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A Comparison of Different Algorithms for Sparse Einsum

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Submitted by Leon Manthey

born on 31.10.1999 in Berlin

Supervisor: Mark Blacher

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Abstract

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1 Introduction

Einstein notation is a powerful and compact notation for representing tensor expressions. It was introduced by Albert Einstein in the early 20th century in order to simplify tensor expressions in "The Foundation of the General Theory of Relativity" [2]. The notation is both elegant and efficient, thus making it a valuable tool in countless fields such as theoretical physics, mathematics, and computer science.

The fundamental operation in Einstein notation is the Einstein summation, often referred to simply as "Einsum". This operation allows for the calculation of various tensor operations, including element-wise multiplications, dot products, outer products, and matrix multiplications. The computational efficiency and expressiveness of Einsum have led to its adoption in numerous applications, ranging from machine learning to scientific computing.

In many practical applications, especially in machine learning and scientific computing, the data involved is often sparse. In sparse tensors most values are zero. Handling sparse tensors efficiently requires specialized algorithms and data structures to avoid unnecessary computations and to save memory. Traditional libraries like NumPy [3] and other major artificial intelligence frameworks [5, 6] typically support Einstein summation for dense tensors, but not for sparse tensors. The only known library that aims to support Einsum operations on sparse tensors is Sparse [8]. However, like NumPy, Sparse only allows for a limited number of symbols to be used as indices, which is why we use opt_einsum [9]. opt_einsum is a package for optimizing the contraction order of Einsum expressions. More importantly for us though, opt_einsum can handle UTF-8 symbols and use Sparse and other libraries like Torch as a backend. Real Einstein summation problems often include expressions with hundreds or even thousands of higher order tensors. In order to express the aforementioned operations we require a large set of unique symbols. Thus, our approaches, just like opt_einsum, are capable of handling all symbols in the UTF-8 encoding.

This thesis explores the implementation and performance of Einstein summation across different computing paradigms, with a particular focus on sparse tensors. Specifically, it focuses on explaining our following implementations and comparing them to multiple libraries:

- SQL-based Implementation: This implementation is based on the algorithm presented in "Efficient and Portable Einstein Summation in SQL" by Blacher et al [1]. It constructs SQL queries dynamically using Python. While SQL is traditionally used for database operations, this approach demonstrates the ability of SQL in performing tensor operations.

- C++ Implementation: The second implementation is written in C++, with multiple versions ranging from naive to optimized approaches. The different versions aim to explore the performance trade-offs between simplicity and optimization, offering insights into how different coding strategies affect computational efficiency.

By comparing these implementations, we aim to provide a comprehensive analysis of the performance and scalability of sparse Einstein summation in various computing environments. The SQL-based implementation serves as a baseline, showcasing the potential of database query languages for tensor operations. Furthermore, the C++ implementations demonstrate the impact of low-level optimizations on computational performance. The code for our implementations is available on GitHub at: https://github.com/Lethey2552/Sparse-Einsum.
By comparing our implementations against the sparse library Sparse and highly performance-tuned dense tensor libraries like Torch, we seek to identify the strengths and weaknesses of each approach, providing guidelines for selecting the appropriate method based on specific use cases and computational requirements. This work contributes to the broader understanding of tensor operations and their efficient implementation, aiming to offer practical insights for researchers and practitioners in fields that rely heavily on tensor computations.

2 Background

The following chapter serves to introduce the necessary background for tensors, Einstein notation and Einstein summation. We will give various examples for operations that can be expressed using Einstein notation. Given the considerable overlap in topics, we will build on related literature [5], adapting and expanding it to meet our specific research requirements.

2.1 Tensors

Tensors are algebraic objects and a fundamental concept in mathematics, physics and computer science. They extend the idea of scalars, vectors and matrices to higher dimensions. In essence, a tensor is a multi-dimensional array with an arbitrary number of dimensions. Each dimension of a tensor is represented by an index with its own range. The number of indices is commonly referred to as the tensor's "rank" or "order." The size of a tensor is determined by the product of the maximum values of each index's range.
For example, consider a tensor T with indices i, j, k and corresponding ranges $i \in \{1, 2\}$, $j \in \{1, 2, 3, 4, 5, 6\}$ and $k \in \{1, 2, 3, 4\}$. The size of tensor T is calculated as follows: $2 \cdot 6 \cdot 4 = 48$. This means tensor T has a total of 48 elements.

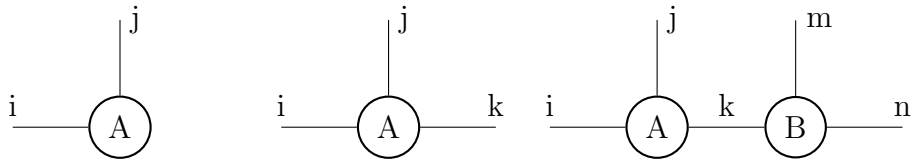

Figure 2.1: A matrix, a tensor and a tensor network visualized as a graph. Each index is represented by an edge. Shared indices in a tensor network are edges between nodes.

In this work, a tensor is simply a multidimensional array containing data of a primitive type. We differentiate between dense and sparse tensors.

Dense Tensors. Dense tensors have a significant number of non-zero entries. However, there is no exact threshold which determines whether a tensor is dense or sparse.

Sparse Tensors. In Sparse tensors most values are zero. They can greatly profit from specialized formats. For our tensor $T \in \mathbb{R}^{I \times J \times K}$ in dense format we need to save $I \cdot J \cdot K$ values no matter whether they are zero or not. Now consider that, if

the vast majority of T's values are zero, we could only save the coordinates of the non-zero values, that is the index of the value for each dimension. This is what we call the coordinate (COO) format. A sparse tensor could be reduced to the COO format as follows:

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 5 & 0 & 0 & 10 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} 0 & 1 & 1 \\ 1 & 2 & 4 \\ 2 & 0 & 5 \\ 2 & 3 & 10 \end{bmatrix}$$

Each row of the COO representation encodes a single value of the tensor with each column holding the position of the value for the corresponding dimension and the last column giving the actual value. This can be done for an arbitrary number of dimensions by simply adding more columns for their respective coordinates.

2.2 Einstein Notation and Einstein Summation

In 1916, Albert Einstein introduced the so called Einstein notation, also known as Einstein summation convention or Einstein summation notation, for the sake of representing tensor expressions in a concise manner. As an example, the contraction of tensors $A \in \mathbb{R}^{I \times J \times K}$ and $B \in \mathbb{R}^{K \times M \times N}$ in figure 2.1,

$$C_{ijmn} = \sum_{k} A_{ijk} \cdot B_{kmn}$$

can be simplified by making the assumption that pairs of repeated indices in the expression are to be summed over. Consequently, the contraction can be rewritten as:

$$C_{ijmn} = A_{ijk} \cdot B_{kmn}$$

To expand upon the expressive power of the original Einstein notation, modern Einstein notation was introduced. This notation is used by most linear algebra and machine learning libraries supporting Einstein summation, that is the evaluation of the actual tensor expressions. Modern Einstein notation explicitly states the indices for the output tensor, enabling further operations like transpositions, traces or summation over non shared indices. In modern Einstein notation, the expression from the previous example would be written as:

$$A_{ijk}B_{kmn} \rightarrow C_{ijmn}$$

When using common Einstein summation APIs, tensor operations are encoded by using the indices of the tensors in a format string and the data itself.

The format string for the above operation would come down to:

$$ijk, kmn \rightarrow ijmn$$

In Modern Einstein notation, indices that are not mentioned in the output are to be summed over. For the sake of simplicity, we will from now on refer to Einstein summation as Einsum, and we will use the original, the modern notation or just the format string, depending on the context.

2.3 Operations with Einsum

Einsum is a powerful tool for performing various tensor operations. Here are some common operations that can be performed using Einsum:

Table 2.1: Example Operations with Einsum.

Operation	**Formula**	**Format string**
Dot Product	$c = \sum_i a_i b_i$	i,i $\rightarrow$
Sum Over Axes	$b_j = \sum_i A_{ij}$	ij $\rightarrow$ j
Outer Product	$C_{ij} = a_i b_j$	i,j $\rightarrow$ ij
Matrix Multiplication	$C_{ij} = \sum_k A_{ik} B_{kj}$	ik,kj $\rightarrow$ ij
Batch Matrix Multiplication	$C_{bij} = \sum_k A_{bik} B_{bkj}$	bik,bkj $\rightarrow$ bij
Tucker Decomposition [7]	$T_{ijk} = \sum_{pqr} D_{pqr} A_{ip} B_{jq} C_{kr}$	pqr,ip,jq,kr $\rightarrow$ ijk

These examples illustrate the versatility of Einsum in performing a wide range of tensor operations with concise and readable notation.

3 Related Work

Previous works
- SQL sparse format idea and query idea [4]
- Einsum to SQL compiling of query by Mark [1]
- Taco compiler
- jcmgrays mapping to batch matrix multiplications
- Sparse library using NUMBA to run einsum

Compared to Einsum with dense tensors, Einsum with sparse tensors has received little attention in the scientific community. Due to the fact that Einsum can be used to compute various expressions the underlying algorithms need to handle many different computations. Here we introduce multiple approaches and ideas, contributing to the field of sparse Einsum.
The incorporation of linear algebra routines into SQL has received more attention recently. (CITE HERE) An approach mapping Einsum problems to SQL queries showed a good performance

Suprisingly, one of the simplest algorithms to compute sparse Einsum problems can be

- many operations not well researched and fine-tuned - recently SQL has gained in popularity in linear algebra operations -

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