Optimal mini-batch and step sizes for SAGA

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Abstract

Recently it has been shown that the step sizes of a family of variance reduced gradient methods called the JacSketch methods depend on the expected smoothness constant. In particular, if this expected smoothness constant could be calculated a priori, then one could safely set much larger step sizes which would result in a much faster convergence rate. We fill in this gap, and provide simple closed form expressions for the expected smoothness constant and careful numerical experiments verifying these bounds. Using these bounds, and since the SAGA algorithm is part of this JacSketch family, we suggest a new standard practice for setting the step sizes and mini-batch size for SAGA that are competitive with a numerical grid search. Furthermore, we can now show that the total complexity of the SAGA algorithm decreases linearly in the mini-batch size up to a pre-defined value: the optimal mini-batch size. This is a rare result in the stochastic variance reduced literature, only previously shown for the Katyusha algorithm. Finally we conjecture that this is the case for many other stochastic variance reduced methods and that our bounds and analysis of the expected smoothness constant is key to extending these results.

1. Introduction

Consider the empirical risk minimization (ERM) problem:

\[ w^* \in \arg \min_{w \in \mathbb{R}^d} \left( f(w) := \frac{1}{n} \sum_{i=1}^{n} f_i(w) \right), \]

where each \( f_i \) is \( L_i \)-smooth and \( f \) is \( \mu \)-strongly convex. Each \( f_i \) represents a regularized loss over a sampled data point. Solving the ERM problem is often time consuming for large number of samples \( n \), so much so that algorithms scanning through all the data points at each iteration are not competitive. Gradient descent (GD) falls into this category, and in practice its stochastic version is preferred.

Stochastic gradient descent (SGD), on the other hand, allows to solve the ERM incrementally by computing at each iteration an unbiased estimate of the full gradient, \( \nabla f_i(w^*) \) for \( i \) randomly sampled in \( [n] := \{1, 2, \ldots, n\} \) (Robbins & Monro, 1951). On the downside, for SGD to converge one needs to tune a sequence of asymptotically vanishing step sizes, a cumbersome and time-consuming task for the user. Recent works have taken advantage of the sum structure in Eq. (1) to design stochastic variance reduced gradient algorithms (Johnson & Zhang, 2013; Shalev-Shwartz & Zhang, 2013; Defazio et al., 2014; Schmidt et al., 2017). In the strongly convex setting, these methods lead to fast linear convergence instead of the slow \( O(1/t) \) rate of SGD. Moreover, they only require a constant step size, informed by theory, instead of sequence of decreasing step sizes.

In practice, most variance reduced methods rely on a mini-batching strategy for better performance. Yet most convergence analysis (with the Katyusha algorithm of Allen-Zhu (2017) being an exception) indicates that a mini-batch size of \( b = 1 \) gives the best overall complexity, disagreeing with practical findings, where larger mini-batch often gives better results. Here, we show both theoretically and numerically that \( b = 1 \) is not the optimal mini-batch size for the SAGA algorithm (Defazio et al., 2014).

Our analysis leverage recent results in (Gower et al., 2018), where the authors prove that the iteration complexity and the step size of SAGA, and a larger family of methods called the JacSketch methods, depend on an expected smoothness constant. This constant governs the trade-off between the increased cost of an iteration as the mini-batch size is increased, and the decreased total complexity. Thus if this expected smoothness constant could be calculated a priori, then we could set the optimal mini-batch size and step size. We provide simple formulas for computing the expected smoothness constant when sampling mini-batches without replacement, and use them to calculate optimal mini-batches and significantly larger step sizes for SAGA.

In particular, we provide two bounds on the expected smoothness constant, each resulting in a particular step sizes.
step size formula. We first derive the simple bound and then develop a matrix concentration inequality to obtain the refined Bernstein bound. We also provide substantial theoretical motivation and numerical evidence for practical motivation of the expected smoothness constant. For illustration, we plot in Figure 1 the evolution of each resulting step size as the mini-batch size grows on a classification problem (Section 5 has more details on our experimental settings).

Furthermore, our bounds provide new insight into the total complexity, denoted $K_{\text{total}}$ hereafter, of SAGA. For example, when using our simple bound we show for regularized generalized linear models (GLM), with $\lambda > 0$ as in Eq. (10), that $K_{\text{total}}$ is piecewise linear in the mini-batch size $b$:

$$K_{\text{total}}(b) = \max \left\{ n \cdot b \left( 1 - \frac{4b}{\mu} + \frac{n - b}{n - 1} \right), n + \frac{n - b}{n - 1} \left( 4b \lambda \right) \right\} \log \left( \frac{1}{\epsilon} \right),$$

with $L_{\max} := \max_{i \in [n]} L_i$, $\bar{L} := \frac{1}{n} \sum_{i=1}^{n} L_i$ and $\epsilon > 0$ is the desired precision. This complexity bound, and others presented in Section 3.3 show that SAGA enjoys a linear speedup as we increase the mini-batch size until an optimal one (as illustrated in Figure 2). After this point, the total complexity increases. We use this observation to develop optimal and practical mini-batch sizes and step sizes.

The rest of the paper is structured as follows. In Section 2 we first introduce variance reduction techniques after presenting our main assumption, the expected smoothness assumption. We highlight how this assumption is necessary to capture the improvement in iteration complexity, and conclude the section by showing that to calculate the expected smoothness constant we need evaluate an intractable expectation. Which brings us to Section 3 where we directly address this issue and provide several tractable upper-bounds of the expected smoothness constant. We then calculate optimal mini-batch sizes and step sizes by using our new bounds. Finally, we give numerical experiments in Section 5 that verify our theory on artificial and real datasets. We also show how these new settings for the mini-batch size and step size lead to practical performance gains.

2. Background

2.1. Controlled stochastic reformulation and JacSketch

We can introduce variance reduced versions of SGD in a principled manner by using a sampling vector.

Definition 1. We say that a random vector $v \in \mathbb{R}^n$ with distribution $D$ is a sampling vector if

$$\mathbb{E}_D[v_i] = 1, \quad \text{for all } i \in [n].$$

With a sampling vector we can re-write (1) through the following stochastic reformulation

$$w^* = \arg \min_{w \in \mathbb{R}^d} \mathbb{E}_D \left[ f_w(w) := \frac{1}{n} \sum_{i=1}^{n} f_i(w) \cdot v_i \right], \quad (2)$$

where $f_i(w)$ is called a subsampled function. The stochastic Problem (2) and our original Problem (1) are equivalent:

$$\mathbb{E}_D [f_w(w)] = \frac{1}{n} \sum_{i=1}^{n} f_i(w) \cdot \mathbb{E}_D [v_i] \overset{\text{Definition}}{=} \frac{1}{n} \sum_{i=1}^{n} f_i(w).$$

Consequently the gradient $\nabla f_w(w)$ is an unbiased estimate of $\nabla f(w)$ and we could use SGD method to solve (2). To tackle the variance of these stochastic gradients we can further modify (2) by introducing control variates which leads to the following controlled stochastic reformulation:

$$w^* \in \arg \min_{w \in \mathbb{R}^d} \mathbb{E}_D \left[ f_w(w) - z_w(w) + \mathbb{E}_D [z_w(w)] \right], \quad (3)$$

Figure 1: Step size as a function of the mini-batch size for a regularized ($\lambda = 10^{-3}$) logistic regression problem applied to the feature-scaled covtype.binary dataset from LIBSVM.

Figure 2: Optimal mini-batch size $b_{\text{simple}}^*$ for the simple bound, where $K_{\text{total}}(b) = \max \{ g_{\text{simple}}(b), h(b) \}$. 

Total complexity

$$\frac{4(n+4)L_{\max}+\lambda}{\mu} n + \frac{4(L_{\max}+\lambda)}{\mu} b_{\text{simple}}^*$$

$$b_{\text{simple}}^*$$
where $z_v(w) \in \mathbb{R}$ are the control variates. Clearly (3) is also equivalent to (1) since $-z_v(w) + \mathbb{E}_D[z_v(w)]$ has zero expectation. Thus, we can solve (3) using an SGD algorithm where the stochastic gradients are given by

$$
g_v(w) := \nabla f_v(w) - \nabla z_v(w) + \mathbb{E}_D[\nabla z_v(w)] .$$  

That is, starting from a vector $w^0$, given a positive step size $\gamma$, we can iterate the steps

$$w_{k+1} = w_k - \gamma g_v(w_k),$$  

where $v^k \sim D$ are i.i.d. samples at each iteration.

The JacSketch algorithm introduced by Gower et al. (2018) fits this format (5) and uses a linear control $z_v(w) = J^T w$, where $J$ is a $d \times n$ matrix of parameters. This matrix is updated at each iteration so as to increase the correlation between $\nabla z_v(w)$ and $\nabla f_v(w)$ and decrease the variance of the resulting stochastic gradients. Carefully updating the covariates through $J$ results in a method that has stochastic gradients with decreasing variance, i.e., $\lim_{w^k \rightarrow w^*} \mathbb{E}[\|g_v(w^k) - \nabla f(w^k)\|^2] = 0$, which is why JacSketch is a stochastic variance reduced algorithm. This is also why the user can set a single constant step size $\gamma$ instead of tuning a sequence of decreasing ones. The SAGA algorithm, and all of its mini-batching variants, are instances of the JacSketch method.

### 2.2. The expected smoothness constant

In order to analyze stochastic variance reduced methods, some form of smoothness assumption needs to be made. The most common assumption is

$$\|\nabla f_i(w) - \nabla f_i(y)\| \leq L_{\max} \|w - y\|,$$

for each $i \in [n]$. That is each $f_i$ is uniformly smooth with smoothness constant $L_{\max}$, as is assumed in (Defazio et al., 2014; Hofmann et al., 2015; Raj & Stich, 2018) for variants of SAGA$^1$. In the analyses of these papers it was shown that the iteration complexity of SAGA is proportional to $L_{\max}$, and the step size is inversely proportional to $L_{\max}$.

But as was shown in (Gower et al., 2018), we can set a much larger step size by making use of the smoothness of the subsampled functions $f_v$. For this Gower et al. (2018) introduced the notion of expected smoothness, which we extend here to all sampling vectors and control variates.

**Definition 2** (Expected smoothness constant). Consider a sampling vector $v$ with distribution $D$. We say that the expected smoothness assumption holds with constant $L$ if for every $w \in \mathbb{R}^d$ we have that

$$\mathbb{E}_D[\|g_v(w) - g_v(w^*)\|^2] \leq 2L(f(w) - f(w^*)) .$$

**Remark 1.** Note that we refer to any positive constant $L$ that satisfies (7) as an expected smoothness constant. Indeed $L \rightarrow \infty$ is a valid constant in the extended reals, but as we will see, the smaller $L$, the better for our complexity results.

Gower et al. (2018) show that the expected smoothness constant plays the same role that $L_{\text{max}}$ does in the previously existing analysis of SAGA, namely that the step size is inversely proportional to $L$ and the iteration complexity is proportional to $L$ (see details in Theorem 1). Furthermore, by assuming that $f$ is $L$-smooth, the expected smoothness constant is bounded

$$L \leq L_{\text{max}} \leq L_{\text{max}},$$

as was proven in Theorem 4.17 in (Gower et al., 2018). Also, the bounds $L_{\text{max}}$ and $L$ are attained when using a uniform single element sampling and a full batch, respectively. And as we will show, the constants $L_{\text{max}}$ and $L$ can be orders of magnitude apart on large dimensional problems. Thus we could set much larger step sizes for larger mini-batch sizes if we could calculate $L$. Though calculating $L$ is not easy, as we see in the next lemma.

**Lemma 1.** Let $v$ be an unbiased sampling vector. Suppose that $f_v(w) = \frac{1}{n} \sum_{i=1}^{n} f_i(v_i) \in L_{\text{v-smooth}}$ and each $f_i$ is convex for $i = 1, \ldots, n$. It follows that the expected smoothness constant holds with $L = \mathbb{E}[L_{v}, v_i]$.

**Proof.** The proof is given in Appendix A.1. \qed

Unfortunately, if the sampling has a very large combinatorial number of possible realizations — for instance sampling mini-batches without replacement — then this expectation becomes intractable to calculate. This observation motivates the development of functional upper-bounds of the expected smoothness constant that can be efficiently evaluated.

### 2.3. Mini-batch without replacement: $b$-nice sampling

Now we will choose a distribution of the sampling vector $v$ based on a mini-batch sampling without replacement. We denote a mini-batch as $B \subseteq [n]$ and its size as $b = |B|$.

**Definition 3** ($b$-nice sampling). $S$ is a $b$-nice sampling if $S$ is a set valued map with a probability distribution given by

$$\mathbb{P}[S = B] = \frac{1}{\binom{n}{b}} , \quad \forall B \subseteq [n] \text{ s.t. } |B| = b .$$

We can construct a sampling vector based on a $b$-nice sampling by setting $v = \frac{n}{b} \sum_{i \in S} e_i$, where $e_1, \ldots, e_n$ is the canonical basis of $\mathbb{R}^n$. Indeed, $v$ is a sampling vector according to Definition 1 since for every $i \in [n]$ we have

$$v_i = \frac{n}{b} \sum_{j \in S} e_j |_i = \frac{n}{b} \mathbb{1}_S(i) .$$

$^1$The same assumption is made in proofs of SVRG (Johnson & Zhang, 2013), S2GD (Konečný & Richtárik, 2017) and the SARAH algorithm (Nguyen et al., 2017).
Algorithm 1 JacSketch version of \( b \)-nice SAGA

**Input**: mini-batch size \( b \), step size \( \gamma > 0 \)

**Initialize**: \( w^0 \in \mathbb{R}^d, J^0 \in \mathbb{R}^{d \times n} \)

for \( k = 0, 1, 2, \ldots \) do

- Sample a fresh batch \( B \subseteq [n] \) s.t. \(|B| = b\)
- \( g^k = \frac{1}{n} J^k e + \frac{1}{b} \sum_{i \in B} (\nabla f_i(w^k) - J^k_i) \)
  
  // update the gradient estimate
  
  \( J^k_{i+1} = \begin{cases} 
  J^k_i, & \text{if } i \notin B \\
  \nabla f_i(w^k), & \text{if } i \in B.
  \end{cases} \)

- \( w^{k+1} = w^k - \gamma g^k \) // take a step

return \( w^k \)

where \( 1_S \) denotes the indicator function of the random set \( S \). Now taking expectation in (9) gives

\[
\mathbb{E} [v_i] = \frac{1}{b} \frac{1}{B \subseteq [n] : |B| = b} \sum_{B \subseteq [n] : |B| = b} 1_B(i) = \frac{1}{b} \left( \frac{n}{b} - 1 \right) = 1,
\]

using \(|\{B \subseteq [n] : |B| = b \land i \in B\}| = \binom{n-1}{b-1}\).

Here we are interested in the mini-batch SAGA algorithm with \( b \)-nice sampling, which we refer to as the \( b \)-nice SAGA. In particular, \( b \)-nice SAGA is the result of using \( b \)-nice sampling, together with a linear model for the control variate \( z_v(w) \). Different choices of the control variate \( z_v(w) \) also recover popular algorithms such as gradient descent, SGD or \( b \)-nice SAGA is the result of using

\[ f_B(w) := \frac{1}{|B|} \sum_{i \in B} \phi_i(a_i^\top w) + \frac{\lambda}{2} \|w\|_2^2 , \]

and its second derivative is thus given by

\[ \nabla^2 f_B(w) = \frac{1}{|B|} \sum_{i \in B} \phi_i''(a_i^\top w)a_i a_i^\top + \lambda I_d \quad (11) \]

where \( I_d \) denotes the identity matrix of size \( d \).

For a symmetric matrix \( M \), we write \( \lambda_{\text{max}}(M) \) (resp. \( \lambda_{\text{min}}(M) \)) for its largest (resp. smallest) eigenvalue. Assumption 1 directly implies the following.

**Lemma 2** (Subsample smoothness constant). Let \( B \subset [n] \), and let \( A_B = [a_i]_{i \in B} \) denote the column concatenation of the vectors \( a_i \) with \( i \in B \). The smoothness constant of the subsampled loss function \( \frac{1}{|B|} \sum_{i \in B} \phi_i(a_i^\top w) \) is given by

\[
L_B := \frac{1}{|B|} \lambda_{\text{max}} \left( \sum_{i \in B} a_i a_i^\top \right) = \frac{1}{|B|} \lambda_{\text{max}} \left( A_B A_B^\top \right). \quad (12)
\]

**Proof.** The proof follows from Assumption 1 as

\[
\frac{1}{|B|} \sum_{i \in B} \nabla^2 \phi_i(a_i^\top w) = \frac{1}{|B|} \sum_{i \in B} \phi_i''(a_i^\top w)a_i a_i^\top \leq \frac{1}{|B|} A_B A_B^\top. \quad \square
\]

Combined with (11), we get that \( f_B \) is \( (L_B + \lambda) \)-smooth.

Another key quantity in our analysis is the strong convexity parameter.
We additionally define the whole function $\epsilon>_{\text{max}}$.

Given an $n$.

Consider the iterates $t=\text{iter}$ of Algorithm 1. Let the step size be given by

$$
\gamma = \frac{1}{n} \max \left\{ \frac{1}{n} \left| \frac{n - b}{n - 1} L_{\text{max}} + \frac{\mu n}{2} \right| \right\}.
$$

(14)

Given an $\epsilon>0$, if $k \geq K_{\text{iter}}(b)$ where

$$
K_{\text{iter}}(b) := \left\{ \frac{4(\mathcal{L}+\lambda)}{\mu}, \frac{n - b}{n - 1} \frac{4(L_{\text{max}}+\lambda)}{\mu} \right\} \log \left( \frac{1}{\epsilon} \right),
$$

(15)

then $\mathbb{E} \left[ \left\| w^k - w^* \right\|^2 \right] \leq \epsilon C$, where $C>0$ is a constant.

Through Theorem 1 we can now explicitly see how the expected smoothness constant $\mathcal{L}$ controls both the step size and the resulting iteration complexity. This is why we need bounds on $\mathcal{L}$ so that we can set the step size. In particular, we will show that the expected smoothness constant is a function of the mini-batch size $b$. Consequently so is the step size, the iteration complexity and the total complexity.

We denote $K_{\text{total}}$ the total complexity defined as the number of stochastic gradients computed, hence with (15),

$$
K_{\text{total}}(b) = b K_{\text{iter}}(b)
$$

(16)

Once we have determined $\mathcal{L}$ as a function of $b$, we will calculate the mini-batch size $b^*$ that optimizes the total complexity $b^* \in \arg \min_{b \in [n]} K_{\text{total}}(b)$.

As we have shown in Lemma 1, computing a precise bound on $\mathcal{L}$ can be computationally intractable. This is why we focus on finding upper bounds on $\mathcal{L}$ that can be computed, but also tight enough to be useful. To verify that our bounds are sufficiently tight, we will always have in mind the bounds $\mathcal{L} \leq \mathcal{L} \leq L_{\text{max}}$ given in (8). In particular, after expressing our bounds of $\mathcal{L} = \mathcal{L}(b)$ as a function of $b$, we would like the bounds (8) to be attained for $\mathcal{L}(1) = L_{\text{max}}$ and $\mathcal{L}(n) = L$.

3.3. Expected smoothness

All bounds we develop on $\mathcal{L}$ are based on the following lemma, which is a specialization of (1) for $b$-nice sampling.

Proposition 1 (Expected smoothness constant). For the $b$-nice sampling, with $b \in [n]$, the expected smoothness constant is given by

$$
\mathcal{L} = \frac{1}{n}\max_{i=1,\ldots,n} \sum_{B \subseteq [n] \cap |B| = b \wedge i \in B} L_B.
$$

(17)

Proof. Let $S$ be the $b$-nice sampling as defined in Definition 3.

Finally from Lemma 1, we have that:

$$
\mathcal{L} = \mathbb{E} \left[ L_{v^i} \right] = \mathbb{E} \left[ L_B \frac{n}{b} \mathbb{1}_{i \in S} \right]
$$

(18)

Taking the maximum over all $i \in [n]$ gives the result. □

The first bound we present is technically the simplest to derive, which is why we refer to it as the simple bound.

Theorem 2 (Simple bound). For a $b$-nice sampling $S$, for $b \in [n]$, we have that

$$
\mathcal{L} \leq \mathcal{L}_{\text{simple}}(b) := \frac{n - b - 1}{b} \frac{1}{n - 1} L + \frac{n - b}{b} \frac{1}{n - 1} L_{\text{max}}.
$$

(19)
**Proof.** The proof, given in Appendix A.2, starts by using the that $L_B \leq \frac{1}{b} \sum_{j \in B} L_j$ for all subsets $B$, which follows from repeatedly applying Lemma 8 in the appendix. The remainder of the proof follows by straightforward counting arguments.

The previous bound interpolates, respectively for $b = 1$ and $b = n$, between $L_{\max}$ and $\bar{L}$. On the one hand, we have that $\mathcal{L}_{\text{simple}}(b)$ is a good bound for when $b$ is small, since $\mathcal{L}_{\text{simple}}(1) = L_{\max}$. Though $\mathcal{L}_{\text{simple}}(b)$ may not be a good bound for large $b$, since $\mathcal{L}_{\text{simple}}(n) = \bar{L} \geq L$, thanks to (13). Thus $\mathcal{L}_{\text{simple}}(b)$ does not achieve the left-hand side of (8). Indeed $\bar{L}$ can be far from $L$. For instance, if $f(w) = \frac{1}{n} \sum_{i \in [n]} \frac{1}{2} (a_i^T w - b_i)^2$ is a quadratic function, then we have that $\mathcal{L} = \frac{1}{n} \text{Tr}(AA^T)$ and $L = \frac{1}{n} \lambda_{\max}(AA^T)$. Thus if the eigenvalues of $AA^T$ are all equal then $\mathcal{L} = dL$. Alternatively, if one eigenvalue is significantly larger than the rest then $\mathcal{L} \approx L$.

Due to this shortcoming of $\mathcal{L}_{\text{simple}}$, we now derive the Bernstein bound. This bound explicitly depends on $L$ instead of $\bar{L}$, and is developed through a specialized variant of a matrix Bernstein inequality (Tropp, 2012; 2015) for sampling without replacement in Appendix C.

**Theorem 3 (Bernstein bound).** The expected smoothness constant is upper bounded by

$$
\mathcal{L} \leq \mathcal{L}_{\text{Bernstein}}(b) := 2 \frac{b - 1}{b} \frac{n}{n - 1} L + \frac{1}{b} \left( \frac{n - b}{n} + \frac{4}{3} \log d \right) L_{\max}.
$$

(19)

Checking again the bounds of $\mathcal{L}_{\text{Bernstein}}(b)$, we have on the one hand that $\mathcal{L}_{\text{Bernstein}}(1) = (1 + \frac{4}{3} \log d) L_{\max} \geq L_{\max}$, thus there is a little bit of slack for $b$ small. On the other hand, using $\frac{3}{n} L_{\max} \leq L$ (see Lemma 10 in appendix), we have that

$$
\mathcal{L}_{\text{Bernstein}}(n) = 2L + \frac{4}{n} \log d L_{\max} \leq \left( 2 + \frac{4}{3} \log d \right) L,
$$

which depends only logarithmically on $d$. Thus we expect the Bernstein bound to be more useful in the large $d$ domains, as compared to the simple bound. We confirm this numerically in Section 5.1.

**Remark 2.** The simple bound is relatively tight for $b$ small, while the Bernstein bound is better for large $b$ and large $d$. Fortunately, we can obtain a more refined bound by taking the minimum of the simple and the Bernstein bounds. This is highlighted numerically in Section 5.

Next we propose a practical estimate of $\mathcal{L}$ that is tight for both small and large mini-batch sizes.

**Definition 5 (Practical estimate).**

$$
\mathcal{L}_{\text{practical}}(b) := \frac{n}{b - 1} \frac{b - 1}{b} L + \frac{1}{b} \left( \frac{n - b}{n} + \frac{4}{3} \log d \right) L_{\max}.
$$

(20)

Indeed $\mathcal{L}_{\text{practical}}(1) = L_{\max}$ and $\mathcal{L}_{\text{practical}}(n) = L$, achieving both limits of (8). The downside to $\mathcal{L}_{\text{practical}}(b)$ is that it is not an upper bound of $\mathcal{L}$. Rather, we are able to show that $\mathcal{L}_{\text{practical}}(b)$ is very close to a valid smoothness constant, but it can be slightly smaller. Our theoretical justification for using $\mathcal{L}_{\text{practical}}(b)$ comes from a mid step in the proof of the Bernstein bound which is captured in the next lemma.

**Lemma 3.** Let $a_j \in \mathbb{R}^d$ for $j \in [n]$ and let $S^i$ be a $(b - 1)$-nice sampling over $[n] \setminus \{i\}$, for every $i \in [n]$. It follows that

$$
\mathcal{L} \leq \mathcal{L}_{\text{practical}}(b) + U \max_{i \in [n]} \mathbb{E} \left[ \lambda_{\max}(N_i) \right],
$$

(21)

with $N_i := \frac{1}{b} \sum_{j \in S^i} a_j a_j^T - \frac{1 - b}{b} \sum_{j \in [n] \setminus \{i\}} a_j a_j^T$.

**Proof.** The proof is given in Appendix A.3.

Lemma 3 shows that the expected smoothness constant is upper-bounded by $\mathcal{L}_{\text{practical}}(b)$ and an additional term. In this additional term we have the largest eigenvalue of a random matrix. This matrix is zero in expectation, and we also find that its eigenvalues oscillate around zero. Indeed, we provide extensive experiments in Section 5 confirming that $\mathcal{L}_{\text{practical}}(b)$ is very close to $\mathcal{L}$ given in (17).

### 4. Optimal mini-batch sizes

Now that we have established the simple and the Bernstein bounds, we can minimize the total complexity (16) in the mini-batch size.

For instance for the simple bound, given $\epsilon > 0$ and plugging in (18) into (16) gives

$$
K_{\text{total}}(b) \leq \max \{ g_{\text{simple}}(b), h(b) \} \log \left( \frac{1}{\epsilon} \right),
$$

where $g_{\text{simple}}(b) := \frac{4L_{\max} + 4(n - 1)\lambda}{\mu(n - 1)} b + \frac{4n(L_{\max} - L)}{\mu(n - 1)}$, and $h(b) := \frac{4(n - 1)\lambda}{\mu(n - 1)} b + n \left( 1 + \frac{1}{n - 1} \frac{4L_{\max} + 4(n - 1)\lambda}{\mu} \right)$.

**Remark 3.** The right-hand side term $h(b)$ is common to all our bounds since it does not depend on $\mathcal{L}$. It linearly decreases from $h(1) = n + \frac{4L_{\max} + 4(n - 1)\lambda}{\mu}$ to $h(n) = n$.

We note that $g_{\text{simple}}(b)$ is a linearly increasing function of $b$, since $L_{\max} \leq n \bar{L}$ (as proven in Lemma 10). One can easily verify that $g_{\text{simple}}(b)$ and $h(b)$ cross, as presented in Figure 2, by looking at initial and final values:
Figure 3: Expected smoothness constant $\mathcal{L}$ and its upper-bounds as a function of the mini-batch size $b$ (staircase eigval dataset, no scaling, $\lambda = 10^{-5}$).

- At $b = 1$, $g_{\text{simple}}(1) = \frac{4}{\mu} (L_{\text{max}} + \lambda) = h(1) - n$. So, $g_{\text{simple}}(1) \leq h(1)$.
- At $b = n$, $g_{\text{simple}}(n) = \frac{4(L_{\text{max}} + \lambda)}{\mu} n = \frac{4(L_{\text{max}} + \lambda)}{\mu} h(n)$. Since $L \geq \mu$, we get $g_{\text{simple}}(n) \geq h(n)$.

Consequently, solving $g_{\text{simple}}(b) = h(b)$ in $b$ gives the optimal mini-batch size

$$b^*_{\text{simple}} = \left[ 1 + \frac{\mu(n-1)}{4(L + \lambda)} \right].$$

(22)

For the Bernstein bound, plugging (19) into (16) leads to

$$K_{\text{total}}(b) \leq \max \left\{ g_{\text{Bernstein}}(b), h(b) \right\} \log \left( \frac{1}{\epsilon} \right),$$

(23)

where

$$g_{\text{Bernstein}}(b) := \frac{4}{\mu(n-1)} (2nL - L_{\text{max}} + (n-1)\lambda) b + \frac{4n}{\mu(n-1)} (L_{\text{max}} - 2L) + \frac{16}{3\mu} \log(d) L_{\text{max}}.$$

The function $g_{\text{Bernstein}}$ is also linearly increasing in $b$ and its initial and final values are

- At $b = 1$, $g_{\text{Bernstein}}(1) = (1 + \frac{4}{3} \log d) \frac{L_{\text{max}} + \lambda}{\mu} + \frac{4\lambda}{\mu}$.
- At $b = n$, $g_{\text{Bernstein}}(n) = n \frac{4(L_{\text{max}} + \lambda)}{\mu} + \frac{16}{3\mu} (L_{\text{max}} + \lambda) \log(d)$.

Since $L \geq \mu$, we get $g_{\text{Bernstein}}(n) \geq h(n)$.

Yet, it is unclear whether $g_{\text{Bernstein}}(1)$ is dominated by $h(1)$. This is why we need to distinguish two cases to minimize the total complexity, which leads to the following solution

$$b^*_{\text{Bernstein}} = \begin{cases} 
1 + \frac{\mu(n-1)}{4(2L+\lambda)}, & \text{if } \frac{4}{3} \frac{L_{\text{max}}}{\mu} \log d \leq n, \\
1, & \text{otherwise}.
\end{cases}$$

Figure 4: Step size estimates as a function the mini-batch size $b$ (staircase eigval dataset, no scaling, $\lambda = 10^{-5}$).

In the first case, the problem is well-conditioned and $g_{\text{Bernstein}}$ and $h$ do cross at a mini-batch size between 1 and $n$. In the second case, the total complexity $K_{\text{total}}$ is governed by $g_{\text{Bernstein}}$ because $g_{\text{Bernstein}}(b) \geq h(b)$ for all $b \in [n]$, and the resulting optimal mini-batch size is $b = 1$.

5. Numerical study

All the experiments were run in Julia and the code is freely available on github.com/gowerrobert/StochOpt.jl.

5.1. Upper-bounds of the expected smoothness constant

First we experimentally verify that our upper-bounds hold and how much slack there is between them and $\mathcal{L}$ given in Equation (17). For artificially generated small data sets, we compute Equation (17) and compare it to our simple and Bernstein bounds, and our practical estimate. Our data are matrices $A \in \mathbb{R}^{d \times n}$ defined as follows

- uniform $(n = 24, d = 50) : [A]_{ij} \sim \mathcal{U}([0,1])$,
- alone eigval $(n = d = 24) : A = \text{diag}(1, \ldots, 1, 100)$,
- staircase eigval $(n = d = 24) : A = \text{diag} \left( 1, 10\sqrt{\frac{1}{n}}, \ldots, 10\sqrt{\frac{(n-2)}{n}}, 10 \right)$.

In Figure 4 we see that $\mathcal{L}_{\text{practical}}$ is arbitrarily close to $\mathcal{L}$, making it hard to distinguish the two line plots. This was the case in many other experiments, which we defer to Appendix E.1. For this reason, we use $\gamma_{\text{practical}}$ in our experiments with the SAGA method.

Furthermore, in accordance with our discussion in Section 3.3, we have that $\mathcal{L}_{\text{simple}}$ and $\mathcal{L}_{\text{Bernstein}}$ are close to $\mathcal{L}$ when $b$ is small and large, respectively. In Appendix E.2 we
show, by using publicly available datasets from LIBSVM\(^6\) and the UCI repository\(^7\), that the simple bound performs better than the Bernstein bound when \(n \gg d\), and conversely for \(d\) significantly larger than \(n\) or when scaling the data.

5.2. Related step size estimation

Different bounds on \(\mathcal{L}\) also give different step sizes (14). Plugging in our estimates \(\mathcal{L}_{\text{simple}}, \mathcal{L}_{\text{Bernstein}}\) and \(\mathcal{L}_{\text{practical}}\) into (14) gives the step sizes \(\gamma_{\text{simple}}, \gamma_{\text{Bernstein}}\) and \(\gamma_{\text{practical}}\), respectively. We compare our resulting step sizes to \(\gamma_{\mathcal{L}}\) where \(\mathcal{L}\) is given by Eq. (17) and to the step size given by Hofmann et al. (2015), which is \(\gamma_{\text{Hofmann}}(b) = \frac{2L_{\text{max}}(1 + K + \sqrt{1 + K^2})}{K}\)

where \(K := \frac{4bL_{\text{max}}}{n\mu}\). We can see in Figure 4, that for \(b = 1\), all the step sizes are approximately the same, with the exceptions of the Bernstein step size. For \(b > 5\), all of our step sizes are larger than \(\gamma_{\text{Hofmann}}(b)\), in particular \(\gamma_{\text{practical}}(b)\) is significantly larger. These observations are verified in other artificial and real data examples in Appendices E.3 and E.4.

5.3. Comparison with previous SAGA settings

Here we compare the performance of SAGA when using the mini-batch size and step size \(b = 1, \gamma_{\text{Defazio}} := 1/3(n\mu + L_{\text{max}})\) given in (Defazio et al., 2014), \(b = 20\) and \(\gamma_{\text{Hofmann}} = 20/n\mu\) given in Hofmann et al. (2015), to our new practical mini-batch size \(b_{\text{practical}} = \left[1 + \frac{1}{\mu(n - 1)}\right]\) and step size \(\gamma_{\text{practical}}\). Our goal is to verify how much our parameter setting can improve practical performance. We also compare with a step size \(\gamma_{\text{gridsearch}}\) obtained by grid search over odd powers of 2. These methods are run until they reach a relative error of \(10^{-4}\).

We find in Figure 5 that our parameter settings \((\gamma_{\text{practical}}, b_{\text{practical}})\) significantly outperforms the previously suggested parameters, and is even comparable to grid search. In Appendix E.5, we show that the settings \((\gamma_{\text{Hofmann}}, b = 20)\) can lead to very poor performance compared to our settings. We also show that our settings are performing very well both in terms of epochs and time.

5.4. Optimality of our mini-batch size

In the last experiment, detailed in Appendix E.6, we show that our estimation of the optimal mini-batch size \(b_{\text{practical}}\) is close to the best one found through a grid search. We build a grid of mini-batch sizes\(^8\) and, as in Section 5.3, compute the empirical complexity required to achieve a relative error of \(10^{-4}\). In Figure 6 we can see that the empirical complexity of the optimal mini-batch size calculated through grid search is very close to the resulting empirical complexity of using \(b_{\text{practical}}\). What is even more interesting, is that \(b_{\text{practical}}\) seems to predict a regime change, where using a larger mini-batch size results in a much larger empirical complexity.

6. Conclusions

We have explained the crucial role of the expected smoothness constant \(\mathcal{L}\) in the convergence of a family of stochastic variance-reduced descent algorithms. We have developed functional upper-bounds of this constant and used them to build larger step sizes and closed-form optimal mini-batch values for the \(b\)-nice SAGA algorithm. Our experiments on artificial and real datasets showed the validity of our upper-bounds and the improvement in the total complexity using our step and optimal mini-batch sizes. Our results suggest a new parameter setting for mini-batch SAGA, that significantly outperforms previous suggested ones, and is even comparable with a gridsearch approach, without the computational burden of the later.

\(^6\)https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/
\(^7\)https://archive.ics.uci.edu/ml/datasets/
\(^8\)Our grid is \(\{2^i, i = 0, \ldots, 14\}, \{2^{10}\}\) being added when needed.
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A. Proofs of the upper bounds of $\mathcal{L}$

A.1. Master lemma

Proof of Lemma 1. Since the $f_i$’s are convex, each realization of $f_v$ is convex, and it follows from equation 2.1.7 in (Nesterov, 2014) that

$$
\|\nabla f_v(x) - \nabla f_v(y)\|^2 \leq 2L_v (f_v(x) - f_v(y) - \langle \nabla f_v(y), x - y \rangle).
$$

(24)

Taking expectation over the sampling gives

$$
E[\|\nabla f_v(x) - \nabla f_v(x^*)\|^2] \leq 2E \left[ L_v (f_v(x) - f_v(x^*) - \langle \nabla f_v(x^*), x - x^* \rangle) \right]
$$

(24)\[ \overset{(24)}{=} \]

$$
= 2n \sum_{i=1}^{n} E \left[ L_v v_i \left( f_i(x) - f_i(x^*) - \langle \nabla f_i(x^*), x - x^* \rangle \right) \right]
$$

(24)

$$
\leq 2 \max_{i=1,\ldots,n} E \left[ L_v v_i \left( f(x) - f(x^*) - \langle \nabla f(x^*), x - x^* \rangle \right) \right]
$$

where in the last equality the full gradient vanishes because it is computed at optimality. The result now follows by comparing the above with the definition of expected smoothness in (7).

A.2. Proof of the simple bound

Proof of Theorem 2. To derive this bound on $\mathcal{L}$ we use that

$$
L_B \leq \frac{1}{b} \sum_{j \in B} L_j,
$$

(25)

which follows from repeatedly applying Lemma 8. For $b \geq 2$, it follows from Equation (17) and Equation (25) that

$$
\mathcal{L} \leq \frac{1}{b^{(n-1)/b-1}} \max_{i=1,\ldots,n} \left\{ \sum_{B \subseteq [n]: |B| = b \wedge i \notin B} \sum_{j \in B} L_j \right\}.
$$

(26)

Using a double counting argument we can show that

$$
\sum_{B \subseteq [n]: |B| = b \wedge i \notin B} \sum_{j \in B} L_j = \sum_{j=1}^{n} \sum_{B \subseteq [n]: |B| = b \wedge j \in B} L_j
$$

$$
= \sum_{j \neq 1} \sum_{B \subseteq [n]: |B| = b \wedge j \in B} L_j + \sum_{B \subseteq [n]: |B| = b \wedge i \in B} L_i
$$

$$
= \sum_{j \neq 1} \left( \frac{n-2}{b-2} \right) L_j + \left( \frac{n-1}{b-1} \right) L_i
$$

$$
= \left( \frac{n-2}{b-2} \right) (n\bar{L} - L_i) + \left( \frac{n-1}{b-1} \right) L_i.
$$

(27)
Optimal mini-batch and step sizes for SAGA

Inserting this into Equation (26) gives

\[ \mathcal{L} \leq \frac{1}{b(n-1)} \max_{i=1,\ldots,n} \left\{ \left( \frac{n-2}{b} \right) \bar{L} + \left( \frac{n-1}{b-1} \right) - \left( \frac{n-2}{b-2} \right) \right\} L_{\text{max}} \]

\[ = \frac{n(n-2)}{b(n-1)} \bar{L} + \frac{(n-1)}{b(n-2)} L_{\text{max}} \]

\[ = \frac{n \cdot b - 1}{b \cdot n - 1} \bar{L} + \frac{1}{b \cdot n - 1} L_{\text{max}} . \quad (28) \]

We also verify that this bound is valid for 1-nice sampling. Indeed, we already have that in this case \( \mathcal{L} = L_{\text{max}} \). \( \Box \)

A.3. Proof of the Bernstein bound

To start the proof of Theorem 3, we re-write the expected smoothness constant as the maximum over an expectation. Let \( S^i \) be a \((b - 1)\)-nice sampling over \([n] \setminus \{i\}\). We can write

\[ \mathcal{L} = \frac{1}{(n-1)} \max_{i=1,\ldots,n} \left\{ \sum_{B \subseteq [n], |B| = b, i \in B} L_B \right\} \]

\[ = \max_{i=1,\ldots,n} \mathbb{E} \left[ L_{S^i \cup \{i\}} \right] \]

\[ \overset{\text{Lemma 2}}{=} \max_{i=1,\ldots,n} \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S^i \cup \{i\}} a_j a_j^\top \right) \right] . \quad (29) \]

One can come back to the definition of the subsample smoothness constant Equation (12) and interpret previous expression as an expectation of the largest eigenvalue of a sum of matrices. This insight allows us to apply a matrix Bernstein inequality, see Theorem 7, to bound \( \mathcal{L} \).

For the proof of Theorem 3, we first need the two following results.

**Lemma 4.** Let \( a_j \in \mathbb{R}^d, i \in \{1,\ldots,n\} \) and let \( S^i \) be a \((b - 1)\)-nice sampling over the set \([n] \setminus \{i\}\). It follows that

\[ \mathbb{E} \left[ \sum_{j \in S^i \cup \{i\}} a_j a_j^\top \right] = a_i a_i^\top + \frac{b-1}{n-1} \sum_{j=1,j \neq i}^n a_j a_j^\top . \quad (30) \]
Proof of Lemma 4. This results follows using a double-counting argument at the fourth line of the computation.

\[
E \left[ \sum_{j \in S \cup \{i\}} a_ja_j^\top \right] = \frac{1}{(n-1)} \sum_{B \subseteq [n] \setminus \{i\}} \sum_{j \in B \cup \{i\}} a_ja_j^\top \\
= \frac{1}{(n-1)} \left( \begin{bmatrix} n-1 \end{bmatrix} a_i a_i^\top + \sum_{B \subseteq [n] \setminus \{i\}} \sum_{j \in B} a_j a_j^\top \right) \\
= a_i a_i^\top + \frac{1}{(n-1)} \sum_{B \subseteq [n] \setminus \{i\}} \sum_{j \in B} a_j a_j^\top \\
= a_i a_i^\top + \frac{1}{(n-1)} \sum_{j=1, j \neq i}^n \sum_{B \subseteq [n] \setminus \{i\}} a_j a_j^\top \\
= a_i a_i^\top + \frac{n-2}{(n-1)} \sum_{j=1, j \neq i}^n a_j a_j^\top \\
= a_i a_i^\top + \frac{b-1}{n-1} \sum_{j=1, j \neq i}^n a_j a_j^\top 
\]

We then introduce another two lemmas which give a first intermediate bound.

Lemma 5. Let \( a_j \in \mathbb{R}^d \) for \( j \in [n] \), let \( i \in [n] \) and let \( S^i \) be a \((b-1)\)-nice sampling over \([n] \setminus \{i\}\). We have

\[
U \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S} a_j a_j^\top \right) \right] \leq \frac{1}{b(n-1)} \left( (n-b)L_i + n(b-1)L \right) \\
+ U \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right) \right]. \tag{31}
\]

Proof of Lemma 5. Expanding the expectation we have

\[
E \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S} a_j a_j^\top \right) \right] \\
\leq \lambda_{\text{max}} \left( E \left[ \frac{1}{b} \sum_{j \in S} a_j a_j^\top \right] \right) + \lambda_{\text{max}} \left( E \left[ \frac{1}{b} \sum_{j \in S} a_j a_j^\top - E \left[ \sum_{j \in S} a_j a_j^\top \right] \right] \right) \\
= \frac{1}{b} \lambda_{\text{max}} \left( a_i a_i^\top + \frac{b-1}{n-1} \sum_{j=1, j \neq i}^n a_j a_j^\top \right) + \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S} a_j a_j^\top - \frac{1}{b} \sum_{j=1, j \neq i}^n a_j a_j^\top \right) \\
= \frac{1}{b} \lambda_{\text{max}} \left( \frac{1}{n-1} \left( (n-b)a_i a_i^\top + (b-1) \sum_{j=1}^n a_j a_j^\top \right) \right) + \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S} a_j a_j^\top - \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right) \\
\leq \frac{1}{b(n-1)} \left( (n-b)\frac{L_i}{U} + n(b-1)\frac{L}{U} \right) + \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S} a_j a_j^\top - \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right),
\]
where in the first inequality we add and remove the mean and then apply Lemma 8. In the second equality we explicit the mean with Lemma 4 and in the last inequality we use again Lemma 8 for the left-hand side term. Finally, we multiply by $U$ on both sides of the inequality.

We recall the following lemma used to introduced the practical estimate given by

$$L_{\text{practical}}(b) := \frac{n}{b} \frac{b - 1}{b - 1} L + \frac{1}{b} \frac{n - b}{n - 1} L_{\text{max}}.$$  

**Lemma 3.** Let $a_j \in \mathbb{R}^d$ for $j \in [n]$ and let $S^i$ be a $(b - 1)$-nice sampling over $[n] \setminus \{i\}$, for every $i \in [n]$. It follows that

$$L \leq L_{\text{practical}}(b) + U \max_{i \in [n]} \mathbb{E} \left[ \lambda_{\text{max}} \left( N_i \right) \right],$$  

with $N_i := \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top$.

**Proof of Lemma 3.** The result comes from applying re-writing $L$ as an expectation of the largest eigenvalue of a sum of matrices. Then we apply Lemma 5 and then taking the maximum over all $i \in [n]$. Thus, we have

$$L \overset{(29)}{=} \max_{i=1, \ldots, n} U \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S^i \cup \{i\}} a_j a_j^\top \right) \right]$$

$$\overset{\text{Lemma 5}}{\leq} \frac{1}{b(n - 1)} \left( (n - b)L_i + n(b - 1)L \right) + U \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right) \right]$$

$$\leq \frac{n}{b} \frac{b - 1}{b - 1} L + \frac{1}{b} \frac{n - b}{b - 1} L_{\text{max}} + \max_{i=1, \ldots, n} U \mathbb{E} \left[ \lambda_{\text{max}} \left( \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right) \right].$$

**Proof of Theorem 3.** Applying the previous lemma we get

$$L \overset{(21)}{\leq} \frac{n}{b} \frac{b - 1}{b - 1} L + \frac{1}{b} \frac{n - b}{b - 1} L_{\text{max}} + \max_{i=1, \ldots, n} U \mathbb{E} \left[ \lambda_{\text{max}} \left( N_i \right) \right],$$  

with $N := \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top$.

To further our argument, we will encode different samplings using unit coordinate vectors. Let $e_1, \ldots, e_n \in \mathbb{R}^n$ be the unit coordinate vectors. Let $S^i = \{S^i_1, \ldots, S^i_k\}$ denote an arbitrary but fixed ordering of the elements of $S^i$. With this we can encode the sampling without replacement as

$$\sum_{j \in S^i} a_j a_j^\top = \sum_{k=1}^{b - 1} \sum_{j \in [n] \setminus \{i\}} (e_j)_{S^i_k} a_j a_j^\top.$$  

Using this notation, the matrix $N$ which can be further decomposed as

$$N = \frac{1}{b} \sum_{j \in S^i} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top$$

$$= \frac{1}{b} \sum_{k=1}^{b - 1} \sum_{j \in [n] \setminus \{i\}} (e_j)_{S^i_k} a_j a_j^\top - \frac{1}{b} \frac{b - 1}{b - 1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top$$

$$= \sum_{k=1}^{b - 1} \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} \left( (e_j)_{S^i_k} - \frac{1}{n - 1} \right) a_j a_j^\top$$

$$:= \sum_{k=1}^{b - 1} M_k .$$
where we have encoded the sampling $S^b$ using unit coordinate vectors. The matrices $M_1, \ldots, M_{b-1}$ are sampled without replacement from the set

$$\left\{ \sum_{j \in [n] \setminus \{i\}} \frac{1}{b} \left( x_j - \frac{1}{n} \right) a_j a_j^\top : x \in \{e_1, \ldots, e_{i-1}, e_{i+1}, \ldots, e_n\} \right\}.$$  

(34)

Now let $X_1, \ldots, X_b$ be matrices sampled with replacement from (34) and let $X_k := \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} \left( z_j^k - \frac{1}{n} \right) a_j a_j^\top$ and $Y := \sum_{k=1}^{b-1} X_k$ thus the vectors $z_j^k$ are sampled with replacement from \{e_1, \ldots, e_{i-1}, e_{i+1}, \ldots, e_n\}. Consequently

$$P[z_j^k = 1] = \frac{1}{n-1}, \quad \forall j \in \{1, \ldots, i, i+1, \ldots, n\}.$$  

We are now in a position to apply the Bernstein matrix inequality. To this end we have

- A sum of centered random matrices: $\mathbb{E}[X_k] = 0$.

- Let $k^*$ be the unique index such that $z_j^{k^*} = 1$. We have a uniform bound of the largest eigenvalue of our $X_k$

$$\lambda_{\max}(X_k) = \frac{1}{b} \lambda_{\max} \left( \sum_{j \in [n] \setminus \{i\}} z_j^k a_j a_j^\top - \frac{1}{n-1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top \right)$$

$$\leq \frac{1}{b} \lambda_{\max} \left( \sum_{j \in [n] \setminus \{i\}} z_j^k a_j a_j^\top \right)$$

$$= \frac{1}{b} \lambda_{\max}(a_{k^*} a_{k^*}^\top)$$

$$\leq \frac{1}{b} L_{\max} U,$$  

(35)

where we applied the Lemma 9 in the first inequality.

- And a bound on the variance too

$$\mathbb{E}[X_k^2] = \mathbb{E} \left( \frac{1}{b} \sum_{j \in [n] \setminus \{i\}} \left( z_j^k - \frac{1}{n-1} \right) a_j a_j^\top \right)^2$$

$$= \frac{1}{b^2} \mathbb{E} \left( \sum_{j, p \in [n] \setminus \{i\}} z_j^k z_p a_j a_j^\top a_p a_p^\top - \frac{2}{n-1} \sum_{j, p \in [n] \setminus \{i\}} z_j^k a_j a_j^\top a_p a_p^\top + \frac{1}{(n-1)^2} \sum_{j, p \in [n] \setminus \{i\}} a_j a_j^\top a_p a_p^\top \right)$$

$$= \frac{1}{b^2} \sum_{j, p \in [n] \setminus \{i\}} \left( \mathbb{E} \left[ z_j^k z_p^k \right] a_j a_j^\top a_p a_p^\top - \frac{2}{n-1} \mathbb{E} \left[ z_j^k \right] a_j a_j^\top a_p a_p^\top + \frac{1}{(n-1)^2} a_j a_j^\top a_p a_p^\top \right)$$

$$= \frac{1}{b^2} \sum_{j, p \in [n] \setminus \{i\}} \left( \mathbb{E} \left[ z_j^k z_p^k \right] a_j a_j^\top a_p a_p^\top - \frac{2}{(n-1)^2} a_j a_j^\top a_p a_p^\top + \frac{1}{(n-1)^2} a_j a_j^\top a_p a_p^\top \right)$$

$$= \frac{1}{b^2} \left( \frac{1}{n-1} \sum_{j \in [n] \setminus \{i\}} a_j a_j^\top a_j a_j^\top - \frac{1}{(n-1)^2} \sum_{j, p \in [n] \setminus \{i\}} a_j a_j^\top a_p a_p^\top \right),$$  

(36)
where, in the last equality, we used that \( z_j^k \neq \sum_{j \neq p} z_j^k x_p = 0 \) if \( j \neq p \) and \( \mathbb{E} \left[ z_j^k z_j^k \right] = \mathbb{E} \left[ z_j^k \right] = \frac{1}{n-1} \), so that

\[
\sum_{j,p \in [n]\{i\}} \mathbb{E} \left[ z_j^k z_p^k \right] a_j^\top a_p^\top = \mathbb{E} \left[ \sum_{j,p \in [n]\{i\}} z_j^k z_p^k \right] a_j^\top a_p^\top
= \sum_{j \in [n]\{i\}} \mathbb{E} \left[ z_j^k z_j^k \right] a_j^\top a_p^\top
= \frac{1}{n-1} \sum_{j \in [n]\{i\}} a_j^\top a_p^\top.
\]

Summing in (36), taking the largest eigenvalue and applying Lemma 9 results in

\[
\lambda_{\text{max}} \left( \sum_{k=1}^{b-1} \mathbb{E} \left[ X_k^2 \right] \right) \leq \lambda_{\text{max}} \left( \sum_{k=1}^{b-1} \frac{1}{b^2} \frac{1}{n-1} \sum_{j \in [n]\{i\}} a_j^\top a_j \right)
\leq \frac{b-1}{b^2} \left( \max_{j \in [n]\{i\}} \lambda_{\text{max}} (a_j^\top a_j) \right) \lambda_{\text{max}} \left( \frac{1}{n-1} \sum_{j \in [n]\{i\}} a_j^\top a_j \right)
\leq \frac{b-1}{b^2} L_{\text{max}} \frac{1}{n^2} L_{[n]\{i\}}.
\]

(37)

Considering Equations (35) and (37) and applying the matrix Bernstein concentration inequality in Theorem 7 we get

\[
U \mathbb{E} \left[ \lambda_{\text{max}} (N) \right] \leq \sqrt{2 \frac{b-1}{b^2} L_{\text{max}} L_{[n]\{i\}} \log d} + \frac{1}{3} \frac{L_{\text{max}}}{b} \log d
\]

Taking the maximum over \( i \) and using \( L_{[n]\{i\}} \leq \frac{n}{n-1} L \) we have that

\[
\max_{i=1,\ldots,n} U \mathbb{E} \left[ \lambda_{\text{max}} (N) \right] \leq \sqrt{2 \frac{b-1}{b^2} \frac{n}{n-1} L_{\text{max}} L \log d} + \frac{1}{3} \frac{L_{\text{max}}}{b} \log d
\]

Combining the above result with (32) leads us to

\[
L \leq \frac{(n-b)L_{\text{max}}}{b(n-1)} + \frac{n(b-1)L}{b(n-1)} + \sqrt{2 \left( \frac{b-1}{b} \frac{n}{n-1} L \right)} \cdot \left( \frac{1}{b} L_{\text{max}} \log d \right) + \frac{1}{3} \frac{L_{\text{max}}}{b} \log d
\]

\[
\leq \frac{(n-b)L_{\text{max}}}{b(n-1)} + \frac{n(b-1)L}{b(n-1)} + \frac{b-1}{b} \frac{n}{n-1} L + 4 \frac{L_{\text{max}}}{3} \frac{1}{b} \log (d)
\]

\[
= \frac{2}{b} \frac{b-1}{b} \frac{n}{n-1} L + \frac{1}{b} \left( \frac{4}{3} \log (d) + \frac{n-b}{n-1} \right) L_{\text{max}}
\]

where in the second inequality we used the inequality \( \sqrt{2ab} \leq a + b \).

\( \square \)

**B. Linear algebra tools**

This appendix is dedicated to the presentation of useful results to manipulate more easily the smoothness constants.

**B.1. Spectral Lemmas**

Let us recall some useful spectral results on Hermitian and positive semi-definite matrices.

**Lemma 6.** *(Weyl’s inequality)* Let \( A, B \in \mathbb{R}^{n \times n} \) symmetric matrices. Assume that the eigenvalues of \( A \) (resp. \( B \)) are sorted i.e., \( \lambda_1(A) \geq \cdots \geq \lambda_n(A) \) (resp. \( \lambda_1(B) \geq \cdots \geq \lambda_n(B) \)). Then, we have

\[
\lambda_{i+j-1}(A + B) \leq \lambda_i(A) + \lambda_j(B)
\]

(38)

whenever \( i, j \geq 1 \) and \( i + j - 1 \leq n \).
Moreover, as a direct consequence of the variational characterization of eigenvalues, namely

$$\lambda_{\text{max}}(A) = \max_{v \neq 0} \frac{v^\top A v}{\|v\|_2^2},$$

we have an inequality between the maximum diagonal term of a positive semi-definite matrices and its maximum eigenvalue.

**Lemma 7.** Let $A \in \mathbb{R}^{n \times n}$ positive semi-definite matrix and the vector containing its diagonal $d := \text{diag}(A)$. Then, we have

$$\max_{i=1,\ldots,n} d_i \leq \lambda_{\text{max}}(A).$$

The following lemma is a direct consequence of Weyl’s inequality for $i = j = 1$.

**Lemma 8.** Let $A, B \in \mathbb{R}^{n \times n}$ symmetric matrices. Then, we have

$$\lambda_{\text{max}}(A + B) \leq \lambda_{\text{max}}(A) + \lambda_{\text{max}}(B).$$

Lastly, we present a result arising from previous lemma.

**Lemma 9.** Let $A, B \in \mathbb{R}^{n \times n}$ symmetric matrices such that $B$ is positive semi-definite. Then, we have

$$\lambda_{\text{max}}(A - B) \leq \lambda_{\text{max}}(A).$$

**Proof.** Let $A, B \in \mathbb{R}^{n \times n}$ symmetric matrices such that $B$ is positive semi-definite. We get directly

$$\lambda_{\text{max}}(A - B) \leq \lambda_{\text{max}}(A) + \lambda_{\text{min}}(-B)
\leq \lambda_{\text{max}}(A) - \lambda_{\text{min}}(B)
\leq \lambda_{\text{max}}(A),$$

where the first inequality stems from Lemma 8 and the second from $B \succeq 0$. \hfill $\Box$

### B.2. Basic properties of the smoothness constants

The complexity results of Gower et al. (2018) depends on smoothness constants defined in Section 3.1. Here are some inequalities giving an idea of the order of those constants.

**Lemma 10.** Let $\emptyset \neq B \subseteq [n] = \{1, \ldots, n\}$ a batch set drawn randomly without replacement. The following inequalities hold

(i) $$L_i \leq L_{\text{max}} \quad \forall i = 1, \ldots, n.$$ (43)

(ii) $$L_B \leq \frac{1}{|B|} \sum_{i \in B} L_i \quad \forall i = 1, \ldots, n.$$ (44)

(iii) $$L^{(a)} \leq L^{(b)} \leq L^{(c)} \leq nL^{(d)} \leq nL.$$ (45)

**Proof.** (i) One directly gets that $L_i \leq \max_{j=1,\ldots,n} L_j = L_{\text{max}}$.

(ii) This inequality states that the smoothness constant $L_B$ of the averaged function $f_B$ is upper bounded by the average of the corresponding smoothness constants $L_i$, over the batch $B$. The proof consists in $|B|$ repetitive calls of Lemma 8.
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(iii) (a) Direct implication of (ii) for $B = [n]$.

(b) Direct calculation

$$ L = \frac{1}{n} \sum_{i=1}^{n} L_i \leq \frac{1}{n} \sum_{i=1}^{n} L_{\text{max}} \leq \hat{L}_{\text{max}}. $$

(c) Let us first recall the matrix formulation of our smoothness constants:

$$ L = \frac{U}{n} \lambda_{\text{max}}(AA^T) = \frac{U}{n} \lambda_{\text{max}}(A^T A) $$

and

$$ L_{\text{max}} = \frac{U}{n} \max_{i=1,\ldots,n} e_i^T A^T A e_i, $$

Using the min-max theorem, we have that

$$ \lambda_{\text{max}}(A^T A) = \max_{x \neq 0} \frac{x^T A^T A x}{\|x\|_2^2} \geq \max_{i=1,\ldots,n} e_i^T A^T A e_i. $$

Dividing the above by $n$ on both sides gives

$$ L \geq \frac{L_{\text{max}}}{n}. $$

(d) Direct consequence of (a).

C. Matrix bernstein inequality: sampling without replacement

In this appendix, we present the matrix Bernstein inequality for independent Hermitian matrices from Tropp (2015). We also provide another version of this theorem for matrices sampled without replacement and prove it as explicitly as possible, taking our inspiration from Tropp (2011). The proof is based on the possibility of transferring the results from sampling with to without through the inequality (50) due to Gross & Nesme (2010). The exact same work can be done for the tail bound, which is for instance used in Bach (2012).

C.1. Original Bernstein inequality for independent matrices

We first present Theorem 4 which gives a Bernstein inequality for a sum of random and independent Hermitian matrices whose eigenvalues are upper bounded. If the matrices $X_k$ are sampled from a finite set $\mathcal{X}$, one can interpret this random sampling of independent matrices as a random sampling with replacement.

**Theorem 4** (Tropp (2015), Theorem 6.6.1: Matrix Bernstein Inequality). Consider a finite sequence $\{X_k\}_{k=1,\ldots,n}$ of $n$ independent, random, Hermitian matrices with dimension $d$. Assume that $E X_k = 0$ and $\lambda_{\text{max}}(X_k) \leq L$ for each index $k$.

Introduce the random matrix

$$ S_X := \sum_{k=1}^{n} X_k. $$

Let $\nu(S_X)$ be the matrix variance statistic of the sum:

$$ \nu(S_X) := \left\| E S_X^2 \right\| = \left\| \sum_{k=1}^{n} E X_k^2 \right\| = \lambda_{\text{max}} \left( \sum_{k=1}^{n} E X_k^2 \right). $$

Then

$$ E \lambda_{\text{max}}(S_X) \leq \sqrt{2\nu(S_X)} \log d + \frac{1}{3} L \log d. $$

This theorem is the one we extend in Theorem 7 to the case when the random matrices $X_k$ are sampled without replacement from a finite set $\mathcal{X}$. We drew our inspiration from the proof of the matrix Chernoff inequality in Tropp (2011) and the one of the matrix Bernstein tail bound in Bach (2012), both in the case of sampling without replacement.
C.2. Technical random matrices prerequisites

Before proving Theorem 7, which extends the matrix Bernstein inequality to sampling without replacement, we need to introduce the key tools of the matrix Laplace transform technique. This technique is precious to prove tail bounds for sums of random matrices such as Chernoff, Hoeffding or Bernstein bounds, as presented in (Tropp, 2012).

Here, \( \| \cdot \| \) denotes the spectral norm, which is defined for any Hermitian matrix \( H \) by

\[
\| M \| = \max \left\{ \lambda_{\text{max}}(H), -\lambda_{\text{min}}(H) \right\}.
\]  

We also introduce the moment generating function (mgf) and the cumulant generating function (cgf) of a random matrix, which are essential in the Laplace transform method approach.

**Definition 6** (Matrix Mgf and Cgf). Let \( X \) be a random Hermitian matrix. For all \( \theta \in \mathbb{R} \), the matrix generating function \( M_X(\theta) := \mathbb{E} e^{\theta X} \) and the matrix cumulant generating function \( \Xi_X(\theta) := \log \mathbb{E} e^{\theta X} \).

**Remark 4.** These expectations may not exist for all values of \( \theta \).

**Proposition 2** (Tropp (2015), Proposition 3.2.2: Expectation Bound of the Maximum Eigenvalue). Let \( X \) be a random Hermitian matrix. Then

\[
\mathbb{E} \lambda_{\text{max}}(X) \leq \inf_{\theta > 0} \left\{ \frac{1}{\theta} \log \mathbb{E} \text{tr} e^{\theta X} \right\}.
\]  

**Remark 5.** This proposition is an adaptation of the Laplace transform method to obtain a bound of the expectation of the maximum eigenvalue of a random Hermitian matrix. Contrary to the tail bounds, there is no exact analog of the expectation bounds in the scalar setting.

**Proof of Proposition 2.** Fix a positive number \( \theta \). Because \( \lambda_{\text{max}}(\cdot) \) is a positive-homogeneous map, we have

\[
\mathbb{E} \lambda_{\text{max}}(X) = \frac{1}{\theta} \mathbb{E} \lambda_{\text{max}}(\theta X)
= \frac{1}{\theta} \mathbb{E} \log e^{\lambda_{\text{max}}(\theta X)}
\leq \frac{1}{\theta} \log \mathbb{E} e^{\lambda_{\text{max}}(\theta X)}
= \frac{1}{\theta} \log \mathbb{E} \lambda_{\text{max}}(e^{\theta X})
\leq \frac{1}{\theta} \log \mathbb{E} \text{tr} e^{\theta X},
\]

where in the third line we used the Jensen’s inequality, in the fourth one the spectral mapping theorem and in the last line the domination by the trace of a positive-definite matrix.

**Theorem 5** (Tropp (2015), Theorem 8.1.1: Lieb). Let \( H \) be a fixed Hermitian matrix with dimension \( d \). The function

\[
X \rightarrow \text{tr} \exp(H + X)
\]

is a concave map on the convex cone of \( d \times d \) positive-definite matrices.

**Proof of Theorem 5.** See Chapter 8 in Tropp (2015).

**Corollary 1.** Let \( H \) be a fixed Hermitian matrix with dimension \( d \). Let \( X \) be a random Hermitian matrix of same dimension. The following inequality holds

\[
\mathbb{E} \text{tr} \exp(H + X) \leq \text{tr} \exp(H + \log \mathbb{E} e^X)
\]

is a concave map on the convex cone of \( d \times d \) positive-definite matrices.
Proof of Corollary 1. Introducing $Y = e^X$, we have directly

$$
\mathbb{E} \text{tr} \exp(H + X) = \mathbb{E} \text{tr} \exp(H + \log e^X)
= \mathbb{E} \text{tr} \exp(H + \log Y)
\leq \text{tr} \exp(H + \log \mathbb{E} Y)
= \text{tr} \exp(H + \log \mathbb{E} e^X)
$$

where the inequality comes from the application of Theorem 5 and Jensen’s inequality. \hfill \square

Lemma 11 (Tropp (2015), Lemma 3.5.1 or Tropp (2012), Lemma 3.4: Subadditivity of Matrix Cgf). Consider a finite sequence $\{X_k\}$ of independent, random, Hermitian matrices of the same dimension. Let $\theta \in \mathbb{R}$, then

$$
\text{tr} \exp\left(\sum_{k=1}^{n} X_k(\theta)\right) = \mathbb{E} \text{tr} \exp\left(\sum_{k=1}^{n} e^X_k\right)
\leq \text{tr} \exp\left(\sum_{k=1}^{n} \log \mathbb{E} e^{\theta X_k}\right)
= \text{tr} \exp\left(\sum_{k=1}^{n} \Xi_{X_k}(\theta)\right).
$$

Proof of Lemma 11. Let us assume, without loss of generality, that $\theta = 1$. Let a finite sequence $\{X_k\}_{k=1}^{n}$ of $n$ independent, random, Hermitian matrices of the same dimension. We write down $\mathbb{E}_k$ the expectation with respect only to the $k$-th random matrix $X_k$.

$$
\text{tr} \exp\left(\sum_{k=1}^{n} X_k(1)\right) = \text{tr} \exp\left(\log \mathbb{E} \exp\left(\sum_{k=1}^{n} X_k\right)\right)
= \mathbb{E} \text{tr} \exp\left(\sum_{k=1}^{n} X_k\right)
= \mathbb{E}_1 \ldots \mathbb{E}_{n-1} \mathbb{E}_n \text{tr} \exp\left(\sum_{k=1}^{n-1} X_k + X_{n+1}\right)
\leq \mathbb{E}_1 \ldots \mathbb{E}_{n-1} \text{tr} \exp\left(\sum_{k=1}^{n-1} X_k + \log \mathbb{E}_n e^{X_{n+1}}\right)
= \mathbb{E}_1 \ldots \mathbb{E}_{n-1} \text{tr} \exp\left(\sum_{k=1}^{n-2} X_k + X_{n-1} + \log \mathbb{E}_n e^{X_{n+1}}\right)
\leq \mathbb{E}_1 \ldots \mathbb{E}_{n-2} \text{tr} \exp\left(\sum_{k=1}^{n-2} X_k + \log \mathbb{E}_{n-1} e^{X_{n-1}} + \log \mathbb{E}_n e^{X_n}\right)
\leq \cdots \leq \text{tr} \exp\left(\sum_{k=1}^{n} \log \mathbb{E} e^{\theta X_k}\right)
= \text{tr} \exp\left(\sum_{k=1}^{n-1} \Xi_{X_k}(\theta)\right).
$$

where first and second inequalities result from Corollary 1, the last one comes the fact that $\mathbb{E}_k e^{X_k} = \mathbb{E} e^{X_k}, \forall k \in [n]$ and the final equality directly comes from an indentification of Definition 6. \hfill \square

Lemma 12 (Tropp (2015), Lemma 6.6.2: Matrix Bernstein Mgf and Cgf Bounds). Let $X$ a random Hermitian matrix such that

$$
\mathbb{E}X = 0 \quad \text{and} \quad \lambda_{\text{max}}(X) \leq L.
$$

Then, for $0 < \theta < 3/L$,

$$
M_{X}(\theta) := \mathbb{E} e^{\theta X} \preceq \exp\left(\frac{\theta^2/2}{1 - \theta L/3} \cdot \mathbb{E} X^2\right).
$$
and

\[ \Xi_X(\theta) := \log \mathbb{E} e^{\theta X} \leq \frac{\theta^2/2}{1 - \theta L/3} \cdot \mathbb{E} X^2. \]

**Proof of Lemma 12.** See Tropp (2015).

### C.3. Extended results for sampling without replacement

This section is dedicated to the main result, Lemma 13, needed for transferring results from sampling with to without replacement. This lemma is actually the matrix version of a classical result from Hoeffding (1963). We then combine it with previous results of Appendix C.2 to produce a new master bound in Theorem 6, which is the key inequality of the proof of Theorem 7.

**Lemma 13 (Gross & Nesme (2010), Domination of the Trace of the Mgf of a Sample Without Replacement).** Consider two finite sequences, of same length \( n \), \( \{X_k\}_{k=1,\ldots,n} \) and \( \{Y_k\}_{k=1,\ldots,n} \) of Hermitian random matrices sampled respectively with and without replacement from a finite set \( \mathcal{X} \). Let \( \theta \in \mathbb{R} \), \( S_X := \sum_{k=1}^n X_k \) and \( S_Y := \sum_{k=1}^n Y_k \), then

\[ \text{tr } M_{S_Y} (\theta) := \mathbb{E} \text{ tr exp} (\theta S_Y) \leq \mathbb{E} \text{ tr exp} (\theta S_X). \]  

**Proof of Lemma 13.** The left-hand side equality directly arises from Definition 6 and the fact that the trace commutes with the expectation because it is a linear operator. For the right-hand side inequality, see the proof in Gross & Nesme (2010).

**Theorem 6 (Master Bound for a Sum of Random Matrices Sampled Without Replacement).** Consider two finite sequences, of same length \( n \), \( \{X_k\}_{k=1,\ldots,n} \) and \( \{Y_k\}_{k=1,\ldots,n} \) of Hermitian random matrices sampled respectively with and without replacement from a finite set \( \mathcal{X} \). Then

\[ \mathbb{E} \lambda_{\max} \left( \sum_{k=1}^n Y_k \right) \leq \inf_{\delta > 0} \left\{ \frac{1}{\theta} \log \mathbb{E} \text{ tr exp} \left( \sum_{k=1}^n \log \mathbb{E} e^{\theta X_k} \right) \right\}. \]  

**Remark 6.** This theorem is a modified version of Theorem 3.6.1 in Tropp (2015) for a sum of matrices sampled without replacement.

**Proof of Theorem 6.** Consider two finite sequences, of same length, \( \{X_k\} \) and \( \{Y_k\} \) of Hermitian random matrices of same size sampled respectively with and without replacement from a finite set \( \mathcal{X} \). Let \( \theta \) a positive number.

\[ \mathbb{E} \lambda_{\max} \left( \sum_{k=1}^n Y_k \right) \leq \inf_{\delta > 0} \left\{ \frac{1}{\theta} \log \mathbb{E} \text{ tr exp} \left( \theta \sum_{k=1}^n Y_k \right) \right\} \leq \inf_{\delta > 0} \left\{ \frac{1}{\theta} \log \mathbb{E} \text{ tr exp} \left( \theta \sum_{k=1}^n X_k \right) \right\}. \]

where we used successively Proposition 2, Lemma 13 and Lemma 11. First, we use the expectation bound for the maximum eigenvalue. We then use the main result of Gross & Nesme (2010) and invoked in Tropp (2011) to extend the matrix Chernoff bound for matrices sampled without replacement. This lemma allows us to transfer our results to sampling with replacement. And finally, we then apply the subadditivity of matrix cgfs to get the desired result.

### C.4. Bernstein inequality for sampling without replacement

The following theorem is almost the same than Theorem 4, but in the case of matrices sampled without replacement from a finite set. The proof stems from results established in previous Appendices C.2 and C.3.

**Theorem 7 (Matrix Bernstein Inequality Without Replacement).** Let \( \mathcal{X} \) be a finite set of Hermitian matrices with dimension \( d \) such that

\[ \lambda_{\max}(X) \leq L, \quad \forall X \in \mathcal{X}. \]

Sample two finite sequences, of same length \( n \), \( \{X_k\}_{k=1,\ldots,n} \) and \( \{Y_k\}_{k=1,\ldots,n} \) uniformly at random from \( \mathcal{X} \) respectively with and without replacement such that

\[ \mathbb{E} X_k = 0 \quad \forall k. \]
Optimal mini-batch and step sizes for SAGA

Introduce the random matrices

$$S_X := \sum_{k=1}^{n} X_k \quad \text{and} \quad S_Y := \sum_{k=1}^{n} Y_k .$$

Let $v(S_X)$ be the matrix variance statistic of the second sum

$$v(S_X) := \| E S_X^2 \| = \left\| \sum_{k=1}^{n} E X_k^2 \right\| = \lambda_{\max} \left( \sum_{k=1}^{n} E X_k^2 \right) .$$

Then

$$E \lambda_{\max} (S_Y) \leq \sqrt{2v(S_X)} \log d + \frac{1}{3} L \log d . \quad (53)$$

Proof of Theorem 7. Consider $\mathcal{X}$ a finite set of Hermitian matrices of dimension $d$ such that

$$\lambda_{\max}(X) \leq L \quad \forall X \in \mathcal{X} .$$

Sample two finite sequences, of same length, $\{X_k\}$ and $\{Y_k\}$ uniformly at random from $\mathcal{X}$ respectively with and without replacement such that

$$E X_k = 0 \quad \forall k .$$

The $\{X_k\}$ matrices are thus independent. Introduce the sums $S_X = \sum_{k=1}^{n} X_k$ and $S_Y = \sum_{k=1}^{n} Y_k$. Let us bound the expectation of the largest eigenvalue of the latter

$$E \lambda_{\max}(S_Y) = E \lambda_{\max} \left( \sum_{k=1}^{n} Y_k \right) \leq \inf_{\theta > 0} \left\{ \frac{1}{\theta} \log \text{tr} \exp \left( \sum_{k=1}^{n} \log E e^{\theta X_k} \right) \right\}$$

$$\leq \inf_{0 < \theta < 3/L} \left\{ \frac{1}{\theta} \log \text{tr} \exp \left( \frac{\theta^2/2}{1-\theta L/3} \sum_{k=1}^{n} E X_k^2 \right) \right\}$$

$$\leq \inf_{0 < \theta < 3/L} \left\{ \frac{1}{\theta} \log d \lambda_{\max} \left( \exp \left( \frac{\theta^2/2}{1-\theta L/3} E S_X^2 \right) \right) \right\}$$

$$\leq \inf_{0 < \theta < 3/L} \left\{ \frac{1}{\theta} \log d \exp \left( \frac{\theta^2/2}{1-\theta L/3} \lambda_{\max} (E S_X^2) \right) \right\}$$

$$\leq \inf_{0 < \theta < 3/L} \left\{ \frac{1}{\theta} \log \left[ d \exp \left( \frac{\theta^2/2}{1-\theta L/3} v(S_X) \right) \right] \right\}$$

$$= \inf_{0 < \theta < 3/L} \left\{ \frac{\log d}{\theta} + \frac{\theta/2}{1-\theta L/3} v(S_X) \right\} .$$

where the inequalities successively derive from Theorem 6, Lemma 12 combined with the monotony of $\text{tr} \exp(\cdot)$, the fact that $\text{tr}(M) \leq d \lambda_{\max}(M), \forall M \in \mathbb{R}^{d \times d}$, the spectral mapping theorem and lastly (48) with $E Y^2 \succeq 0$. Finally, one can complete the infimum, for instance using a computer algebra system, to finish the proof as it was stated in the original proof by Tropp (2015)\(^9\). In conclusion,

$$E \lambda_{\max}(S_Y) \leq \sqrt{2v(S_X)} \log d + \frac{1}{3} L \log d .$$

\(\square\)

D. Miscellaneous

Lemma 14 (Double counting). Let $a_{i,C} \in \mathbb{R}$ for $i = 1, \ldots, n$ and $C \in \mathcal{C}$, where $\mathcal{C}$ is a collection of subsets of $[n]$. Then

$$\sum_{C \in \mathcal{C}} \sum_{i \in C} a_{i,C} = \sum_{i=1}^{n} \sum_{C \in \mathcal{C} : i \in C} a_{i,C} . \quad (54)$$

\(^9\)For instance: Minimize[(log(d)/x) + ((x/2)/(1-(L/3)*x))]*v, x > 0, x < (3/L), x] in Wolfram Alpha.
Algorithm 2 JacSketch Practical implementation of $b$-nice SAGA

**Input:** mini-batch size $b$, step size $\gamma > 0$

**Initialize:** $w^0 \in \mathbb{R}^d$, $J^0 \in \mathbb{R}^{d \times n}$, $u^0 = \frac{1}{n} J^0 e$

for $k = 0, 1, 2, \ldots$ do

Sample a fresh batch $B \subseteq [n]$ s.t. $|B| = b$

\[ \text{aux} = \sum_{i \in B} (\nabla f_i(w^k) - J^k_i) \]  // update the auxiliary vector

\[ g^k = u^k + \frac{1}{b} \text{aux} \]  // update the unbiased gradient estimate

\[ u^{k+1} = u^k + \frac{1}{n} \text{aux} \]  // update the biased gradient estimate

\[ J^{k+1}_i = \begin{cases} J^k_i & i \notin B \\ \nabla f_i(w^k) & i \in B. \end{cases} \]  // update the Jacobian estimate

\[ w^{k+1} = w^k - \gamma g^k \]  // take a step

end for

E. Additional experiments

E.1. Experiment 1 on artificial datasets

As described in Section 5, we compute our the simple and Bernstein bounds, our practical estimate and the true $L$ for small artificial datasets: uniform ($n = 24, d = 50$), staircase eigval ($n = d = 24$) and alone eigval ($n = d = 24$). Figure 7 shows first that the practical estimate is a very close approximation of $L$. On the one hand, we observe in Figure 7a that the Bernstein bound performs poorly since the feature dimension is very small $d = 50$. On the other hand, Figure 7b shows a regime change for $b \approx 10$, which highlight the usefulness of combining our bounds to approximate the expected smoothness constant. Finally, we observe that for the alone eigval dataset Figure 7b, which has one very large eigenvalue far from the rest of the spectrum, the simple bound matches $L$ because the gap between $\bar{L}$ and $L$ shrinks. Indeed, $\bar{L} \approx L \approx \frac{L_{\text{max}}}{n}$. When the spectrum is more concentrated, like for staircase eigval, we get a significant gap between $\bar{L}$ and $L$ as shown in Figure 7c, where the simple bound is far from $L$ when $b = n$.  

![Figure 7](image_url)

Figure 7: Expected smoothness constant $L$ and its upper-bounds the mini-batch size $b$ varies (unscaled datasets, $\lambda = 10^{-1}$).

We also report the influence of changing the value of the regularization parameter $\lambda$. Figure 8 shows that this parameter has little impact on the general shape of the bounds and of $L$.

Finally, we study the impact of scaling or standardizing (i.e., removing the mean and dividing by the standard deviation for each feature) our artificial datasets. In order not to benefit from the diagonal shape of the alone eigval and staircase eigval datasets we also give examples of the bounds of $L$ after a rotation of the data. The rotation aims at preserving the spectrum while erasing the diagonal structure of the covariance matrix $AA^\top$. This rotation procedure consists in transforming $A$ into $Q^\top AQ$, where $Q$ is the orthogonal matrix given by the QR decomposition of a random squared matrix (with dimension the same as the one of $A$) with uniformly random coefficients $M$, such that $M = QR$.  

![Figure 8](image_url)
E.2. Experiment 1 for real datasets

In Figure 10, we also used publicly available datasets from LIBSVM\textsuperscript{10} provided by Chang & Lin (2011). For real regression data sets such as \textit{YearPredictionMSD} ($n = 515, 345, d = 90$), and for binary classification with logistic regression \textit{covtype} ($n = 581, 012, d = 54$), \textit{ijcnn1} ($n = 141, 691, d = 22$) and \textit{slice-localization} from the UCI repository\textsuperscript{11} provided by Dheeru & Karra Taniskidou (2017) the simple bound performs better than the Bernstein bound when $n \gg d$, and conversely when $d$ gets of the order of $n$ or larger or when scaling the data.

We recall the datasets we used for ridge regression problems: \textit{YearPredictionMSD} ($n = 515, 345, d = 90$) from LIBSVM and \textit{slice} ($n = 53, 500, d = 384$) from UCI. And for binary classification with logistic regression we used: \textit{ijcnn1} ($n = 141, 691, d = 22$), \textit{covtype.binary} ($n = 581, 012, d = 54$) \textit{real-sim} ($n = 72, 309, d = 20, 958$), \textit{rcv1.binary} ($n = 697, 641, d = 47, 236$) and \textit{news20.binary} ($n = 19, 996, d = 1, 355, 191$) from LIBSVM. When a test set was available, we concatenated it with the train set to have more samples.

E.3. Experiment 2 for artificial datasets

In this section we give the step sizes estimate corresponding to the expected smoothness constant, the simple and Bernstein upper-bounds and the practical estimate for our small artificial datasets. In Figure 12, we show that the practical step size

\textsuperscript{10}https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/

\textsuperscript{11}https://archive.ics.uci.edu/ml/datasets/
estimate is larger than all others. Moreover, for except for small value of \( b \), our \( \gamma_{\text{simple}} \) or \( \gamma_{\text{Bernstein}} \) estimates are larger than the one proposed in (Hofmann et al., 2015).

E.4. Experiment 2 for real datasets

Here we show the step sizes estimate corresponding to the simple and Bernstein upper-bounds and the practical estimate for real datasets detailed in Appendix E.1. On these real data, unscaled in Figure 13 scaled in Figure 14, we see that the gap between our step size estimates and \( \gamma_{\text{Hofmann}} \) are even larger. We observe in Figure 13 that simple bound leads to higher step sizes for small \( d \) than the Bernstein, and vice versa. Yet, Figure 14 seems show that scaling the data leads to \( \gamma_{\text{Bernstein}} \) larger than \( \gamma_{\text{simple}} \).

E.5. Experiment 3: comparison with previous SAGA settings

In this section we provide more example of the performance of our practical settings compared to previously known SAGA settings. We run our experiments on real datasets introduced in detail in Appendix E.1. SAGA implementations are run until they reach a relative error of \( 10^{-4} \), except in some cases where the Hofmann’s exceeded our maximal number of epochs like in Figure 15.

In Figures 16 to 21, we experimentally show that our settings \((b_{\text{practical}}, \gamma_{\text{practical}})\) outperforms whether the classical \((b = 1, \gamma_{\text{Defazio}})\) or the \((b = 20, \gamma_{\text{Hofmann}})\) settings both in terms of epochs and running time.

E.6. Experiment 4: Optimality of the mini-batch size

This experiment aims to estimate how close is our practical estimate \( b_{\text{practical}} \) to the empirical best mini-batch size one could get running a grid search. We recall that we use the following grid for the mini-batch sizes: \( \{2^i, i = 0, \ldots, 14\} \), with \( \{2^{16}\} \) added in some cases. We show in the log-scaled Figures 22 to 27 the empirical complexity, e.g., the number of computed gradients to reach a relative error of \( 10^{-4} \), as a function of the mini-batch \( b \).

We almost always observe this change of regime in the empirical complexity, except in Figure 27a. For small values of \( b \), the complexity is of the same order of magnitude, then, for values greater than the empirical optimal mini-batch size, the complexity explodes. The observed saturation in Figure 26b is due to the fact that the algorithm reached the maximum number of epochs, which is similar to an exploding complexity compared to the regime for small \( b \).

This experiment shows that our optimal mini-batch size \( b_{\text{practical}} \) is correctly designating the largest mini-batch achieving the best complexity as it as large as possible, without reaching the regime where the total complexity explodes.
Figure 9: Upper-bounds of the expected smoothness constant $\mathcal{L}$ for not rotated (left) and rotated (right) data sets ($\lambda = 10^{-3}$).
Figure 10: Upper-bounds of the expected smoothness constant for real unscaled datasets ($\lambda = 10^{-1}$).

(a) icnn1

(b) covtype.binary

(c) YearPredictionMSD

(d) slice

(e) real-sim

(f) rcv1.binary

(g) news20.binary

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Optimal mini-batch and step sizes for SAGA
**Optimal mini-batch and step sizes for SAGA**

Figure 11: Upper-bounds of the expected smoothness constant of $L$ for real feature-scaled datasets ($\lambda = 10^{-1}$).

Figure 12: Step size estimates as a function the mini-batch size for unscaled artificial datasets ($\lambda = 10^{-1}$).
Figure 13: Step size estimates as a function the mini-batch size for real unscaled datasets ($\lambda = 10^{-1}$).
Figure 14: Step size estimates as a function the mini-batch size for real feature-scaled datasets ($\lambda = 10^{-1}$).

Figure 15: Poor performance of Hofmann’s settings for the feature-scaled dataset slice ($\lambda = 10^{-1}$).
Figure 16: Performance of SAGA implementations for the feature-scaled dataset *ijcnn1*.

Figure 17: Performance of SAGA implementations for the feature-scaled dataset *covtype.binary*. 
Figure 18: Performance of SAGA implementations for the feature-scaled dataset YearPredictionMSD.

Figure 19: Performance of SAGA implementations for the feature-scaled dataset slice.
## Optimal mini-batch and step sizes for SAGA

### Figure 20: Performance of SAGA implementations for the unscaled dataset slice.

![Performance of SAGA implementations for the unscaled dataset slice](image)

### Figure 21: Performance of SAGA implementations for the unscaled dataset real-sim.

![Performance of SAGA implementations for the unscaled dataset real-sim](image)
Figure 22: Empirical total complexity versus mini-batch size for the feature-scaled *ijcnn1* dataset.

Figure 23: Empirical total complexity versus mini-batch size for the feature-scaled *covtype.binary* dataset.

Figure 24: Empirical total complexity versus mini-batch size for the feature-scaled *YearPredictionMSD* dataset.
Figure 25: Empirical total complexity versus mini-batch size for the feature-scaled slice dataset.

Figure 26: Empirical total complexity versus mini-batch size for the unscaled slice dataset.

Figure 27: Empirical total complexity versus mini-batch size for the unscaled real-sim dataset.