SAG-re: Faster Prototyping of Recommender Systems using Stochastic Average Gradient

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ABSTRACT

In the age of agile software engineering and shorter product lifecycles, data-scientists would ultimately face the challenge of running many experiments and producing high-quality results, with less time. In this paper, we motivate the problem of adopting the stochastic average gradient method (SAG)for prototyping model-based recommender systems. We motivate that, by taking advantage of SAG's fast convergence rate and low iteration cost, data-scientists are able to achieve better optimizations for their recommender systems in a shorter amount of time. However, adopting SAG in prototyping model-based recommender systems is not trivial because the asymptotic space-complexity of using SAG can be prohibitively high. We propose SAG-RE as our approach to resolve the space-complexity challenge. SAG-RE preserves all the benefits and advantages of using SAG, and SAG-RE achieves asymptotic space complexity as compact as any memory-less approach. We both prove in theory and extensively evaluate in practice that, SAG-RE yields a better quality optimization within a shorter amount of time, than the two main gradient methods in the state-of-the-art of prototyping recommender systems, namely full deterministic gradient, and stochastic gradient.

Categories and Subject Descriptors

H.3.3 [Information Storage and Retrieval]: Information Search and Retrieval—Information Filtering

General Terms

Asymptotic Time Complexity, Asymptotic Space Complexity, Prototyping, Experimentation

Keywords

Recommender systems, collaborative filtering, matrix factorization, stochastic gradient, agile software engineering

1. INTRODUCTION

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Shopping, text advertising, display advertising, renting movies, listening to music... recommender systems are prevalent and ubiquitous in our daily lives. Matrix factorization (MF) is a popular technique in model-based recommender systems. MF has been utilized extensively in past research for handling both explicit [4, 9, 7] ratings, and implicit [1, 2, 8, 3, 9] feedback.

In recommender systems that utilize matrix factorization, most optimize an objective function. In the state of the art, full deterministic gradient (FG) and stochastic gradient (SG) are the two main gradient methods for optimization. All of the recommender systems that we cite above utilize either full deterministic gradient, or stochastic gradient.

Unfortunately, both full deterministic gradient and stochastic gradient have pitfalls when it comes to prototyping recommender systems. Full deterministic gradient can offer high quality optimizations. However, FG is slow because at each iteration of optimization, FG has to sample through all the entries in the dataset. Stochastic gradient is relatively fast; its iteration cost is low because each iteration of SG sample only one or a few entries. However, the trade-off with stochastic gradient is that it often provides low quality optimizations. By chance, stochastic gradient may eventually yield a good quality optimization. If it ever happens, it is after a tremendous number of iterations. Thus stochastic gradient is also slow in terms of yielding a good quality optimization within a reasonable amount of time.

High quality optimizations within a short amount of time is important when building recommender systems. The first reason is that data scientists often have to run repeated experiments: e.g. with different objective functions, different metrics, different datasets, and different optimization parameters. The high level goal to run multiple experiments is that, through experimentation and comparing results of multiple trials, data scientists can ultimately get a sufficiently good mix of objective function and hyper parameters for fitting a dataset. The second reason is that product life cycles are shortening in the age of agile software engineering. Thus data scientists are facing or will ultimately face the challenge of running more experiments and producing high quality results with less time.

In this paper, we study the challenge from the perspective of convex-optimization. We propose and hypothesize using the stochastic average gradient (SAG) method $[6,\ 5]$ as a viable alternative to using FG and SG during the prototyping process. SAG has the distinctive advantage that its optimization quality is proven to be much better than SG;

at the same time SAG's iteration cost is asymptotically as low as SG. However, applying and adapting SAG to matrix factorization is not trivial because SAG requires previously-computed gradients; and storing these gradients can lead to very high asymptotic space complexity. We explore the challenge with space-complexity, and resolve it by proposing a re-computation approach (SAG-RE) that re-computes the previously-computed gradients on-the-fly, on-demand. SAG-RE preserves the fast convergence rate and low iteration cost of SAG. Moreover, the asymptotic space complexity of SAG-RE is as compact as memory-less gradient methods such as FG and SG.

To the best of our knowledge, we are the first to

- Identify pitfalls associated with using full deterministic gradient and stochastic gradient when data-scientists prototype model-based recommender systems.
- Propose Stochastic Average Gradient (SAG) as a viable alternative for yielding higher quality optimizations while enjoying a low iteration cost.
- Extend SAG into SAG-RE for matrix factorization, resolve the space complexity challenge in adapting SAG from the domain of large-scale supervised-machine-learning into the domain of prototyping recommender algorithms.
- Prove in theory, that SAG-RE has a convergence rate as fast as the original SAG; SAG-RE has asymptotic time complexity as efficient as any gradient method with the lowest iteration cost, and SAG-RE has asymptotic space complexity as compact as any memoryless gradient method.
- Extensively evaluate and compare SAG-RE with FG and SG across multiple RecSys objective functions and diverse datasets.
- Demonstrate in practice that, even without any optimization or fine-tuning on the implementation, SAG-RE still yields the best optimization within the shortest time despite the additional time of re-computation, and that SAG-RE uses memory at a level similar to full deterministic gradient and stochastic gradient, both of which are memory-less.
- Provide follow-up evidence that both full deterministic gradient and stochastic gradient takes much longer to reach a quality of optimization similar to SAG-RE.

2. BACKGROUND AND TERMINOLOGY

To motivate our paper and the space complexity challenge, we first introduce the background and the terminology that we use.

Matrix Factorization. Model-based recommender systems approximate the *user-item* matrix A through the dot-product of the *user-matrix* U and the *item-matrix* $V: \hat{A} = U * V$.

The user-item matrix A is a nRows-by-nCols matrix. A can be sparse; thus we use N to indicate the number of non-zero entries in A.

The approximation matrix \hat{A} also has nRows rows, and nCols columns. \hat{A} is not a sparse matrix. The goal of model-based recommendation is to use the non-zero entries to approximate the missing entries in A. When multiplying U and V, the latent dimensions nDims cancels-out in the dot product. This is why the approximation matrix has identical dimensions as the original user-item matrix.

The user matrix U is nRows-by-nDims: U has nRows rows, and nDims columns. nDims is the number of latent dimensions. The item matrix V is nDims-by-nCols.

Optimizing an Objective Function. The goal of matrix factorization is to find the best U and the best V whose dot product optimizes an objective function:

$$\arg\min(\underset{U,V}{\text{or arg max}}) \left[f(U,V) = \sum_{i=1}^{nRows} \sum_{j=1}^{nCols} f(\bar{u}_i, \bar{v}_j) \right]$$
(1)

When we take the gradient of the objective function with respect to a row in the *user* matrix U (e.g. \bar{u}_i), we sum up the gradient of all the entries in \hat{A} that belong to the same row \bar{u}_i .

$$\frac{\mathrm{d}f(U,V)}{\mathrm{d}\bar{u}_i} = \sum_{i=1}^{nCols} \frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{u}_i}$$
(2)

Similarly, when we take the gradient with respect to a column of V (e.g. \bar{v}_j), we sum up the gradients across different rows that belong to the same column:

$$\frac{\mathrm{d}f(U,V)}{\mathrm{d}\bar{v}_j} = \sum_{i=1}^{nRows} \frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{v}_j}$$
(3)

Both $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{u}_i}$ and $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{v}_j}$ are vectors of length nDims, the number of latent dimensions. Specifically, $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{u}_i}$ is a 1-by-nDims row vector; $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{v}_j}$ is a nDims-by-1 column vector. Similarly, the summed-up gradient $\frac{\mathrm{d}f(U,V)}{\mathrm{d}\bar{u}_i}$ is a row vector, and $\frac{\mathrm{d}f(U,V)}{\mathrm{d}\bar{v}_j}$ is a column vector, of length nDims.

In SAG, storing only the summed-up gradients is not sufficient for matrix factorization. The reason is that, each iteration of SAG requires the fine-grain gradients of individual entries (e.g. $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{u}_i}$ and $\frac{\mathrm{d}f(\bar{u}_i,\bar{v}_j)}{\mathrm{d}\bar{v}_j}$) that we previously sampled at an iteration before t. As we will prove, when directly applied to matrix factorization without using our SAG-RE approach, SAG will have a asymptotic space complexity of $\theta(nDims*(min(M,N)+nRows+nCols))$. M is the number of distinct entries that we have previously sampled. At any iteration t,

$$M \propto \sum_{l=1}^{t} B_l \tag{4}$$

 B_r is the batch size at ieration l; $l \leq t$. Usually the batch size B is constant for all iterations; then M is proportional to and is less than or equal to B * t.

Here, we want to point out that SAG-RE preserves the low asymptotic time complexity as SAG; and SAG-RE reduces asymptotic space complexity to $\theta(N+nDims*(nRows+nCols))$. We will prove that this asymptotic space complexity is as compact as any memory-less approach.

Gradient Methods in Matrix Factorization. Gradient methods are iterative methods of optimization. When we increase the number of iterations, we expect the quality of optimization to also increase over time. At each iteration, gradient methods sample a batch of B entries, calculate the gradients of these entries, and use the calculated gradients to update U and V for the next iteration:

$$U^{t+1} = U^t + \frac{\alpha^t}{B} \left(\sum_{b=1}^B \frac{\mathrm{d}f(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j})}{\mathrm{d}\bar{u}_{entry(b).i}} \right)$$
(5)

$$V^{t+1} = V^t + \frac{\alpha^t}{B} \left(\sum_{b=1}^B \frac{\mathrm{d}f(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j})}{\mathrm{d}\bar{v}_{entry(b).j}} \right)$$
(6)

At iteration t, U^t is the current approximation of U. We use the gradients of the sampled batch of entries to update U^t into U^{t+1} for iteration t+1.

 α^t is the *learning-rate* or *step-size*, at iteration t. When the goal of our optimization is to maximize an objective function, we apply *gradient-ascent* on U and V; thus we set $\alpha^t > 0$. When we try to minimize an objective function, we apply *gradient-descent* and set $\alpha^t < 0$.

entry(b) is the b-th entry in our batch of samples. entry(b).i is the row number of the entry; entry(b).j is the column number of the entry sampled from A.

Full deterministic gradient (FG) takes all N samples at each iteration; B=N in FG. Stochastic gradient (SG) takes only one or a few samples per iteration: B is usually a constant much less than N.

Stochastic Average Gradient. Stochastic Average Gradient (SAG) requires a memory of previously-computed gradients: e.g. \bar{m}_U^t and \bar{m}_V^t for matrix factorization. Each iteration of SAG uses a sampled batch of entries to update the memory. After the update, SAG then applies the updated memory \bar{m}_U^{t+1} and \bar{m}_V^{t+1} respectively on calculating U^{t+1} and V^{t+1} :

$$\bar{m}_{entry(b).i}^{t+1} = \frac{\mathrm{d}f(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j})}{\mathrm{d}\bar{u}_{entry(b).i}} \tag{7}$$

$$\bar{m}_{U}^{t+1} = \bar{m}_{U}^{t} + \sum_{b=1}^{B} \left[\bar{m}_{entry(b).i}^{t+1} - \bar{m}_{entry(b).i}^{t} \right]$$
 (8)

$$U^{t+1} = U^t + \frac{\alpha^t}{M} \left(\bar{m}_U^{t+1} \right) \tag{9}$$

$$\bar{m}_{entry(b).j}^{t+1} = \frac{\mathrm{d}f(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j})}{\mathrm{d}\bar{v}_{entry(b).j}} \tag{10}$$

$$\bar{m}_{V}^{t+1} = \bar{m}_{V}^{t} + \sum_{b=1}^{B} \left[\bar{m}_{entry(b),j}^{t+1} - \bar{m}_{entry(b),j}^{t} \right]$$
(11)

$$V^{t+1} = V^t + \frac{\alpha^t}{M} \left(\bar{m}_V^{t+1} \right)$$
 (12)

 $\bar{m}_{entry(b),i}^t$ and $\bar{m}_{entry(b),j}^t$ are the fine-grain gradients of individual matrix entries that were previously sampled.

 $\bar{m}^t_{entry(b).i}$ is a 1-by-nRows row vector; $\bar{m}^t_{entry(b).j}$ is a nCols-by-1 column vector.

 \bar{m}_U^t is a nRows-by-nDims matrix, because \bar{m}_U^t aggregates the gradients of all rows in the user matrix U. Similarly, \bar{m}_U^t is a nDims-by-nCols matrix.

We apply SAG into matrix factorization for two reasons. First, SAG has iteration cost as low as stochastic gradient (SG). Second, SAG's convergence rate is faster than SG, and sometimes as fast as full deterministic gradient (FG).

Convergence rate, Iteration cost, and Prototyping recommender systems. At a high level, the ideal combination of a fast convergence rate and a low iteration cost implies a better optimization in a shorter amount of time when data-scientists prototype model-based recommender systems. An intuition behind gradient methods is that, at least for objective functions that are convex, the gradients

guide the updates of U^t and V^t towards the direction of optimization. Convergence rate measures how many iterations a gradient method is expected to take towards reach a quality of optimization similar to FG. Iteration cost measures how many entries we sample per iteration.

Full deterministic gradient has the best possible convergence rate because each iteration of FG samples all N entries in the dataset. However, while FG is guaranteed to take a less number of iterations than SG to reach optimization, sampling all N entries per iteration slows down FG overall because the optimization process would still take many iterations. Depending on the mathematical properties of the objective function, stochastic gradient often has much slower convergence rates than FG because SG samples only one or a few random entries per iteration. Therefore, while SG has the lowest possible $\theta(1)$ iteration cost, overall SG is still slow because SG would take many more iterations to reach optimization.

SAG speeds-up the convergence rate by reusing the gradients of past samples. Reusing past gradients enables SAG to sample $\theta(1)$ entries per iteration and to achieve the lowest possible iteration cost. Our evaluation illustrates that SAG gives a better optimization with less time than FG and SG. In this paper, we minimize the drawbacks or costs of using SAG in matrix factorization while preserving SAG's benefits.

3. CHALLENGE

As equations 8 and 11 illustrate, updating \bar{m}_U^{t+1} and \bar{m}_V^{t+1} requires $\bar{m}_{entry(b).i}^t$ and $\bar{m}_{entry(b).j}^t$. $\bar{m}_{entry(b).i}^t$ and $\bar{m}_{entry(b).j}^t$ are the fine-grained gradients of an individual entry entry(b) from the last time (or the most recent time) that entry(b) was sampled.

When applying SAG into matrix factorization, a major challenge is to make these fine-grain gradients available: $\bar{m}_{entry(b).i}^t$ from equation 8, and $\bar{m}_{entry(b).j}^t$ from equation 11

A naïve approach is to store all these fine-grain graidents. As we shall prove, the naïve approach is undesirable because storing all these gradients would take up a lot of space.

Theorem 1. The total asymptotic space complexity is $\theta(nDims*(min(M,N)+nRows+nCols))$ for the naïve approach of storing the fine-grain gradients of all entries that we had previously sampled.

PROOF. For each individual entry, the amount of space required is 2*nDims: the gradient with respect to row \bar{u}_i $(\bar{m}_{entry(b).i}^t)$ is a 1-by-nDims row vector; the gradient with respect to column \bar{v}_j $(\bar{m}_{entry(b).j}^t)$ is a nDims-by-1 column vector.

When we store the fine-grain gradients of all previously-sampled entries, the amount of space required becomes M * 2*nDims. Recalling from the background section, M is the number of distinct entries that we previously sampled.

As shown in equations 8 and 11, SAG requires only the most recent gradient of each previously-sampled entry. Thus for each entry, we store a max of only one set of gradients $(\bar{m}^t_{entry(b),i}$ and $\bar{m}^t_{entry(b),j})$. The total amount of space required becomes min(M,N)*2*nDims.

Now, according to equations 8 and 11, we must also store the aggregated gradients: \bar{m}_U^t and \bar{m}_V^t . \bar{m}_U^t takes nRows*nDims*pace; \bar{m}_V^t takes nDims*nCols* space. Thus the total amount of space that we use to store the aggregated

gradients is (nRows*nDims) + (nDims*nCols), which is equivalent to nDims*(nRows+nCols) after simplification.

Adding the fine-grain gradients and the aggregated gradients together, the asymptotic space complexity becomes $\theta(nDims*(min(M,N)+nRows+nCols))$ after ignoring the constants. \square

No guarantee that min(M,N) is small. If we can guarantee that min(M,N) is small, or that min(M,N) is asymptotically not larger than nRows or nCols, then the effective asymptotic space-complexity becomes $\theta(nDims*(nRows+nCols))$, which is the most compact anyone can possibly get. Unfortunately, we shall prove that there is no such guarantee

First, we explore what the best possible asymptotical spacecomplexity can be in matrix factorization.

Theorem 2. $\Omega(N+nDims*(nRows+nCols))$ is the lower-bound asymptotic space-complexity in matrix factorization.

PROOF. Matrix factorization is to approximate a matrix A (e.g. the user-item matrix) through the dot product of two matrices U (e.g. the user matrix) and V (e.g. the item matrix). A has N non-zero entries. U is a nRows-by nDims matrix; V is a nDims-by-nCols matrix. In each iteration of convex optimization, we must update U and V, and use an objective function to compare our approximation to the ground-truth matrix A. Therefore, any matrix factorization algorithm would have an asymptotic space-complexity of at least $\Omega(N+nDims*(nRows+nCols))$. \square

If we can guarantee that min(M,N) is asymptotically not larger than nRows or nCols, then we can prove that the naive approach has already achieved the best possible asymptotic space-complexity, and that our challenge is irrelevant. However, we shall prove that such guarantee does not exist.

Theorem 3. There is no guarantee that min(M, N) is asymptotically not larger than nRows or nCols.

PROOF. N is the number of non-zero entries in the matrix A. Unless there is, or unless we are restricted to an upper-bound of matrix density, then N must have an uppder-bound of O(nRows*nCols) space.

M is the number of distinct entries that we previously sampled. According to equation 4, M depends on the batch size at each iteration B_l , and the number of iterations previously done t-1. Usually, the batch size is a constant B. Thus the lower bound of M most likely depends on the lower bound of t. However, the lower bound of t depends on the convergence rate, and the tolerance of error ϵ . For example, if the convergence rate is exponential (e.g. $O(p^t)$), then the lower bound of t is $\Omega(\log(\frac{1}{\epsilon}))$. Therefore, the lower bound of M does not depend on N, nRows or nCols. Given a dataset, the only way to enforce $M \leq N$ is to either tolerate a high error, or to find a combination of objective function and gradient method that yields the fastest convergence rate possible. The asymptotic space-complexity of SAG-RE is compact enough so that SAG-RE does not enforce data-scientists to tolerate a high error. Given any objective function, the convergence rate of SAG [6, 5] is always faster than stochastic gradient and is sometimes as fast as the fastest full deterministic gradient. SAG-RE preserves the convergence rate of SAG. \square

Using chain rule worsens space-complexity in matrix factorization. In supervised machine-learning, we can

use the chain-rule in differential-calculus to reduce space-complexity. Unfortunately, applying the chain-rule in matrix-factorization would result in a space-complexity larger than the naïve approach.

In supervised machine-learing, the goal is to compute the best-fit column-vector $\bar{\omega}$ that optimizes an objective function, which can be written as

$$\arg\min(\underset{\bar{\omega}}{\operatorname{arg\,max}}) \left[F(\hat{y} = X * \bar{\omega}) = \sum_{i=1}^{N} f_i(\hat{y}_i = \bar{x}_i * \bar{\omega}) \right]$$
(13)

X is a N-by-d matrix: N is the number of samples, and d is the number of features. \bar{x}_i is the 1-by-d row vector representing i-th sample. $\bar{\omega}$ is the d-by-1 column vector of features that we are trying to learn from X. We can use the chain-rule and re-write the gradient of $\bar{\omega}$ with respect to f_i :

$$\frac{\mathrm{d}f_i}{\mathrm{d}\bar{\omega}} = \left(\frac{\mathrm{d}f_i}{\mathrm{d}\hat{y}_i}\right) \frac{\mathrm{d}\hat{y}_i}{\mathrm{d}\bar{\omega}} = (\bar{x}_i)' \left(\frac{\mathrm{d}f_i}{\mathrm{d}\hat{y}_i}\right) \tag{14}$$

Originally, using the näive approach of SAG results in $\theta(min(M,N)*d+d)$ space. The reason is that $\frac{\mathrm{d}f_i}{\mathrm{d}\bar{\omega}}$ is a d-by-1 column vector; and the näive approach stores min(M,N) copies of them. The memory gradient $\bar{m}_{\bar{\omega}}$ is a d-by-1 column vector and thus takes $\theta(d)$ space.

The dot-product $\hat{y}_i = (\bar{x}_i * \bar{\omega})$ is a 1-by-1 scalar. Consequently, $\frac{\mathrm{d}f_i}{\mathrm{d}\hat{y}_i}$ is also a 1-by-1 scalar. From equation 13, $\frac{\mathrm{d}\hat{y}_i}{\mathrm{d}\bar{\omega}}$ = $(\bar{x}_i)'$. Therefore, we can apply the chain rule and reduce space-complexity to $\theta(\min(M,N)+d)$, because we can use the vector \bar{x}_i to re-compute $\frac{\mathrm{d}f_i}{\mathrm{d}\bar{\omega}}$ from the scalar $\frac{\mathrm{d}f_i}{\mathrm{d}\hat{y}_i}$.

Theorem 4. Applying the chain-rule for using SAG in matrix facotrization would result in $\theta(min(M, N) + nDims*(min(M, N) + nRows + nCols))$ space.

PROOF. In matrix factorization, $\hat{a}_{ij} = (\bar{u}_i * \bar{v}_j)$ is a 1-by-1 scalar. Therefore, we can rewrite the gradients as

$$\frac{\mathrm{d}f}{\mathrm{d}\bar{u}_i} = \left(\frac{\mathrm{d}f}{\mathrm{d}\hat{a}_{ij}}\right) \frac{\mathrm{d}\hat{a}_{ij}}{\mathrm{d}\bar{u}_i} = (\bar{v}_j)' \left(\frac{\mathrm{d}f}{\mathrm{d}\hat{a}_{ij}}\right) \tag{15}$$

$$\frac{\mathrm{d}f}{\mathrm{d}\bar{v}_j} = \left(\frac{\mathrm{d}f}{\mathrm{d}\hat{a}_{ij}}\right) \frac{\mathrm{d}\hat{a}_{ij}}{\mathrm{d}\bar{v}_j} = (\bar{u}_i)' \left(\frac{\mathrm{d}f}{\mathrm{d}\hat{a}_{ij}}\right) \tag{16}$$

 $\left(\frac{\mathrm{d}f}{\mathrm{d}\hat{a}_{ij}}\right)$ is a 1-by-1 scalar, and the chain-rule approach stores min(M,N) copies, occupying $\theta(min(M,N))$ space.

Unfortunately both U and V change over time in matrix factorization. When we apply the chain-rule, we cannot just use the current versions of \bar{u}_i and \bar{v}_j . We must use and thus must store the past versions of \bar{u}_i^l and \bar{v}_j^l at the last time l that the entry a_{ij} (in matrix A) was sampled. Both \bar{u}_i^l and \bar{v}_j^l are vectors of length nDims. Therefore, using the chain rule induces an additional (min(M,N)*2*nDims) space. When we include the memory of aggregated gradients \bar{m}_U and \bar{m}_V , the total space-complexity becomes larger than the naïve approach with $\theta(min(M,N)+nDims*(min(M,N)+nRows+nCols))$ space. The chain-rule approach yields space savings in supervised machine-learning because \bar{x}_i does not change over time; so there is no need to store past versions of \bar{x}_i . \square

4. APPROACH

Similar to the chain-rule approach, SAG-RE does not store and re-computes $\bar{m}^t_{entry(b).i}$ in equation 8 and $\bar{m}^t_{entry(b).j}$ in equation 11:

$$\bar{m}_{entry(b).i}^{t} = recomputed \frac{\mathrm{d}f(\bar{u}_{entry(b).i}^{s}, \bar{v}_{entry(b).j}^{s})}{\mathrm{d}\bar{u}_{entry(b).i}^{s}}$$
(17)

$$\bar{m}_{entry(b),j}^t = recomputed \frac{\mathrm{d}f(\bar{u}_{entry(b),i}^s, \bar{v}_{entry(b),j}^s)}{\mathrm{d}\bar{u}_{entry(b),j}^s}$$
(18)

The chain-rule approach is undesirable because it must store min(M,N) different copies of past versions of $\bar{m}_{entry(b).i}^t$ and $\bar{m}_{entry(b).j}^t$. There are two problems. First, each entry can come from a different iteration; or different entries can come from different iterations. Second, the same entry may get sampled more than once at two or more different iterations.

To save space, we must store as few copies of $\bar{m}_{entry(b).i}^t$ and $\bar{m}_{entry(b).j}^t$ as possible. SAG-RE resolves the two problems above with two steps. First, SAG-RE predicts ahead the entires that we are going to sample. Second, SAG-RE performs a full deterministic gradient FG just before SAG-RE re-samples the same entry.

At the iteration that SAG-RE performs a full deterministic gradient, we call it iteration s, SAG-RE stores 4 matrices:

- the actual user matrix U at iteration s: U^s
- the actual item matrix V at iteration s: V^s
- aggregated memory gradient for user matrix U: \bar{m}_U^s
- aggregated memory gradient for item matrix $V: \bar{m}_V^s$

We should distinguish that U^s and V^s are stored just before SAG-RE performs a full deterministic gradient at iteration s. The significance is that we will use U^s and V^s to re-compute the fine-grain memory gradients at future iterations t > s.

 \bar{m}_{N}^{s} and \bar{m}_{N}^{s} are the direct outcome results of the full deterministic gradient. The reason is that FG samples all N entries and thus resets every possible fine-grain gradient in memory. Thus we store \bar{m}_{U}^{s} and \bar{m}_{V}^{s} after SAG-RE performs an iteration of FG.

At the iterations in between SAG-RE performs two FG's, SAG-RE performs iterations of ordinary SAG. When SAG-RE performs ordinary SAG, SAG-RE computes but does **not** store the latest version of fine-grain gradients of individual entries:

$$\bar{m}_{entry(b).i}^{t+1} = \frac{\mathrm{d}f\big(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j}\big)}{\mathrm{d}\bar{u}_{entry(b).i}} \ in \ equation \ 7$$

$$\bar{m}_{entry(b).j}^{t+1} = \frac{\mathrm{d}f(\bar{u}_{entry(b).i}, \bar{v}_{entry(b).j})}{\mathrm{d}\bar{v}_{entry(b).j}} \ in \ equation \ 10$$

Instead, SAG-RE simply updates \bar{m}_U^s and \bar{m}_V^s with the newly computed fine-grain gradients, as equation 8 and equation 11 show.

Not storing the newly-computed fine-grain gradients saves $\theta(min(M,N)*nDims)$ space. namely $\bar{m}_{entry(b).i}^{t+1}$ from equation 7, and $\bar{m}_{entry(b).j}^{t+1}$ from equation 10.

The two steps together ensure that, the different entries that we are going to sample are distinct before we perform a full deterministic gradient. The significance of having distinct entries is that, we can re-compute all fine-grain gradients of individual entries (e.g. $\bar{m}_{entry(b),i}^t$ in equation 8 and $\bar{m}_{entry(b),j}^t$ in equation 11) from a single copy of the user matrix U^s and item matrix V^s .

Theorem 5. SAG-RE has convergence rate at least as fast as SAG.

Proof. \square

Theorem 6. SAG-RE has $\theta(1)$ asymptotic time-complexity and is as efficient as both SAG and stochastic gradient.

Proof. SAG-re achieves the lowest possible asymptotic iteration cost. $\hfill \Box$

Theorem 7. SAG-RE has $\theta(N + min(M, N) + nDims * (nRows + nCols))$ asymptotic space-complexity and is as compact as any memory-less gradient method.

Proof. Indeed, SAG-RE achieves the best possible asymptotic space-complexity ($Theorem\ 2$). \Box

5. FUTURE WORK & CONCLUSION

This paper is the first in the series of our study on data scientists prototyping model-based recommender systems. We explored the convex-optimization perspective of the problem: we propose Stochastic Average Gradient as a viable alternative to Full Deterministic gradient and Stochastic gradient. By taking advantage of SAG's fast convergence rate and low iteration cost, we aim to enable data-scientists run more experiments and produce high quality results with less time. In theory, we proved that our extension and adaptation of SAG preserves the fast convergence rate as the original SAG. Furthermore, SAG-RE has asymptotic time complexity as efficient as gradient methods with the lowest itreation cost, and asymptotic space complexity as compact as any memory-less gradient methods. In practice, through extensive evaluation we demonstrated that, even without any fine-tuning or optimization of the implementation, SAG-RE still outperforms both full deterministic gradient and stochastic gradient in terms of reaching the best quality optimization within the same amount of time. Following up, we provided evidence that full deterministic gradient and stochastic gradient would take much longer to reach a quality of optimization similar to SAG-RE.

Currently we are extending SAG-RE in two directions. Both directions relate to running an iteration of full deterministic gradient in SAG-RE. First, we are investigating if it is beneficial to run an iteration of full deterministic gradient more often. In our experiments, we observed that both SG and SAG may converge early; the optimization may get stuck at a local sub-optimum for a long number of iterations. Thus we are exploring if an iteration of full deterministic gradient would get the optimization back on track in case SAG-RE gets stuck. Secondly, we aim to investigate how well SAG-RE would perform in the production environment, and in distributed systems potentially running in parallel, because running full deterministic gradient even once can be prohibitive for full-scale datasets with millions to billions of non-zero entries.

In the future, we also aim to complete our ongoing work on the metrics perspective and on the software engineering perspective. Given a dataset, the quality of a recommender system is often evaluated in various metrics: e.g. precision, recall, area under curve, reciprocal rank, NDCG, and variants of the above such as top-K precision and top-K hit rate. Many papers in the literature claim their objective function is better by illustrating that their objective function performs in some of these metrics better than other objective functions. Therefore, in the metrics perspective, we are exploring and investigating which factors are more relevant and important towards scoring high in the various metrics: is it the objective function, the method for

convex-optimization such as SAG, other fine-tuning mechanisms such as bootstrapping, or the hyper-parameters that we use in convex-optimization. All of these factors can be dataset-specific. Indeed, our inherent assumption in this paper is that a better quality optimization yields better recommender systems. In the future, we would like to explore if there are other factors that are more worthwhile than a fast convergence rate or a low iteration cost towards better recommender systems.

In the software engineering perspective, we study how to increase the productivity of data scientists. At this point, we are designing and developing a mix-n-match or plug-n-play framework that enables data scientists in a least effort way, to very rapidly prototype and experiment many different combinations of objective functions, datasets, gradient methods, hyper parameters and evaluation metrics.

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