J. Liu, K. Scheinberg, and M. Takáč, *Sarah: A novel method for machine learning problems using stochastic recursive gradient*, 2017.

[7] S. J. Reddi, S. Kale, and S. Kumar, *On the convergence of adam and beyond*, 2019.

[8] B. Wang, Y. Zhang, H. Zhang, Q. Meng, Z.-M. Ma, T.-Y. Liu, and W. Chen, *Provable adaptivity in adam*, 2022.

[9] Z. Yang, *Sarah-m: A fast stochastic recursive gradient descent algorithm via momentum*, Expert Systems with Applications, 238 (2024), p. 122295.