Stochastic Gradients for Large-Scale Tensor Decomposition

Tamara G. Kolda† and David Hong‡

Abstract. Tensor decomposition is a well-known tool for multiway data analysis. This work proposes using stochastic gradients for efficient generalized canonical polyadic (GCP) tensor decomposition of large-scale tensors. GCP tensor decomposition is a recently proposed version of tensor decomposition that allows for a variety of loss functions such as logistic loss for binary data or Huber loss for robust estimation. The stochastic gradient is formed from randomly sampled elements of the tensor. For dense tensors, we simply use uniform sampling. For sparse tensors, we propose two types of stratified sampling that give precedence to sampling nonzeros. Numerical results demonstrate the advantages of the proposed approach and its scalability to large-scale problems.

Key words. tensor decomposition, stochastic gradients, stochastic optimization, stratified sampling

1. Introduction. Tensor decomposition is the higher-order analogue of matrix decomposition and is becoming an everyday tool for data analysis. It can be used for unsupervised learning, dimension reduction, tensor completion, feature extraction in supervised machine learning, data visualization, and more. For a given $d$-way data tensor $X$ of size $n_1 \times n_2 \times \cdots \times n_d$, the goal is to find a low-rank approximation $M$, i.e.,

\begin{equation}
X \approx M \quad \text{where} \quad M = \sum_{j=1}^{r} a_1(:,j) \odot a_2(:,j) \odot \cdots \odot a_d(:,j).
\end{equation}

The low-rank structure of $M$ reveals patterns within the data, as defined by the factor matrices. The $k$th factor matrix of size $n_k \times r$ is denoted $A_k$. The $j$th factor (column) in mode $k$ is denoted $a_k(:,j)$. Each component of $M$ is a $d$-way outer product (denoted by $\odot$) of $d$ factors, forming a rank-one tensor. We say $\text{rank}(M) \leq r$ because $M$ can be written as the sum of $r$ rank-one tensors.

The standard canonical polyadic or CANDECOMP/PARAFAC (CP) tensor decomposition seeks the best low-rank approximation with respect to sum of squared errors [7, 15]. The generalized CP (GCP) tensor decomposition is a novel approach that allows for an arbitrary elementwise loss function that is summed across all tensor entries [18]; i.e., the user provides a scalar loss function $f : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ resulting in the optimization problem

\begin{equation}
\text{minimize} \quad F(X,M) \equiv \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} f(x_{i_1 \ldots i_d}, m_{i_1 \ldots i_d}) \quad \text{subject to} \quad \text{rank}(M) \leq r.
\end{equation}
GCP is useful in situations where non-standard choices of the scalar loss function $f$ may be appropriate, such as logistic loss, $f(x, m) = \log(m + 1) - x \log(m)$, for binary-valued data tensors with entries in $\{0, 1\}$ or Gamma loss, $f(x, m) = x/m + \log(m)$, for positive data tensors. Standard CP tensor decomposition corresponds to $f(x, m) = (x - m)^2$, and Poisson tensor decomposition [45, 9] to $f(x, m) = m - x \log m$.

In this paper, we consider the problem of fitting GCP for large-scale tensors. The total size of $X$ is $n^d$ where we define $n = \left(\prod_{k=1}^d n_k\right)^{1/d}$. We assume $r \ll n^d$. The GCP gradient requires $O(rn^d)$ flops as well as $n^d$ storage for intermediate computations. The computational and storage costs of computing the gradient may thus be prohibitive, especially if $X$ is sparse. Our solution is a flexible framework for stochastic gradient computation for GCP, which can be used with stochastic gradient descent or popular variants such as ADAM [21]. The stochastic gradient uses $s \ll n^d$ tensor entries, reducing the gradient cost to $O(sr)$ flops and $O(s)$ intermediate storage.

Past work on stochastic approaches for tensor decomposition has focused primarily on standard CP. Much of the work has focused on the recommender systems context, sampling only nonzeros and ignoring zero entries in the belief that they represent missing data. Other work has focused on the streaming setting where one hyperslice of a tensor is added at each step. To the best of our knowledge, ours is the first work to compute a stochastic gradient of the complete tensor. We survey related work in section 2 and provide notation and background in section 3.

Like standard CP, the GCP gradient involves a sequence of $d$ matricized-tensor times Khatri-Rao product (MTTKRP) computations with a dense tensor of size $n^d$. Our stochastic framework replaces the dense tensor with a (stochastic) sparse tensor that equals the dense tensor in expectation. The resulting MTTKRPs requires work proportional to the number of nonzero elements in the stochastic sparse tensor. A distinguishing feature of our framework is stratified sampling. If $X$ is sparse, uniform sampling of the indices rarely samples nonzeros even though they are extremely important to finding an appropriate minimizer. Stratified sampling explicitly samples nonzeros, which can reduce the variance of the stochastic gradient, thereby accelerating convergence. Since stratified sampling can itself be expensive, we also introduce a semi-stratified sampling approach to further improve efficiency. These methods are discussed in section 4.

We present computational experiments on both artificial and real-world problems in section 5, demonstrating the reliability and efficiency of using stochastic gradients. Experimentally, the number of gradient samples is comparable to the sum of the tensor dimensions, i.e., $d\bar{n}$. For dense problems, stochastic optimization can be an order of magnitude faster than non-stochastic optimization. For sparse problems, stochastic optimization enables computing GCP for sparse tensors that would otherwise be intractable. Additionally, stratified and semi-stratified sampling of zeros and nonzeros have a clear advantage over uniform sampling in this setting. We also compare to CP-APR [9, 14] on real-world Chicago crime data. In our experiments, the stochastic methods are faster and find equivalent solutions.

---

1Both standard and Poisson CP have special structure that allows the gradient to be formed implicitly, as described in Appendix A.
2. Related Work. To the best of our knowledge, ours is the first work to consider SGD for a complete tensor. However, SGD has been applied in the recommender systems and streaming settings. Additionally, there is related work in tensor sketching.

Randomization of the least squares problems within CP-ALS. Alternating least squares (CP-ALS) is a primary method for fitting the CP model, and there are several randomized variations. Vervilet and De Lathauwer [43] sample a complete sub-block of the tensor at each outer iteration and base the updates on the sub-block. Battaglino, Ballard, and Kolda [5] propose CP-ARLS (alternating randomized least squares) using a sketched version of the least squares problem that in turn relies on a sampled Khatri-Rao product (SKRP). For sparse tensors, Cheng et al. [8] propose a sparse ALS method (SPALS) based on sampling from the Khatri-Rao product using leverage scores.

Streaming tensors. In the streaming context, one dimension is typically treated as time with a new slice arriving at each time step. Mardani, Mateos, and Giannakis [29] use a form of SGD to update the factorization of a third-order time-evolving tensor. Maehara, Hayashi, and Kawarabayashi [28] factorize tensors that arise as sums of streaming tensor samples. Similar to our approach, they apply SGD on the samples to update the factorization of the sum. However, they primarily consider applications where a stream of samples is already given, whereas a focus of our work is on how to sample complete tensors effectively. There are also other works, not based on SGD. Nion and Sidiropoulos [32] propose an online updating scheme for third order tensors in the context of subspace tracking, extended to arbitrary order and other applications by Zhou et al. [47]. Ma, Yang, and Wang [27] develop a streaming version of CP-ARLS [5] using the SKRP. Gujral, Pasricha, and Papalexakis [13] develop a sampling-based batch incremental tensor decomposition (SamBaTen).

Recommender systems. In recommender systems, matrix factorization is used to predict which products are most likely to be interesting to a consumer. This is generally a problem with missing data [24] where zeros represent missing values and are ignored in factorization; nevertheless, many of the ideas are similar. In this context, Gemulla et al. [12] and Zhuang et al. [48] consider the problem of high-performance large-scale matrix factorization with SGD, and Smith, Park and Karypis [36] consider the tensor completion setting. The main differences with our work are that we both consider the tensor case and explicitly include zeros (even if they are stored implicitly).

Other work. For the special case of orthogonal CP decomposition of symmetric tensors, Song, Woodruff, and Zhang [38] sketch the input tensor and provide provable guarantees for a sublinear algorithm. Wang et al. [44] propose a sketching method in a specific symmetric scenario where the tensor itself is already available in factored form (but with a larger rank). Ge et al. [11] consider SGD for symmetric tensor decomposition and argue that it finds a local minimizer rather than a saddle point. Acar et al. [1] show that, for dense tensors, it is heuristically possible to recover a full tensor decomposition with only a sketch of the data based on uniformly sampled elements; however, they did not evaluate whether or not their tensors were incoherent.

3. Notation and background. We provide some brief context for the discussions in the remainder of the paper.
3.1. **Probability notation and sampling background.** In this paper, we use a tilde to indicate random variables and instances thereof, e.g., \( \tilde{x} \). The expected value is denoted \( \mathbb{E}[\tilde{x}] \). If \( \tilde{x} \in \{ v_1, v_2, \ldots, v_m \} \) is a discrete random variable that samples \( v_i \) with probability \( p_i \), then

\[
\mathbb{E}[\tilde{x}] \equiv \sum_{i=1}^{m} p_i \cdot v_i.
\]

The random sample is **uniform** if each element has equal probability; i.e., \( p_i = 1/m \) for \( i = 1, 2, \ldots, m \). Sampling with replacement means that the same \( v_i \) can be sampled more than once, i.e., that subsequent samples are independent identically distributed (i.i.d.) draws. If we let \( \tilde{s}_i \) denote the number of times that \( v_i \) is sampled from a uniform distribution over \( s \) draws with replacement, then

\[
\mathbb{E}[\tilde{s}_i] = \frac{s}{m},
\]

since there are \( s \) independent draws and each draw selects sample \( v_i \) with probability \( 1/m \).

3.2. **Tensor notation.** For a \( d \)-way data tensor \( X \) of size \( n_1 \times n_2 \times \cdots \times n_d \), we define

\[
n = \sqrt[d]{\prod_{k=1}^{d} n_k}
\]

and \( \bar{n} = \frac{1}{d} \sum_{k=1}^{d} n_k \).

These quantities provide convenient measures of how large the tensor is. We treat \( d \) as constant for big-O notation. Throughout, we let \( i = (i_1, i_2, \ldots, i_d) \) where \( i_k \in \{1, 2, \ldots, n_k\} \) and refer to this as a **multi-index** or simply an **index**. Every multi-index has a corresponding linear index between 1 and \( n^d \) [22]. We let \( \Omega \) denote the set of all tensor indices, so necessarily \( |\Omega| = n^d \). Excepting the discussion of missing data in subsection 4.4, we assume all tensor entries are known. We let \( \text{nnz}(X) \) denote the number of nonzeros in \( X \) and say that \( X \) is **sparse** if \( \text{nnz}(X) \ll n^d \).

If \( X \) is dense, then the storage is \( n^d \). If \( X \) is sparse, then only the nonzeros and their indices are stored, so the storage is \( (d+1) \cdot \text{nnz}(X) \) using coordinate format [2]. The total storage for a rank-\( r \) approximation \( M \) as in (1.1) is the storage for the factor matrices, i.e., \( \bar{n}dr \), and is usually significantly less than the storage for \( X \).

3.3. **MTTKRP background.** Given a tensor \( Y \) of size \( n_1 \times n_2 \times \cdots \times n_d \) and factor matrices \( A_k \) (from a low-rank \( M \)) of size \( n_k \times r \) for \( k = 1, \ldots, d \), the MTTKRP in mode \( k \) is

\[
Y_{(k)} \left[ \underbrace{A_d \odot \cdots \odot A_{k+1} \odot A_{k-1} \odot \cdots \odot A_1}_{Z_k} \right].
\]

The matrix \( Z_k \) is of size \( n^d/n_k \times r \) and is the Khatri-Rao product (denoted by \( \odot \)) of all the factor matrices except \( A_k \), and the matrix \( Y_{(k)} \) is of size \( n_k \times n^d/n_k \) and denotes the mode-\( k \) unfolding of \( Y \).

Much work has gone into efficient computation of MTTKRP. Bader and Kolda [2] consider both dense and sparse \( Y \) tensors, showing that the cost is \( O(rn^d) \) for dense \( Y \) and \( O(r \cdot \text{nnz}(Y)) \) for sparse \( Y \). Phan, Tichavsky, and Cichocki [33] propose methods to reuse partial
computations when computing the MTTKRP for all $d$ modes in sequence. Much recent work has focused on more efficient representations of sparse tensors and parallel MTTKRP computations [37, 20, 25, 34]. There is also continued work on improving the efficiency of dense MTTKRP calculations [16, 4].

4. Stochastic GCP Gradient. GCP tensor decomposition generalizes CP tensor decomposition, minimizing the GCP loss function in (1.2). From [18, Theorem 3], the GCP gradient is calculated via a sequence of MTTKRP computations. Key to this calculation is the elementwise partial gradient tensor $\mathbf{Y}$ that is the same size as $\mathbf{X}$ and defined as

\begin{equation}
y_i = \frac{\partial f}{\partial m}(x_i, m_i).
\end{equation}

That is, $\mathbf{Y}$ is the tensor of first derivatives of $f$ evaluated elementwise w.r.t. $\mathbf{X}$ and $\mathbf{M}$. The partial derivative, denoted $G_k$, of the objective function $F$ in (1.2) w.r.t. $\mathbf{A}_k$ is

\begin{equation}
G_k = \mathbf{Y}(k)\mathbf{Z}_k,
\end{equation}

where $\mathbf{Z}_k$ is the Khatri-Rao product defined in (3.1). The problem is that $\mathbf{Y}$ is dense even when $\mathbf{X}$ is sparse, which means that $\mathbf{Y}$ requires $n^d$ storage and the cost of computing MTTKRP for gradients $G_k$ is $O(rn^d)$. Such costs may be prohibitive. For instance, if $n = 1000$ and $d = 4$, then $\mathbf{Y}$ would require 8 TB of storage. There are a couple of special cases (see Appendix A) where dense computation can be avoided because $\mathbf{Y}$ is formed implicitly, notably for standard CP [2], but this is not the case for general loss functions and so motivates stochastic approaches.

We develop a stochastic gradient whose general form is

\begin{equation}
\mathbf{G}_k = \tilde{\mathbf{Y}}(k)\mathbf{Z}_k
\end{equation}

where $\mathbf{E}[\tilde{\mathbf{Y}}] = \mathbf{Y}$ and $\text{nnz}(\tilde{\mathbf{Y}}) \leq s \ll n^d$. By linearity of expectation, $\mathbf{E}[\tilde{\mathbf{Y}}] = \mathbf{Y}$ implies $\mathbf{E}[\tilde{\mathbf{G}}_k] = \mathbf{G}_k$. Requiring $\tilde{\mathbf{Y}}$ to be sparse unlocks efficient sparse computation of the MTTKRP. Consequently, storage for $\tilde{\mathbf{Y}}$ is $O(s)$ and the cost to compute the gradients is $O(rs)$, a reduction of roughly $n^d/s$ compared to computing the full gradient.

In the remainder of this section, we discuss the pros and cons of several different choices for $\tilde{\mathbf{Y}}$ based on uniform sampling, stratified sampling, and semi-stratified sampling.

4.1. Uniform Sampling. To create a random instance of $\tilde{\mathbf{Y}}$, we sample $s$ indices uniformly with replacement. The number of times that $i$ is sampled is denoted as $\tilde{s}_i$, so $\sum_{i \in \Omega} \tilde{s}_i = s$. Using this sampling strategy, in expectation we have

\begin{equation}
\mathbf{E}[\tilde{s}_i] = \frac{s}{n^d} \quad \text{for all} \quad i \in \Omega.
\end{equation}

Note that the $\tilde{s}_i$ values are not stored as a dense object but rather as just a list of the samples or in some other sparse data structure. We then define the stochastic tensor $\tilde{\mathbf{Y}}$ to be

\begin{equation}
\tilde{y}_i = \frac{n^d}{s} \cdot y_i \quad \text{for all} \quad i \in \Omega.
\end{equation}
The stochastic $\tilde{Y}$ is sparse because at most $s$ entries are nonzero (since at most $s$ values of $\tilde{s}_i$ are nonzero). Clearly $E[\tilde{Y}] = Y$ since

$$E[\tilde{y}_i] = E[\tilde{s}_i] \cdot \frac{n^d}{s} \cdot y_i = y_i \quad \text{for all } i \in \Omega.$$  

A similar argument applies for sampling without replacement, but there is no practical difference when $s \ll n^d$ and so we omit the discussion.

The most straightforward procedure to generate a random index $i$ is to generate $d$ random mode indices $i_k$ as follows:

$$i_k = \text{randi}(n_k) \quad \text{for } k \in \{1, 2, \ldots, d\}.$$  

Here, $\text{randi}(m)$ indicates selecting a random integer between 1 and $m$. This requires $d$ random numbers per random tensor index. Alternatively, we can generate a random linear index via $\text{randi}(n^d)$ and then convert it to a tensor index. Either way is $O(1)$ work (we treat $d$ as a constant). Generating $d$ separate entries prevents overflow if $n^d > 2^{64}$, i.e., the total number of entries in the tensor is more than the size of the largest integer. Clearly, this cannot be the case for a dense tensor (else it would not be even storable in memory), but it can be the case for a sparse tensor where only the nonzeros are stored.

The procedure is presented in Algorithm 4.1. The function $\text{MTTKRP}$ corresponds to (3.1), and this can be computed efficiently because specialized sparse implementations exist as discussed in subsection 3.3. The model entries $m_i$ and elementwise partial gradient tensor entries $y_i$ are only computed for the $s$ randomly selected indices. The most expensive operations are computing the model entries $m_i$ and the corresponding MTTKRP calculations. In the implementation, we are able to share some intermediate computations across these two steps.

Algorithm 4.1 Stochastic Gradient with Uniform Sampling

1: function $\text{StocGrad}(X, \{A_k\}, s)$
2: $\omega \leftarrow \prod_k n_k$ // $\omega =$ # entries in $X$
3: $\tilde{Y} \leftarrow 0$ // initialize $\tilde{Y}$ to all-zero sparse tensor
4: for $c = 1, 2, \ldots, s$ do  // loop to sample $s \ll \omega$ indices for $\tilde{Y}$
5: for $k = 1, 2, \ldots, d$ do $i_k \leftarrow \text{randi}(n_k)$, end  // sample random index $i \equiv (i_1, i_2, \ldots, i_d)$
6: $m_i \leftarrow \sum_{j=1}^{r} \prod_{k=1}^{d} a_k(i_k, j)$ // compute $m_i$ at sampled index
7: $\tilde{y}_i \leftarrow \tilde{y}_i + (\omega/s) \cdot g(x_i, m_i)$ // compute $\tilde{y}_i$ at sampled index, $g \equiv \partial f/\partial m$
8: end for
9: for $k = 1, 2, \ldots, d$, do $\tilde{G}_k \leftarrow \text{MTTKRP}(\tilde{Y}, A_k, k)$, end // use stochastic sparse $\tilde{Y}$ to compute $\tilde{G}_k$
10: return $\{\tilde{G}_k\}$
11: end function

4.2. Stratified Sampling. Uniform sampling may not be appropriate for sparse tensors since the nonzeros will rarely be sampled. We would need $s > n^d/\text{nnz}(X)$ samples to ensure an average of just one nonzero per sample. Intuitively, however, we expect nonzeros in a sparse tensor to be important to the factorization.

Theoretical support for explicitly sampling nonzeros exists, at least for some choices of loss function. In the context of SGD, Needall et al. [31] justify biased sampling toward functionals with higher Lipschitz smoothness constants to reduce the variance in the gradient...
estimate. In our case, this corresponds to choosing specific tensor entries whose corresponding elementwise loss function \( f_i \equiv f(x_i, m_i) \) has a higher Lipschitz smoothing constant for the fixed value of \( x_i \). Consider the case of Bernoulli tensor factorization which is GCP with \( f(x, m) = \log(m + 1) - x \log m \) where we assume \( x \in \{0, 1\} \). If \( x = 0 \), then \( \frac{\partial f}{\partial m}(m, 0) = 1/(m + 1) \) and so the Lipschitz smoothness constant is bounded as \( L \leq 1 \); conversely, if \( x \geq 1 \), then \( \frac{\partial f}{\partial m}(x, m) = -1/(m^2 + m) \), so the Lipschitz smoothness constant is unbounded as \( m \downarrow 0 \). Therefore, the nonzeros have higher Lipschitz smoothness constants and so should be sampled more often. Separately sampling zeros and nonzeros can help reduce the variance of the stochastic gradients.

Consider a generic partition of \( \Omega \) into \( p \) partitions \( \Omega_1, \Omega_2, \ldots, \Omega_p \). If we partition into zeros and nonzeros, then \( p = 2 \). Let \( s_\ell > 0 \) be the number of samples from partition \( \Omega_\ell \) so that the total number of samples is \( s = \sum_\ell s_\ell \). Within each partition, we sample uniformly with replacement. Therefore, the expectation of the number of times that index \( i \) is sampled depends on its partition and is given by

\[
E[\tilde{s}_i] = s_\ell \frac{|\Omega_\ell|}{|\Omega_\ell|} \quad \text{where} \quad i \in \Omega_\ell \quad \text{for all} \quad i \in \Omega.
\]

We then define the stochastic tensor \( \tilde{\mathbf{Y}} \) to be

\[
\tilde{y}_i = \tilde{s}_i \cdot \frac{|\Omega_\ell|}{s_\ell} \cdot y_i \quad \text{where} \quad i \in \Omega_\ell \quad \text{for all} \quad i \in \Omega.
\]

Once again, at most \( s \) entries of \( \tilde{\mathbf{Y}} \) are nonzero, and \( E[\tilde{\mathbf{Y}}] = \mathbf{Y} \) since

\[
E[\tilde{y}_i] = E[\tilde{s}_i] \cdot \frac{|\Omega_\ell|}{s_\ell} \cdot y_i = y_i \quad \text{for all} \quad i \in \Omega.
\]

Interestingly, the weight \( (|\Omega_\ell|/s_\ell) \) for index \( i \) is completely independent of the overall sample or tensor size — it depends only on the partition size and the number of samples for that partition.

The stratified sampled procedure for sparse tensors is presented in Algorithm 4.2. We assume that we will sample \( p \) nonzeros and \( q \) zeros. Sampling the \( p \) nonzeros is straightforward because they are stored as a list in coordinate format. However, sampling \( q \) zeros requires sampling a random index as was done for uniform sampling and then rejecting the sample if it is actually a nonzero.

We can estimate how many random multi-indices are needed to obtain at least \( q \) valid zero samples. Let

\[
\eta = \text{nnz}(\mathbf{X}) \quad \text{and} \quad \zeta = n^d - \eta.
\]

We expect a very small proportion \( (\eta/n^d) \) of indices to be rejected. The number of samples needed to produce an average of \( q \) zero indices is

\[
q \approx \frac{1 - \eta/n^d}{\zeta} \cdot q \approx q.
\]
Algorithm 4.2 Stochastic Gradient with Stratified Sampling for Sparse Tensor

1: function StocGrad($X$, $\{A_k\}$, $p$, $q$)
2: \hspace{1em} $\eta \leftarrow \text{nnz}(X)$ \hspace{0.5em} // $\eta = \# \text{ of nonzeros in } X$
3: \hspace{1em} $\zeta \leftarrow \prod_k n_k - \text{nnz}(X)$ \hspace{0.5em} // $\zeta = \# \text{ of zeros in } X$
4: \hspace{1em} $\bar{y} \leftarrow 0$
5: for $c = 1, 2, \ldots, p$ do \hspace{0.5em} // loop to sample $p \ll (\eta + \zeta)$ nonzero indices for $\bar{y}$
6: \hspace{1em} $\xi \leftarrow \text{randi}(\eta)$ \hspace{0.5em} // sample random nonzero index in $\{1, \ldots, \eta\}$
7: \hspace{1em} $i \leftarrow \text{index of } \xi \text{th nonzero}$ \hspace{0.5em} // extract corresponding tensor index
8: \hspace{1em} $m_i \leftarrow \sum_{j=1}^d \prod_{k=1}^d a_k(i_k, j)$ \hspace{0.5em} // compute $m_i$ at sampled index
9: \hspace{1em} $\bar{y}_i \leftarrow \bar{y}_i + (\eta/p) \cdot g(x_i, m_i)$ \hspace{0.5em} // compute $\bar{y}_i$ at sampled index, $g \equiv \partial f/\partial m$
10: end for
11: $c \leftarrow 0$
12: while $c < q$ do \hspace{0.5em} // loop to sample $q \ll (\eta + \zeta)$ zero indices for $\bar{y}$
13: \hspace{1em} for $k = 1, 2, \ldots, d$, do $i_k \leftarrow \text{randi}(n_k)$, end \hspace{0.5em} // sample random index $i \equiv (i_1, i_2, \ldots, i_d)$
14: \hspace{1em} if $x_i \neq 0$ then \hspace{0.5em} // check against list of nonzeros
15: \hspace{1em} \hspace{1em} reject sample
16: \hspace{1em} else \hspace{0.5em} // increment count of accepted zero samples
17: \hspace{1em} \hspace{1em} $c \leftarrow c + 1$
18: \hspace{1em} \hspace{1em} $m_i \leftarrow \sum_{j=1}^d \prod_{k=1}^d a_k(i_k, j)$ \hspace{0.5em} // compute $m_i$ at sampled index
19: \hspace{1em} \hspace{1em} $\bar{y}_i \leftarrow \bar{y}_i + (\zeta/q) \cdot g(x_i, m_i)$ \hspace{0.5em} // compute $\bar{y}_i$ at sampled index, $g \equiv \partial f/\partial m$
20: \hspace{1em} end if
21: end while
22: for $k = 1, 2, \ldots, d$, do $\tilde{G}_k \leftarrow \text{MTTKRP}(\bar{y}, A_k, k)$, end \hspace{0.5em} // use stochastic sparse $\bar{y}$ to compute $\tilde{G}_k$
23: return $\{\tilde{G}_k\}$
24: end function

This is only on average, so we oversample to get the desired number of indices. In other words, sample $\rho \cdot (n^d/\zeta) \cdot q$ indices where $\rho > 1$ is the oversample rate. A default of $\rho = 1.1$ is justified in Appendix B.

The most expensive operations are still computing the model entries $m_i$ and the corresponding MTTKRP calculation, but the rejection sampling for zeros can be nearly as expensive since we have to scan the entire list of nonzeros for each sample. Hash tables hold the promise of $O(1)$ lookups, but the cost of hashing and the actual lookups can still be expensive in practice.

4.3. Semi-Stratified Sampling. To avoid rejection sampling, we propose a variant that we call semi-stratified sampling. We sample zeros incorrectly but then correct for it when sampling nonzeros. Specifically, we sample without rejection to obtain “zeros”, knowing that a small proportion are actually nonzeros. We still sample nonzeros explicitly but now add a correction to account for the possibility that they were also wrongly sampled as “zeros.”

To create a random instance of $\bar{y}$, sample $p$ nonzeros and $q$ “zeros” from $\Omega$ (the entire set of indices). Let $\tilde{p}_i$ be the number of times that index $i$ was sampled as a nonzero where $\sum_i \tilde{p}_i = p$. Clearly, $\tilde{p}_i = 0$ if $x_i = 0$. Let $\tilde{q}_i$ be the number of times that index $i$ is sampled as a “zero” from the full set of possible indices where $\sum_i \tilde{q}_i = q$. It is possible that some nonzeros are sampled, i.e., we can have $\tilde{q}_i > 0$ when $x_i \neq 0$. Using these counts and recalling
\[ \eta = \text{nnz}(X), \text{we define } \tilde{y} \text{ as} \]
\[ \tilde{y}_i = \frac{\eta}{p} \cdot (y_i - c_i) + \frac{n^d}{q} \cdot c_i \]
where \[ c_i = \frac{\partial f}{\partial m_t}(0, m_i). \]
This still satisfies \( E[\tilde{y}_i] = y_i \). For \( i \) such that \( x_i = 0 \), we have \( \tilde{p}_i = 0 \) and \( c_i = y_i \), so
\[ E[\tilde{y}_i] = E[\tilde{q}_i] \cdot \frac{n^d}{q} \cdot c_i = \frac{q}{n^d} \cdot \frac{n^d}{q} \cdot y_i = y_i. \]
For \( i \) such that \( x_i \neq 0 \), we have
\[ E[\tilde{y}_i] = E[\tilde{p}_i] \cdot \frac{\eta}{p} \cdot (y_i - c_i) + E[\tilde{q}_i] \cdot \frac{n^d}{q} \cdot c_i \]
\[ = \frac{p}{\eta} \cdot \frac{\eta}{p} \cdot (y_i - c_i) + \frac{q}{n^d} \cdot \frac{n^d}{q} \cdot c_i \]
\[ = (y_i - c_i) + c_i = y_i. \]

The procedure is implemented in Algorithm 4.3. The procedure for the nonzero samples is identical to that in Algorithm 4.2 except for the adjustment term \(-g(0, m_i)\) to ensure that the expectations are correct. The procedure for the “zeros” differs because it samples over the entire index space and does not reject nonzeros; it assumes that \( x_i = 0 \) in computing \( y_i \).

**Algorithm 4.3** Stochastic Gradient with Semi-Stratified Sampling for Sparse Tensor

1: \textbf{function} StocGrad \((X, \{A_k\}, p, q)\) \hfill // \# of nonzeros in \( X \)
2: \( \eta \leftarrow \text{nnz}(X) \)
3: \( \omega \leftarrow \prod_k n_k \) \hfill // \# entries in \( X \)
4: \( \hat{Y} \leftarrow 0 \)
5: \textbf{for} \( c = 1, 2, \ldots, p \) \textbf{do} \hfill // loop to sample \( p \ll \omega \) indices for \( \hat{Y} \)
6: \( \xi \leftarrow \text{randi}(\eta) \) \hfill // sample random nonzero index in \( \{1, \ldots, \eta\} \)
7: \( i \leftarrow \text{index of } \xi \text{th nonzero} \) \hfill // extract corresponding tensor index
8: \( m_i \leftarrow \sum_{k=1}^{\eta} \prod_{k=1}^{\eta} a_k(i_k, j) \) \hfill // compute \( m_i \) at sampled index
9: \( \tilde{y}_i \leftarrow \tilde{y}_i + (\eta/p) \cdot [g(x_i, m_i) - g(0, m_i)] \) \hfill // compute \( \tilde{y}_i \) at sampled index with correction term
10: \textbf{end for}
11: \textbf{for} \( c = 1, 2, \ldots, q \) \textbf{do} \hfill // loop to sample \( q \ll \omega \) “zero” indices for \( \hat{Y} \)
12: \( k \leftarrow \text{randi}(n_k) \), \textbf{end} \hfill // sample index \( i \equiv (i_1, i_2, \ldots, i_d) \)
13: \( m_i \leftarrow \sum_{k=1}^{\eta} \prod_{k=1}^{\eta} a_k(i_k, j) \) \hfill // compute \( m_i \) at sampled index
14: \( \tilde{y}_i \leftarrow \tilde{y}_i + (\omega/q) \cdot g(0, m_i) \) \hfill // compute \( \tilde{y}_i \) at sampled index, assuming \( x_i = 0 \)
15: \textbf{end for}
16: \textbf{for} \( k = 1, 2, \ldots, d \), do \( \tilde{G}_k \leftarrow \text{MTTKRP}(\tilde{Y}, A_k, k) \), \textbf{end} \hfill // use sparse \( \tilde{Y} \) to compute \( \tilde{G}_k \)
17: \textbf{return} \( \{ \tilde{G}_k \} \)
18: \textbf{end function}

**4.4. Adapting to Weighted Formulations.** Stratified sampling can be easily adapted to the weighted version of GCP that replaces the loss function in (1.2) with the weighted version

\[ (4.6) \quad \text{minimize } F(X, M) \equiv \sum_i w_i \cdot f(x_i, m_i) \quad \text{subject to } \text{rank}(M) \leq r. \]
In estimating the gradient, the only change in the methods is to replace $y_i$ in (4.1) with

$$y_i = w_i \cdot \frac{\partial f}{\partial m}(x_i, m_i).$$

We do not explicitly study the weighted formulation in this work, but we briefly mention two scenarios where such methods may be useful.

**Adapting to Weighted Formulations.** In the context of recommender systems, zeros are generally treated as missing data. The data is assumed to be missing at random (MAR), meaning that the probability of a data item being present does not depend on its value. However, it has been argued in the matrix case that this may be a flawed assumption [30]. Instead, we may consider including the zero terms but *downweighting* them by using a weighted scheme, i.e., $w_i = 1$ for $x_i \neq 0$ and $w_i = 0.1$ for $x_i = 0$. Many large-scale tensor applications have a recommender system flavor, where down-weighting of the zero entries may be appropriate. More generally, down-weighting can be appropriate for entries that are less reliable or noisier, as has been done in various matrix factorization applications [10, 19, 40, 46]. See also [39, 41] for work on computing weighted matrix factorizations and [17] for a recent analysis of matrix factorization weights when columns have heterogeneous noise levels.

**Weighted Formulations for Missing Data.** Conversely, if some portion of data is missing, there are various strategies that can be used to avoid sampling missing elements. However, this can also be handled easily by setting the weights of missing entries to be zero.

5. **Experimental Results.** All experiments were run using MATLAB (Version 2018a) on a Dual Socket Intel E5-2683v3 2.00GHz CPU with 256 GB memory. The methods are implemented in *gcp_opt* in the Tensor Toolbox for MATLAB [3].

5.1. **Stochastic optimization algorithm.** The stochastic gradients can be used with any number of stochastic optimization methods. We use Adam [21], which uses momentum and is less sensitive to the learning rate than standard SGD. The method is detailed in Algorithm 5.1. If the total number of gradient samples is $s$, then we use $s$ samples for uniform sampling in Algorithm 4.1 and $p = \lfloor s/2 \rfloor$ and $q = \lceil s/2 \rceil$ for the stratified sampling in Algorithm 4.2 and semi-stratified sampling in Algorithm 4.3. The parameter $\alpha$ is the learning rate and defaults to 0.01. The Adam parameters are set to the values recommended in the original paper: $\beta_1 = 0.9$, $\beta_2 = 0.999$, and $\epsilon = 10^{-8}$. We employ a few standard modifications. We group the iterates into epochs, and the number of iterations per epoch defaults to $\tau = 1000$. In order to track progress, we estimate the function value once per epoch. When the function value ceases to decrease, we can either decay the weight by $\eta = 0.1$ (as motivated by [26]) or quit (after more than $\kappa = 1$ failures). We enforce the lower bound by simple projection.

In order to measure progress of the stochastic optimization, we estimate $F(X, M)$ (via the function EstObj) in a way that is analogous to the stochastic gradient computation. There are two key differences. First, we use a much larger number of samples to ensure reasonable accuracy, which is less important for the gradient computation. Second, the set of samples used for function estimation are fixed across all iterations for consistent evaluation across epochs. For uniform sampling, let $\tilde{s}_i$ be the number of times that index $i$ is selected and then
Algorithm 5.1 GCP with Adam (GCP-Adam)

1: function GCPAdam(\(X, r, s, \alpha, \beta_1, \beta_2, \epsilon, \tau, \kappa, \nu, \ell\))
2:   for \(k = 1, 2, \ldots, d\) do
3:      \(A_k \leftarrow \) random matrix of size \(n_k \times r\)
4:      \(B_k, C_k \leftarrow \) all-zero matrices of size \(n_k \times r\) // temporary variables used for Adam
5:   end for
6:   \(\hat{F} \leftarrow \text{EstObj}(X, \{A_k\})\) // estimate loss with fixed set of samples
7:   \(c \leftarrow 0\) // \(c = \#\) of bad epochs (i.e., without improvement)
8:   \(t \leftarrow 0\) // \(t = \#\) of Adam iterations
9:   while \(c \leq \kappa\) do // \(\kappa = \max\ #\) of bad epochs
10:      Save copies of \(\{A_k\}, \{B_k\}, \{C_k\}\) // save in case of failed epoch
11:      \(\hat{F}_{\text{old}} \leftarrow \hat{F}\) // save to check for failed epoch
12:      for \(\tau\) iterations do // \(\tau = \#\) iterations per epoch
13:         \(\{\tilde{G}_k\} \leftarrow \text{StocGrad}(X, \{A_k\}, s)\) // \(s = \#\) samples per stochastic gradient
14:            for \(k = 1, \ldots, d\) do
15:               \(B_k \leftarrow \beta_1 B_k + (1 - \beta_1) \tilde{G}_k\)
16:               \(C_k \leftarrow \beta_2 C_k + (1 - \beta_2) \tilde{G}_k^2\)
17:               \(\hat{B}_k \leftarrow B_k / (1 - \beta_1)\)
18:               \(\hat{C}_k \leftarrow C_k / (1 - \beta_2)\)
19:               \(\hat{A}_k \leftarrow A_k - \alpha \cdot (\hat{B}_k \odot \sqrt{\hat{C}_k} + \epsilon)\)
20:          end for
21:      end for
22:      \(t \leftarrow t + 1\)
23:   end while
24:   \(\hat{F} \leftarrow \text{EstObj}(X, \{A_k\})\) // estimate loss with fixed set of samples
25:   if \(\hat{F} > \hat{F}_{\text{old}}\) then // check for failure to decrease loss
26:      Restore saved copies of \(\{A_k\}, \{B_k\}, \{C_k\}\) // revert to last epoch’s variables
27:      \(\hat{F} \leftarrow \hat{F}_{\text{old}}\) // revert to prior function value
28:      \(t \leftarrow t - \tau\) // wind back the iteration counter
29:      \(\alpha \leftarrow \alpha \cdot \nu\) // reduce the step length
30:      \(c \leftarrow c + 1\) // increment \# of bad epochs
31:   end if
32: end function
33: return \(\{A_k\}\)
34: end function

(5.1) \[ \hat{F} \equiv \sum_{i \in \Omega} \tilde{s}_i \cdot \frac{n^d}{s} \cdot f(x_i, m_i). \]

For stratified sampling, let \(\tilde{p}_i\) denote the number of times that nonzero \(i\) is selected and \(\tilde{q}_i\) be the same for zero \(i\) and then estimate

(5.2) \[ \hat{F} \equiv \sum_{x_i \neq 0} \tilde{p}_i \cdot \frac{n}{p} \cdot f(x_i, m_i) + \sum_{x_i = 0} \tilde{q}_i \cdot \frac{\zeta}{q} \cdot f(x_i, m_i). \]

In either case, it is easy to show that \(E[\hat{F}] = F\). When we perform multiple runs of the same problem, we use the same set of samples for the function estimation across all runs so
that they can be easily compared. The only exception is the non-stochastic method, which computes the full objective function.

5.2. Sample Size and Comparison to Full Method for Dense Tensors. We study the effect of sample size to understand the trade-offs in the number of samples. Using larger samples sizes results in lower variance stochastic gradients but higher cost per iteration.

We compute the GCP decomposition on an artificial four-way tensor of size $200 \times 150 \times 100 \times 50$ and rank $r = 5$ using the gamma loss function: $f(x, m) = x/m - \log m$ with a nonnegativity constraint on the factor matrices. Appendix C provides the details of the data generation.

Figure 5.1 shows the results of GCP-Adam with various sample sizes ranging from $s = 125$ to $s = 2000$. For comparison, we also include non-stochastic results based on the bound-constrained limited-memory BFGS method [6] using full gradients. The same set of 25 initial guesses is used for every instance. The initial guesses comprise factor matrices with entries drawn uniformly from $(0, 1)$. For GCP-Adam, we estimate the loss $\hat{F}$ using 100,000 uniformly sampled entries that are fixed across all epochs and trials. For the stochastic gradient, we use uniform sampling.

In the top two subfigures, we plot the function value versus time. In Figure 5.1a, we consider just the stochastic methods and see the variation between them. There are $d\bar{n}r = 2500$ free parameters and $\max_k n_k = 200$. Common wisdom is to make one pass through the data per epoch, which would require $s = n^d/\tau = 150,000$ samples per iteration. However, we see that two orders of magnitude fewer samples are needed in practice, arguably due to the low-rank structure in the data. Another option is to set $s$ large enough so that we get at least one sample per row of $\tilde{Y}_{(k)}$ and thus every row of $A_k$ is updated. At a minimum, therefore, we may want $s \geq \max_k n_k = 200$. Fewer samples generally corresponds to less progress per epoch; however, sometimes fewer samples is advantageous because it enables the method to escape local minima more quickly. For instance, we see that $s = 2000$ initially makes better progress, but $s = 500$ and $s = 1000$ find the minimum more quickly. At the other extreme, $s = 125$ is the lowest cost per epoch, but its progress in reducing the loss is hindered by too few samples.

In Figure 5.1b we show a longer time range on the x-axis so that the non-stochastic method is visible. The non-stochastic method is approximately an order of magnitude slower.

It may not be clear that the final function value tells the whole story, so we provide another measure of success. Each instance is run with 25 random starts. Figure 5.1c shows the number of times that each instance recovers the true solution, meaning that the cosine similarity score between the true solution and the recovered solution is at least 0.9. (See Appendix E for details of the cosine similarity score.) The only time the true solution is not recovered is one run for $s = 125$ samples per gradient.

Figure 5.1d shows box plots of the cost per epoch, which is 1000 stochastic gradient evaluations (with $s$ specified on the x-axis) plus one function value estimation with 100,000 samples.

---

2This does not necessarily guarantee that every row is updated every time. Roughly $10 \cdot \max_k n_k$ samples ensures a 99.99% probability of having at least one sample in each row. From [23, Appendix A]: To sample $\rho n$ distinct “types” (i.e., row indices) from a set of $t$ types where $\rho \in (0, 1)$, the expected number of draws is $t \log(1/(1 - \rho)) + O(1)$. Therefore, if we want to sample 99.99% of the members of a set with $t$ types, the expected number of samples is less than $10 \cdot t$. 

---
Figure 5.1: GCP with Gamma loss $f(x, m) = x/m + \log m$ on artificial dense data tensor of size $200 \times 150 \times 100 \times 50$ and rank $r = 5$, comparing various numbers of samples for the stochastic gradient in GCP-Adam and the non-stochastic GCP. For each instance, we do 25 runs with different initial guesses. (The same 25 initial guesses are used for each instance.)
Figure 5.2: Factorization with the lowest overall score. GCP with $\beta$-divergence loss $f(x, m) = 2m^\beta + 2xm^{-\beta}$ with $\beta = 1/2$, rank $r = 4$, and $s = 1000$ on real-world dense gas data tensor of size $71 \times 1250 \times 5 \times 140$. Sensor components are scaled proportional to component magnitude; the rest are normalized to length one. Trial symbols are color coded by gas.

samples. In each box plot, the middle line indicates the median, and the bottom and top edges of the box indicate the 25th and 75th percentiles, respectively. The whiskers extend to the most extreme data points not considered outliers, and the outliers are plotted individually as red ‘+’ symbols. Clearly, the cost per epoch grows with the number of samples, but not very quickly. Notably, $s = 2000$ uses 16 times as many samples as $s = 125$ but is generally only around twice as slow.

5.3. Application to Dense Gas Measurements Tensor. We consider a tensor based on chemo-sensing data collected by Vergara et al. [42]. The dataset consists of measurements as a gas is blown over an array of conductometric metal-oxide sensors in a wind tunnel. The tensor modes correspond to

- 71 sensors,
- 1250 time points,
- 5 temperatures,
- 140 trials (7 gases with 20 repeats each).

This is a dense, relatively small 0.5 GB tensor. Vervliet and De Lathauwer [43] and Battaglino, Ballard and Kolda [5] applied CP tensor decomposition to another tensor with only three gases but more time points, formed from the same data. As the tensor is nonnegative and may have some outliers, $\beta$-divergence is an attractive choice for the loss function. So, we use $\beta = 1/2$ and the resulting loss function is $f(x, m) = 2m^{1/2} + 2xm^{-1/2}$ with nonnegativity constraints. We use rank $r = 4$ because this small rank captures distinctions between the different gases.

We run GCP-Adam using uniform sampling and the non-stochastic GCP under the same experimental conditions as in the previous subsection; initial guesses are scaled to match the magnitude of the data tensor. Figure 5.2 shows the results of the best overall run in terms of the final objective value. The components are ordered by magnitude, the sensor mode

---

3Available at http://archive.ics.uci.edu/ml/datasets/Gas+sensor+arrays+in+open+sampling+settings. There is data for eleven gases, of which we use seven with the most distinctive behaviors. The tests are run at six different sensor positions, and we use the third position which is in the middle of the wind tunnel and where some of the interesting behaviors occur. The data is recorded at approximately 100 Hz, and we sample in time at 5 Hz, using the nearest measurement in time for each sample, and skip the first 9 seconds. Finally, we remove sensor 33 (out of 72), which seemed to have erratic measurements.
is normalized to the magnitude of the component, and the other modes are normalized to unit length. The trial mode is color coded by gas. The first two components focus largely on sensor variations due to temperature. The final two components capture some temporal patterns for each gas that impact sensors near the middle of the array, where the gas is likely most concentrated. The factorization identifies generally smooth temporal profiles and tends to group the same gas (indicated by color) in the trial mode.

Performance results are shown in Figure 5.3. Figure 5.3a shows a boxplot of the runtimes for the varying sample sizes as well as the non-stochastic GCP (“full”). The smaller sample sizes take longer because they converge more slowly even though each epoch is cheaper. The non-stochastic instance is overall slowest. Figure 5.3b shows the range of objective function values for each instance, which is very small. For the stochastic instances, larger sample sizes tend to achieve a marginally better loss, as indicated by improved median and percentile losses. The stochastic instances with $s \geq 500$ samples per gradient perform at least as well as the non-stochastic instance, while being much faster. Figure 5.3c shows performance on a clustering task. The fourth component for each run (for a given random start and instance) is clustered according to k-means, and we measure what percentage of the 140 trials (7 gases with 20 trials each) are clustered correctly. Increasing the sample size generally improves clustering performance. Non-stochastic GCP generally performs similarly to $s = 2000$ samples per gradient.

---

4We use 500 replicates with MATLAB’s built-in `kmeans` command to avoid local minima.
(a) Individual runs. Each dashed line represents a single run, and the markers signify epochs. The marker is an asterisk if the true solution was recovered and a dot otherwise. Solid lines represent the median. Dashed black line is the function value estimate for the true solution. The same set of samples is used to estimate the loss across every individual run.

(b) Number of times the true solution was recovered, i.e., cosine similarity $\geq 0.9$.

(c) Boxplot of mean time per epoch. Each epoch is 1000 stochastic gradients plus one estimation of the function value.

Figure 5.4: GCP with Bernoulli loss $f(x, m) = \log(m + 1) - x \log m$ on artificial sparse data tensor of size $200 \times 150 \times 100 \times 50$ and rank $r = 5$ with $524,468$ (0.35%) nonzeros. Comparing various numbers of samples for the stochastic gradient in GCP-Adam. For each instance, we do 25 runs with different initial guesses. (The same 25 initial guesses are used for each instance.)

5.4. Sample Size for Sparse Tensors. We consider a four-way sparse binary tensor of size $200 \times 150 \times 100 \times 50$ and rank $r = 5$ generated according to an odds model tensor, i.e., where $m_i$ gives the odds that $x_i = 1$. The procedure to generate the data is described in detail in Appendix D. The factor matrices in the solution $\mathbf{M}$ have $(r - 1)$ sparse columns and one constant column. The result is a tensor that has 150,452 ‘structural’ nonzeros (from the sparse columns) and 374,435 ‘noise’ nonzeros (from the dense column), with an overall density of 0.35%. We use the loss corresponding to Bernoulli data with an odds link, i.e., $f(x, m) = \log(m + 1) - x \log m$ and a nonnegativity constraint on the factor matrices.

The results of GCP-Adam with various sample sizes ranging from $s = 125$ to $s = 2000$ are shown in Figure 5.4. The same set of 25 initial guesses is used for every instance. The initial guesses comprise factor matrices with entries drawn uniformly from $(0, 1)$ and then scaled to be the same magnitude as the true solution tensor. For GCP-Adam, we estimate the loss $\hat{F}$
using 100,000 uniformly sampled entries that are fixed across all epochs and trials. For the stochastic gradient, we use stratified sampling, and the gradient samples are evenly divided between zeros and nonzeros.

Figure 5.4a plots the individual runs. For the stochastic method, the overall run time is about four times more than for the (easier) Gamma case. We do not compare to the non-stochastic method since it is again significantly slower. This is arguably a difficult test problem in terms of being able to recover the true factors, especially as compared to the Gamma test problem in subsection 5.2. From Figure 5.4b, observe that $s = 125$ fails to find the true solution more often than it succeeds. For $s \geq 250$, the true solution is recovered in the majority of cases, and the recovery rate improves as the number of samples increases. The time per epoch in Figure 5.4c shows that stratified sampling on the sparse tensor is slightly more expensive than uniform sampling on a same-sized dense tensor. Overall, we see a correlation between increased number of samples, increased time to solution, and increased recovery of the true solution.

5.5. Comparison of Sampling Strategies for Sparse Tensors. In this section, we show the advantage of stratified sampling over uniform, and further show that semi-stratified sampling reduces the sampling cost with only a minor impact on optimization performance. We use the same procedure as in the last section to create a sparse binary tensor (detailed in Appendix D). We generate a tensor of size $400 \times 300 \times 200 \times 100$ that is 0.38% dense. This example has 4,402,374 ‘structural’ nonzeros and 4,788,052 ‘noise’ nonzeros, with a total of 9,181,549 nonzeros (less than the sum due to overlap). If this tensor were dense, it would require 19 GB of storage, versus 0.37 GB as a sparse tensor.

The results of uniform, stratified, and semi-stratified sampling are shown in Figure 5.5. We calculate the estimated loss $\hat{F}$ once per epoch using 100,000 stratified sampled entries, evenly divided between zeros and nonzeros. We use $s = 1000$ samples per stochastic gradient evaluation ($s = d\bar{n}$), evenly divided between nonzeros and zeros (or “zeros”) for the stratified samplers. We use 25 initial guesses with random positive values, scaled so that the norm of the initial guess is the same as the norm of the tensor. Note that uniform sampling on a sparse tensor is not as fast as it is on a dense tensor since only nonzeros are stored explicitly and every sampled index has to be checked against the list of nonzeros to determine its value.

The proportion of nonzeros is arguably higher than what is observed in many real-world datasets, which is a favorable condition for uniform sampling because every sample will include nonzeros. Nevertheless, stratified and semi-stratified approaches clearly outperform uniform sampling. They converge faster and more often find the true solution, all at less cost per epoch. This result is expected because stratified sampling should reduce the variance. Semi-stratified sampling is highly competitive with stratified sampling even though its variance is likely higher. The time advantage of the semi-stratified approach is minimal for this small example but is likely to be important for larger sparse tensor with hundreds of millions or billions of nonzeros. In particular, the speed of the MATLAB implementation of stratified sampling depends on the ability to use linearized indices, which means that the total size of the tensor must be less than $2^{64}$. For larger tensors, where we cannot use this approach, the sampling efficiency can degrade by more than an order of magnitude. The semi-stratified approach has no such limitation.
5.6. Application to Sparse Count Crime Data and Comparison to CP-APR. We consider a real-world crime statistics dataset comprising more than 15 years of crime data from the city of Chicago. The data is available at www.cityofchicago.org, and we downloaded a 4-way tensor version from FROSTT [35]. The tensor modes correspond to

- 6,186 days from 2001 to 2017,
- 24 hours per day,
- 77 communities,
- 32 types of crimes.

Each $X(i, j, k, \ell)$ is the number of times that crime $\ell$ happened in neighborhood $k$ during hour $j$ on day $i$. The tensor has 5,330,673 nonzeros. Stored as a sparse tensor, it requires 0.21 GB of storage.
Since this is count data, we use GCP with a Poisson loss function, i.e., \( f(x, m) = m - x \log m \) and nonnegativity constraints. We run GCP-Adam with both stratified and semi-stratified sampling using \( s = d\bar{n} = 6319 \) samples for the stochastic gradient. We compare to the state-of-the-art for CP alternating Poisson Regression (CP-APR) \([9]\), using the Quasi-Newton method described in \([14]\). We run each method with 20 different starting points. We compute rank \( r = 10 \) factorizations.

Timing results are shown in Figure 5.6. The CP-APR method has to do extensive pre-processing, which is why the first iteration does not complete until approximately 140 seconds. The GCP-Adam methods descend much more quickly but do not reduce the loss quite as much, though this failure to achieve the same final minima is likely an artifact of the function estimation and/or nuance of the Adam parameters.

Although the final loss functions values are slightly different, the factorizations computed by the three methods are similar. We show the results from the first random starting point in Figure 5.7. Each rank-1 component corresponds to a row in the figure. The first column is the day, shown as a line graph. Components in this column are scaled to capture the magnitude of the overall component, while all the other components are normalized. The second column is hour of the day, shown as a bar graph. The third column is the neighborhood, shown as a bar graph. (The third column is somewhat difficult to interpret visualized this way but we show it on a map in Appendix F.) The fourth column is the crime type, sorted by overall frequency, and only showing the 13 most prevalent crimes. When working with real-world data, we generally have to experiment. Nevertheless, certain trends emerge over and over again for different starting points, ranks, and methods. In this case, we see strong commonalities among the three methods, as follows.

- Component 1 for CP-APR is similar to component 2 for the GCP-Adam methods,
Figure 5.7: Visualization of factorizations of the Chicago crime tensor as produced by three different methods.
with “theft” being the most prevalent crime and a similar pattern in time.

- Component 2 for CP-APR is similar to component 1 for the GCP-Adam methods.
- Component 3 for the semi-stratified GCP-Adam has a very strong seasonal signature, becoming most active in summer months. Component 4 for stratified GCP-Adam is similar, as is component 6 for CP-APR.
- Component 8 in CP-APR and component 6 in both GCP-Adam methods has a special pattern of a spike on the first of each year and again on the first of each month. There is also a spike at midnight in the hour mode. This is likely a feature of how the associated crimes were recorded in the dataset.

To help further with interpretation of the rank-1 components, we zoom in on the components from the semi-stratified GCP-Adam solution in Appendix F, where we show each individual component, including drawing a heatmap of the neighborhoods on a map.

6. Conclusions. We propose a stochastic gradient for GCP tensor decomposition with general loss functions. The structure of the GCP gradient means that there is no general way to maintain sparsity in its computation even when the input tensor is sparse. Our investigation was prompted by the sparse case, but the stochastic approach applies equally well to dense tensors. To the best of our knowledge, this work is also novel in the context of standard CP because past work has focused only on the recommender systems settings, where zeros are ignored, or the streaming setting, where past time steps are ignored.

In the case of dense tensors, the methodology is straightforward, relying on uniform sampling. For sparse tensors, we explained stratified sampling and demonstrated its effectiveness. A major cost in stratified sampling is the rejection of candidate zero samples that are actually nonzeros. To avoid this cost, we propose a novel semi-stratified sampling that eliminates the rejection step.

We tested the stochastic gradient in our implementation of Adam [21] for GCP tensor decomposition. The numerical results show the following.

- Stochastic gradient methods are effective in practice in terms of driving down the objective function and recovering the true solutions.
- For dense problems, stochastic gradient methods can be much faster than the non-stochastic approach, using L-BFGS-B [6].
- For sparse problems, we can avoid ever forming the dense tensor needed by the gradient, making it possible to solve much larger problems.
- For sparse problems, stratified and semi-stratified sampling are typically superior to uniform sampling.

Overall, stochastic methods have proven to be a promising approach for GCP tensor decomposition. We can likely further improve the results by using more sophisticated stochastic optimization methods. For instance, we can potentially use more sophisticated weight decay strategies in ADAM [26].

An interesting consequence of sampling in the context of parallel tensor decomposition [37, 20, 25, 34] is that we can reduce the computation and/or communication by sampling only a subset of the entries. Moreover, we may be able to stratify the samples in such a way that is amenable to more structured communications. This is a topic of future research.
Appendix A. Special Cases where Gradient Does Not Require Dense Calculations.

Computing the gradient is not a major issue for standard CP due to its special structure. Specifically, the computation of $G_k$ can be simplified so that the primary work is computing $X_k Z_k$, which is a sparse MTTKRP whenever $X$ is sparse [18, Appendix A]. For Poisson CP [9], the primary work is computing $V(k) Z_k$ where $V$ is the sparse tensor defined as

$$v_i = \begin{cases} x_i/m_i & \text{if } x_i \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

In these cases, the gradient can be computed in $O(\text{nnz}(X) \cdot rd)$ flops with $O(\text{nnz}(X))$ additional storage. Generally, however, we may not have such structure and we have to compute with a dense $Y$ tensor at a cost of $O(rd)$ flops and $O(\text{nnz}(X))$ extra storage.

Appendix B. Determining the Oversampling Rate. Subsection 4.2 mentions that we need to oversample because samples may be rejected. Here we discuss the oversampling rate.

We can use the inverse cumulative distribution function (CDF) of a negative binomial distribution in this determination. The negative binomial distribution models the number of failures before a given number of successes with a specified success rate. In our case, we want $s_{\text{zero}}$ successes (e.g., the desired number of zero samples), and the success rate is $p_{\text{zero}} = 1 - \frac{\text{nnz}(X)}{nd}$ (the proportion of excluded entries in the tensor). We can use the inverse CDF to determine the number of rejections at the 99.9999% percentile. For instance, the MATLAB call is:

$$s_{\text{reject}} = \text{icdf('Negative Binomial', 0.999999, s, p)}.$$ 

This means we want to choose the oversampling rate $\rho$ so that

$$\rho \geq \frac{s_{\text{zero}} + s_{\text{reject}}}{s_{\text{zero}}} \cdot p_{\text{zero}}.$$

In Figure B.1, we plot the oversample rate that would be needed in different scenarios. The x-axis is the proportion of nonzeros. The y-axis is the oversample rate. We plot four lines corresponding to different values for $s_{\text{zero}}$. We observe two trends:

1. For fixed $p_{\text{zero}}$, $\rho$ decreases as $s_{\text{zero}}$ increases, and
2. For fixed $s_{\text{zero}}$, $\rho$ decreases as $p_{\text{zero}}$ increases.

For most real-world examples of sampling zeros from a sparse tensor, $p_{\text{zero}} \geq 0.99$ because the tensors are extremely sparse. Additionally, we usually use a sample size of at least $s_{\text{zero}} = 1000$. Therefore, it is clear that oversampling by $\rho = 1.1$ should be adequate for most scenarios that we expect to encounter.

We could also determine the oversampling rate for any individual problem using this procedure, but the inverse CDF calculation can be expensive.

Appendix C. Creating Gamma-Distributed Test Problems. To create the Gamma-distributed test problem used in subsection 5.2, we generate factor matrices whose entries are drawn from the uniform distribution on $(0, 1)$:

$$A_k(i_k, j) \sim \text{uniform}(0, 1) \quad \text{for all } i_k = 1, \ldots, n_k, j = 1, \ldots, r, \text{ and } k = 1, \ldots, d.$$
Using these factor matrices, we create $\mathbf{M}_{\text{true}}$. The data tensor $\mathbf{X}$ is generated as

$$x_i \sim \text{gamma}(k, m_i) \quad \text{with} \quad k = 1.$$ 

**Appendix D. Details of Creating Binary Test Problems.** We assume an odds link with the data, so the factor matrices must be nonnegative. The probability of a one is given by $m/(1 + m)$ where $m$ corresponds to the odds. For simplicity in the model and in generating the data tensor, we assume that factors 1 through $(r - 1)$ are relatively sparse (i.e., sparsity specified by $\delta \in (0, 1/2)$ and factor $r$ is dense. The idea here is the last dense component corresponds to noise in the model, i.e., random but infrequent observations of ones. Otherwise, the ones have a pattern as dictated by the sparse components.

We specify a density of factor matrix nonzeros and a probability of a one for nonzero values in the resulting model, denoted $\rho_{\text{high}}$. To obtain that probability, the nonzero factor matrix entries should be $\sqrt[4]{\rho_{\text{high}}/(1 - \rho_{\text{high}})}$. We modify that slightly by setting the nonzero factor matrix entries to be drawn from a normal distribution with the mean as the target value and a standard deviation of 0.5. Since only a few entries are nonzero, we can identify all the possible nonzeros corresponding to the first four factors and then compute the exact probability computed by the model and then generate an observation.

For the final dense component, we want the probability of a one, denoted $\rho_{\text{low}}$, to be relatively low. This means that approximately $\rho_{\text{low}}$ of the data tensor entries will correspond to this last “noise” column. The entries of the factor matrix are set to $\sqrt[4]{\rho_{\text{low}}/(1 - \rho_{\text{low}})}$. We use this value exactly so that we can generate nonzero “noise” observations in bulk.

For the test problems in subsection 5.2, we use $\delta = 0.15$, $\rho_{\text{high}} = 0.9$, and $\rho_{\text{low}} = 0.0025$. For the test problems in subsection 5.5, we use $\delta = 0.15$, $\rho_{\text{high}} = 0.9$, and $\rho_{\text{low}} = 0.002$.

**Appendix E. Cosine Similarity Score.** If the true factor matrices are known, we can compute a cosine similarity score between the true and recovered solutions.
is denoted by $A_k$ and the estimated solution is $\hat{A}_k$, then the cosine similarity score is

$$\frac{1}{r} \sum_{j=1}^{r} \prod_{k=1}^{d} \cos(a_k(:,j), \hat{a}_k(:, \pi(j)))$$

where $\pi$ is a permutation that should yield the highest possible similarity. Recall that the cosine of two vectors $a$ and $b$ is $a^\top b/(\|a\|_2 \|b\|_2)$. We say that the true solution is recovered if the similarity score is at least 0.9. Assume that $M$ holds $\hat{A}_k$ and $M_{\text{true}}$ holds $A_k$, the cosine similarity is computed using the Tensor Toolbox for MATLAB [3] via the following command:

```
score(M,Mtrue,'lambda_penalty',false)
```

**Appendix F. Individual components of Chicago crime tensor factorization.** In this appendix, we show the remaining 10 components for the factorization of the Chicago crime tensor discussed in subsection 5.6 in Figures F.1 to F.10. Here we have scaled the date to show the overall weight of the component, and the other components are normalized.

**Appendix G. Acknowledgments.** We gratefully acknowledge Jed Duersch for preliminary investigations on handling large-scale tensors with GCP and many insightful discussions about the work presented in this paper. Thanks also to Cliff Anderson-Bergman for stimulating discussions about this project, including providing the information for Appendix B.

**REFERENCES**

[1] E. Acar, D. M. Dunlavy, T. G. Kolda, and M. Mørup, *Scalable tensor factorizations for incomplete data*, Chemometrics and Intelligent Laboratory Systems, 106 (2011), pp. 41–56, doi: 10.1016/j.chemolab.2010.08.004.

[2] B. W. Bader and T. G. Kolda, *Efficient MATLAB computations with sparse and factored tensors*, SIAM Journal on Scientific Computing, 30 (2007), pp. 205–231, doi:10.1137/060676489.

[3] B. W. Bader, T. G. Kolda, et al., *MATLAB Tensor Toolbox Version, Version 3.1*. Available online, June 2019, https://www.tensortoolbox.org.
Figure F.2: Component 2 for Chicago crime tensor using semi-stratified sampling.

Figure F.3: Component 3 for Chicago crime tensor using semi-stratified sampling.

Figure F.4: Component 4 for Chicago crime tensor using semi-stratified sampling.
Figure F.5: Component 5 for Chicago crime tensor using semi-stratified sampling.

Figure F.6: Component 6 for Chicago crime tensor using semi-stratified sampling.

Figure F.7: Component 7 for Chicago crime tensor using semi-stratified sampling.
Figure F.8: Component 8 for Chicago crime tensor using semi-stratified sampling.

Figure F.9: Component 9 for Chicago crime tensor using semi-stratified sampling.

Figure F.10: Component 10 for Chicago crime tensor using semi-stratified sampling.
[4] G. Ballard, N. Knight, and K. Rouse, Communication lower bounds for matricized tensor times Khatri–Rao product, 2017, arXiv:1708.07401v1 [cs.DC].

[5] C. Battaglino, G. Ballard, and T. G. Kolda, A practical randomized CP tensor decomposition, SIAM Journal on Matrix Analysis and Applications, 39 (2018), pp. 876–901, doi:10.1137/17M1122303, arXiv:1701.06600.

[6] R. H. Byrd, P. Lu, J. Nocedal, and C. Zhu, A limited memory algorithm for bound constrained optimization, SIAM J. Sci. Comput., 16 (1995), pp. 1190–1208, doi:10.1137/0916069.

[7] J. D. Carroll and J. J. Chang, Analysis of individual differences in multidimensional scaling via an N-way generalization of “Eckart-Young” decomposition, Psychometrika, 35 (1970), pp. 283–319, doi:10.1007/BF02310791.

[8] D. Cheng, R. Peng, I. Perros, and Y. Liu, SPALS: Fast alternating least squares via implicit leverage scores sampling, in NIPS’16, 2016, https://papers.nips.cc/paper/6436-spals-fast-alternating-least-squares-via-implicit-leverage-scores-sampling.pdf.

[9] E. C. Chi and T. G. Kolda, On tensors, sparsity, and nonnegative factorizations, SIAM Journal on Matrix Analysis and Applications, 33 (2012), pp. 1272–1299, doi:10.1137/110859063.

[10] R. A. Harshman, Foundations of the PARAFAC procedure: Models and conditions for an “explanatory” multi-modal factor analysis, UCLA working papers in phonetics, 16 (1970), pp. 1–84. Available at http://www.psychology.uwo.ca/faculty/harshman/wpppfac0.pdf.

[11] D. Hong, T. G. Kolda, and B. W. Bader, Tensor decompositions and applications, SIAM Review, 51 (2019), pp. C424–C452, doi:10.1137/100806678.

[12] T. G. Kolda, A. Pinar, T. Plantenga, and C. Seshadhri, A scalable generative graph model with community structure, SIAM Journal on Scientific Computing, 36 (2014), pp. C424–C452, doi:10.1137/130914218.
[24] Y. Koren, R. Bell, and C. Volinsky, *Matrix factorization techniques for recommender systems*, Computer, 42 (2009), pp. 30–37, doi:10.1109/MC.2009.203.

[25] J. Li, J. Choi, I. Perros, J. Sun, and R. Vuduc, *Model-driven sparse CP decomposition for higher-order tensors*, in 2017 IEEE International Parallel and Distributed Processing Symposium (IPDPS), IEEE, 2017, pp. 1048–1057, doi:10.1109/ipdps.2017.80.

[26] I. Loshchilov and F. Hutter, *Fixing weight decay regularization in Adam*, 2017, arXiv:1711.05101v2 [cs.LG].

[27] C. Ma, X. Yang, and H. Wang, *Randomized online CP decomposition*, in Proc. Tenth Int. Conf. Advanced Computational Intelligence (ICACI), Mar. 2018, pp. 414–419, doi:10.1109/ICACI.2018.8377495.

[28] T. Maehara, K. Hayashi, and K.-i. Kawarabayashi, *Expected tensor decomposition with stochastic gradient descent*, in AAAI, 2016, pp. 1919–1925.

[29] M. Mardani, G. Mateos, and G. B. Giannakis, *Subspace learning and imputation for streaming big data matrices and tensors*, IEEE Transactions on Signal Processing, 63 (2015), pp. 2663–2677, doi:10.1109/TSP.2015.2417491.

[30] B. Marlin, R. S. Zemel, S. Roweis, and M. Slaney, *Collaborative filtering and the missing at random assumption*, in Proceedings of the Twenty-Third Conference on Uncertainty in Artificial Intelligence (UAI'07), 2007, pp. 267–275, arXiv:1206.5267v1.

[31] D. Needell, N. Srebro, and R. Ward, *Stochastic gradient descent, weighted sampling, and the randomized Kaczmarz algorithm*, Mathematical Programming, 155 (2015), pp. 549–573, doi:10.1007/s10107-015-0864-7.

[32] D. Nion and N. D. Sidiropoulos, *Adaptive algorithms to track the PARAFAC decomposition of a third-order tensor*, IEEE Transactions on Signal Processing, 57 (2009), pp. 2299–2310, doi:10.1109/TSP.2009.2016885.

[33] A.-H. Phan, P. Tichavsky, and A. Cichocki, *Fast alternating LS algorithms for high order CANDECOMP/PARAFAC tensor factorizations*, IEEE Transactions on Signal Processing, 61 (2013), pp. 4834–4846, doi:10.1109/TSP.2013.2269903, http://dx.doi.org/10.1109/TSP.2013.2269903.

[34] E. Phipps and T. G. Kolda, *Software for sparse tensor decomposition on emerging computing architectures*, SIAM Journal on Scientific Computing, (2019), arXiv:1809.09175, in press.

[35] S. Smith, J. W. Choi, J. Li, R. Vuduc, J. Park, X. Liu, and G. Karypis, *FROSTT: The formidable repository of open sparse tensors and tools*, 2017, http://frostt.io/.

[36] S. Smith, J. Park, and G. Karypis, *An exploration of optimization algorithms for high performance tensor completion*, in Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC ’16, IEEE Press, 2016, pp. 31:1–31:13, doi:10.1109/sc.2016.30, http://dl.acm.org/citation.cfm?id=3014904.3014946.

[37] S. Smith, N. Ravindran, N. D. Sidiropoulos, and G. Karypis, *SPLATT: Efficient and parallel sparse tensor-matrix multiplication*, in IPDPS 2015: IEEE International Parallel and Distributed Processing Symposium, May 2015, pp. 61–70, doi:10.1109/ipdps.2015.27.

[38] Z. Song, D. P. Woodruff, and H. Zhang, *Sublinear time orthogonal tensor decomposition*, in Advances in Neural Information Processing Systems (NIPS) 30, 2016, https://papers.nips.cc/paper/6495-sublinear-time-orthogonal-tensor-decomposition.pdf.

[39] N. Srebro and T. Jaakkola, *Weighted low-rank approximations*, in IMCL-2003: Proceedings of the Twentieth International Conference on Machine Learning, Machine Learning, 2003, pp. 720–727, https://www.aaai.org/Papers/ICML/2003/ICML03-094.pdf.

[40] O. Tamuz, T. Maze, and S. Zucker, *Correcting systematic effects in a large set of photometric light curves*, Monthly Notices of the Royal Astronomical Society, 356 (2005), pp. 1466–1470, doi:10.1111/j.1365-2966.2004.08585.x.

[41] M. Udell, C. Horn, R. Zadeh, and S. Boyd, *Generalized low rank models*, FNT in Machine Learning, 9 (2016), pp. 1–118, doi:10.1109/2200000055, http://dx.doi.org/10.1109/2200000055.

[42] A. Vergara, J. Fonollosa, J. Mañues, M. Trincavelli, N. Rulkov, and R. Huerta, *On the performance of gas sensor arrays in open sampling systems using inhibitory support vector machines*, Sensors and Actuators B: Chemical, 185 (2013), pp. 462 – 477, doi:http://dx.doi.org/10.1016/j.snb.2013.05.027.

[43] N. Verlief and L. De Lathauwer, *A randomized block sampling approach to canonical polyadic
decomposition of large-scale tensors, IEEE J. Sel. Top. Signal Process., 10 (2016), pp. 284–295, doi: 10.1109/JSTSP.2015.2503260.

[44] Y. Wang, H.-Y. Tung, A. J. Smola, and A. Anandkumar, Fast and guaranteed tensor decomposition via sketching, in Advances in Neural Information Processing Systems (NIPS) 28, 2015, pp. 991–999, http://papers.nips.cc/paper/5944-fast-and-guaranteed-tensor-decomposition-via-sketching.pdf.

[45] M. Welling and M. Weber, Positive tensor factorization, Pattern Recognition Letters, 22 (2001), pp. 1255–1261, doi:10.1016/S0167-8655(01)00070-8.

[46] H. H. Yue and M. Tomoyasu, Weighted principal component analysis and its applications to improve FDC performance, in 2004 43rd IEEE Conference on Decision and Control (CDC) (IEEE Cat. No.04CH37601), IEEE, 2004, doi:10.1109/cdc.2004.1429421.

[47] S. Zhou, N. X. Vinh, J. Bailey, Y. Jia, and I. Davidson, Accelerating online CP decompositions for higher order tensors, in KDD’16: Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 2016, doi:10.1145/2939672.2939763.

[48] Y. Zhuang, W.-S. Chin, Y.-C. Juan, and C.-J. Lin, A fast parallel SGD for matrix factorization in shared memory systems, in RecSys’13: Proceedings of the 7th ACM Conference on Recommender Systems, ACM, 2013, pp. 249–256, doi:10.1145/2507157.2507164.