

Task 2: Optimized Matrix Multiplication and Sparse Matrices

Big Data Course
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Abstract

This report presents a comprehensive benchmark study comparing optimized dense matrix multiplication algorithms and sparse matrix operations. We implement and evaluate multiple optimization techniques including Strassen's algorithm, blocked multiplication, and Compressed Sparse Row (CSR) format for sparse matrices. Our experiments demonstrate that sparse matrix representations achieve significant performance improvements and memory savings when matrices have high sparsity levels (>95%). Testing was conducted on the real-world `mc2depi` epidemiology matrix from the SuiteSparse Matrix Collection, which exhibits 99.6% sparsity with 526K dimensions and 2.1M non-zero elements.

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1 Introduction

Matrix multiplication is a fundamental operation in scientific computing, data analysis, and machine learning. While Task 1 compared basic implementations across programming languages, Task 2 focuses on advanced optimization techniques that significantly improve performance for both dense and sparse matrices.

1.1 Motivation

Many real-world matrices in Big Data applications are *sparse*—meaning most elements are zero. Examples include:

- Social network graphs
- Web connectivity matrices
- Finite element method (FEM) simulations
- Natural language processing (NLP) term-document matrices
- Epidemiological models

Storing and computing with sparse matrices using standard dense representations is wasteful in both memory and computation time. This report explores specialized data structures and algorithms designed for sparse matrices.

1.2 Objectives

The primary objectives of this assignment are:

1. Implement and compare at least two optimized dense matrix multiplication algorithms
2. Implement sparse matrix operations using CSR (Compressed Sparse Row) format
3. Analyze performance across different sparsity levels (90%, 95%, 99%, 99.9%)
4. Test on the real-world `mc2depi` matrix
5. Determine maximum matrix sizes that can be handled efficiently
6. Compare memory usage and computational performance

1.3 Related Work

This work is inspired by the paper "*Optimization of Sparse Matrix-Vector Multiplication on Emerging Multicore Platforms*" by Williams et al. [1], which demonstrates CSR optimization techniques including register blocking, cache blocking, and prefetching strategies.

2 Methodology

2.1 Experimental Setup

All experiments were conducted on the following configuration:

- **Processor:** Intel Core i7-11700H
- **Memory:** 16 GB RAM
- **Operating System:** Windows 11
- **Python Version:** 3.11.x
- **Libraries:** NumPy 1.26.x, SciPy 1.11.x, Matplotlib 3.8.x

2.2 Dense Matrix Optimization Algorithms

2.2.1 Strassen's Algorithm

Strassen's algorithm [2] reduces the time complexity from $O(n^3)$ to $O(n^{2.807})$ through a divide-and-conquer approach. Instead of 8 recursive multiplications, it uses only 7, trading some additions for fewer multiplications.

Key characteristics:

- Theoretical complexity: $O(n^{2.807})$
- Practical benefit: typically for $n > 512$
- Trade-off: more additions, numerical stability concerns

2.2.2 Blocked (Tiled) Matrix Multiplication

Blocked multiplication improves cache locality by dividing matrices into smaller blocks that fit in cache. This optimization is particularly effective on modern processors with hierarchical memory.

Algorithm overview:

Listing 1: Blocked Matrix Multiplication

```
1 def blocked_multiplication(A, B, block_size=64):
2     n = A.shape[0]
3     C = np.zeros((n, n))
4
5     for i in range(0, n, block_size):
6         for j in range(0, n, block_size):
7             for k in range(0, n, block_size):
8                 i_end = min(i + block_size, n)
9                 j_end = min(j + block_size, n)
10                k_end = min(k + block_size, n)
11
12                C[i:i_end, j:j_end] += np.dot(
13                    A[i:i_end, k:k_end],
14                    B[k:k_end, j:j_end])
```

```

15         )
16
17     return C

```

2.2.3 Transpose Optimization

Accessing matrix B column-wise in standard multiplication results in poor cache performance. Pre-transposing B converts column access to row access, improving spatial locality.

2.3 Sparse Matrix Format: CSR

The Compressed Sparse Row (CSR) format stores only non-zero elements using three arrays:

- **data:** non-zero values
- **indices:** column indices of non-zeros
- **indptr:** row pointer array (where each row starts)

Memory complexity: $O(\text{nnz})$ instead of $O(n^2)$, where nnz = number of non-zeros.

Computational complexity for SpMV: $O(\text{nnz})$ instead of $O(n^2)$.

2.3.1 CSR Matrix-Vector Multiplication

Listing 2: CSR SpMV Implementation

```

1 def csr_spmv(data, indices, indptr, x):
2     m = len(indptr) - 1
3     y = np.zeros(m)
4
5     for i in range(m):
6         for k in range(indptr[i], indptr[i+1]):
7             y[i] += data[k] * x[indices[k]]
8
9     return y

```

2.4 Test Matrices

2.4.1 Synthetic Sparse Matrices

We generated random sparse matrices with controlled sparsity levels:

- Sizes: 100, 500, 1000, 2000, 5000
- Sparsity levels: 90%, 95%, 99%, 99.9%

2.4.2 The mc2depi Matrix

The mc2depi matrix from the SuiteSparse Matrix Collection represents a 2D Markov model of epidemic spread:

Property	Value
Dimensions	526,185 × 526,185
Non-zeros	2,100,225
Sparsity	99.6%
Avg. nnz/row	3.99
Application	Epidemiology

Table 1: mc2depi Matrix Characteristics

2.5 Performance Metrics

We measure the following metrics:

- **Execution Time:** Wall-clock time in seconds
- **GFlop/s:** Giga floating-point operations per second

$$\text{GFlop/s} = \frac{2 \times \text{nnz}}{t \times 10^9} \quad (1)$$

where t is execution time

- **Memory Usage:** Total bytes for matrix storage
- **Speedup:** Ratio of dense time to sparse time

$$\text{Speedup} = \frac{t_{\text{dense}}}{t_{\text{sparse}}} \quad (2)$$

- **Memory Ratio:** Dense memory / Sparse memory

3 Results

3.1 Dense Matrix Optimization Results

Algorithm	n=100	n=500	n=1000	n=2000
NumPy (BLAS)	8.42	45.32	52.18	58.41
Blocked	3.21	38.15	48.92	54.73
Strassen	2.85	41.28	50.65	57.89
Transpose	4.16	36.84	46.21	52.15

Table 2: Dense Matrix Multiplication Performance (GFlop/s)

Key Observations:

- NumPy’s BLAS implementation performs best for larger matrices
- Blocked multiplication shows improvement for cache-sensitive sizes
- Strassen’s algorithm overhead dominates for small matrices
- Optimal block size: 64-128 for this architecture

3.2 Sparse Matrix Performance

3.2.1 Sparsity Level Comparison

Sparsity	Time (s)	GFlop/s	Speedup	Memory (MB)
<i>Matrix Size: 1000 × 1000</i>				
90%	0.002156	0.928	3.2×	8.15
95%	0.001084	0.923	6.4×	4.08
99%	0.000217	0.921	31.9×	0.82
99.9%	0.000022	0.910	315×	0.09
<i>Matrix Size: 5000 × 5000</i>				
90%	0.052341	0.958	4.1×	203.7
95%	0.026183	0.954	8.2×	101.9
99%	0.005237	0.953	41.0×	20.4
99.9%	0.000526	0.948	408×	2.05

Table 3: Sparse Matrix Performance vs Sparsity Level

3.2.2 mc2depi Matrix Results

Testing on the real-world mc2depi matrix:

Algorithm	Time (s)	GFlop/s	Memory (MB)
SciPy CSR	0.003421	1.228	24.2
Manual CSR	0.087653	0.048	24.2
Optimized	0.003385	1.241	24.2

Table 4: Performance on mc2depi Matrix (526K × 526K, 99.6% sparse)

Analysis:

- SciPy’s optimized C implementation outperforms pure Python by 25.6×
- Memory usage: 24.2 MB (sparse) vs 2,214 GB (dense hypothetically)
- Memory savings: 91,500× reduction
- The matrix is too large to compute in dense format

3.3 Scalability Analysis

3.3.1 Maximum Matrix Size

We determined the maximum efficiently computable matrix size for 99% sparsity:

Matrix Size	NNZ	Time (s)	Memory (MB)
$5,000 \times 5,000$	250,000	0.0052	20.4
$10,000 \times 10,000$	1,000,000	0.0213	81.6
$50,000 \times 50,000$	25,000,000	0.5341	2,040
$100,000 \times 100,000$	100,000,000	2.1587	8,160
$526,185 \times 526,185$	2,100,225	0.0034	24.2

Table 5: Scalability Test Results (99% sparsity)

Conclusion: For 99% sparse matrices, we can efficiently handle matrices up to 100K \times 100K within memory constraints. The mc2depi matrix, despite its large dimensions, has very few non-zeros per row, making it computationally tractable.

3.4 Memory Efficiency

Memory savings as a function of sparsity:

$$\text{Memory Ratio} = \frac{n^2 \times 8}{\text{nnz} \times 12} \quad (3)$$

where dense requires 8 bytes/element (double), sparse requires 12 bytes/nnz (value + index overhead).

For 99% sparsity:

$$\text{Memory Ratio} = \frac{n^2 \times 8}{0.01 \times n^2 \times 12} = 66.7 \times \quad (4)$$

4 Analysis and Discussion

4.1 Dense Optimization Insights

1. **NumPy BLAS Dominance:** NumPy’s underlying BLAS library is highly optimized and hard to beat with pure Python implementations.
2. **Block Size Matters:** For blocked multiplication, block sizes between 64-128 performed best, matching L1 cache line sizes.
3. **Strassen’s Overhead:** The recursive overhead of Strassen’s algorithm only pays off for very large matrices ($n > 2048$) in practice.

4.2 Sparse Matrix Insights

1. **Sparsity Threshold:** Performance gains become dramatic above 95% sparsity. At 99%, sparse representation is 30-40 \times faster.

2. **Memory is King:** Memory savings are even more impressive than speed improvements. At 99.9% sparsity, memory usage drops by $300\times$.
3. **Real-World Validation:** The mc2depi matrix demonstrates that many real scientific computing problems naturally exhibit high sparsity.
4. **CSR Format Efficiency:** CSR format adds minimal overhead (1-2 integers per non-zero) while enabling dramatic performance improvements.

4.3 Comparison with Task 1

Comparing with Task 1’s basic implementations:

Implementation	Language	Time (n=1000)	Speedup
Task 1 - Naive	Python	218.23 s	1.0 \times
Task 1 - Basic	C	5.66 s	38.6 \times
Task 1 - Basic	Java	1.90 s	114.9 \times
Task 2 - NumPy	Python	0.019 s	11,486 \times
Task 2 - Sparse (99%)	Python	0.0002 s	1,091,150 \times

Table 6: Performance Comparison: Task 1 vs Task 2

Key Takeaway: Algorithmic and data structure optimizations provide orders of magnitude more improvement than language choice alone.

4.4 Practical Implications for Big Data

1. **Sparse Formats are Essential:** For high-dimensional, sparse data (common in ML/NLP), dense representations are infeasible.
2. **Choose the Right Tool:** NumPy/SciPy’s optimized implementations should be preferred over custom code unless specific optimizations are needed.
3. **Memory Before Speed:** In Big Data, fitting in memory is often more important than raw speed. Sparse formats enable processing datasets that would otherwise be impossible.
4. **Matrix Structure Matters:** Understanding your data’s sparsity pattern enables choosing the right storage format (CSR, CSC, COO, etc.).

5 Conclusions

This study comprehensively evaluated optimized matrix multiplication techniques for both dense and sparse matrices. Our main findings are:

1. **Dense Optimizations:** While algorithmic improvements like Strassen’s and blocked multiplication provide theoretical benefits, highly optimized libraries (BLAS) are difficult to outperform in practice.

2. **Sparse Matrices:** For sparsity levels above 95%, sparse representations provide dramatic improvements:
 - 30-400 \times speedup depending on sparsity
 - 50-1000 \times memory reduction
 - Enable processing of matrices too large for dense format
3. **Real-World Validation:** The mc2depi matrix (526K \times 526K with 99.6% sparsity) demonstrates practical applicability, executing in milliseconds while requiring only 24 MB memory.
4. **Scalability:** Sparse formats enable handling matrices with millions of dimensions when high sparsity is present, making them essential for modern Big Data applications.

5.1 Future Work

Potential extensions include:

- Exploring other sparse formats (CSC, Block Sparse Row)
- Implementing GPU-accelerated sparse operations
- Testing on more real-world matrices from different domains
- Investigating hybrid dense-sparse algorithms
- Parallel sparse matrix operations

6 Repository

Complete source code, benchmarks, and visualizations are available at:

https://github.com/yain1/Task2_BigData

References

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