

# GATTO: Can Topological Information Improve Node Classification via GAT?

Proposal for Learning from Network's project

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## I. MOTIVATION

In the field of computer science, sorting algorithms are fundamental tools used to organize data. Whether the task is to arrange numbers, words, or any other data types, sorting is a critical operation that enhances the efficiency of subsequent data processing and analysis. The importance of sorting is evident in various applications, from database management to search optimization and even in everyday computational tasks.

The choice of a sorting algorithm is often determined by the size and nature of the dataset, as well as the performance requirements of the system. For example, simple algorithms like Bubble Sort and Insertion Sort are easy to implement and understand, making them suitable for small datasets or educational purposes. On the other hand, other algorithms such as Quick Sort, Merge Sort, and Heap Sort are preferred in professional applications due to their superior performance on large datasets.

As data continues to grow exponentially in today's digital world, the role of sorting algorithms remains as vital as ever, serving as the backbone of effective data organization and retrieval. However, even a robust sequential algorithm like Merge Sort may not be as effective in real-life scenarios: in real-time computation, the timespan is constrained to be very small, making computation time a critical factor.

To address these limitations, parallelization is required.

As shown in the pseudocode, the algorithm operates by splitting the input array into two

halves, repeatedly doing so until each subarray contains a single element. It then merges these subarrays in a way that results in a sorted array. The merging process is the key to Merge Sort's efficiency, as it combines elements in linear time, leading to its overall  $O(n \log n)$  complexity.

One of the strengths of Merge Sort is its performance consistency, as it maintains the same complexity in the worst, best, and average cases. However, Merge Sort requires additional space proportional to the size of the input data, which can be a drawback in environments with limited memory.

### A. Parallelization of Merge Sort Algorithm

Due to its nature, there are multiple ways to parallelize the Merge Sort algorithm. One straightforward approach is to leverage the hypercube architecture, which provides efficient parallel processing capabilities. This chapter explores a naive solution based on the Bitonic Sorting Paradigm, implemented on a hypercube network.

1) *Hypercube Architecture:* A hypercube [boman1990hypercube] is a  $d$ -dimensional structure with  $2^d$  nodes, where each node is connected to  $d$  other nodes. The diameter of the hypercube is  $\log_2 P$ , where  $P$  is the number of processors.

2) *Bitonic Sorting Paradigm:* In the Bitonic Sorting Paradigm [batcher1968sorting] on a hypercube, data is exchanged among nodes based on edges connecting nodes that differ by specific bit positions. The process proceeds as follows:

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**Algorithm 1:** Merge Sort

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**Input:** Array  $A$  with indices  $start$  to  $end$

**Output:** Sorted array  $A$

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1: Function Merge( $A, start, mid, end$ ):
2:    $n_1 \leftarrow mid - start + 1$ ;
3:    $n_2 \leftarrow end - mid$ ;
4:    $A_L[0 \dots n_1 - 1], A_R[0 \dots n_2 - 1]$ 
5:   for  $i \leftarrow 0$  to  $n_1 - 1$  do
6:      $A_L[i] \leftarrow A[start + i]$ ;
7:   end
8:   for  $j \leftarrow 0$  to  $n_2 - 1$  do
9:      $A_R[j] \leftarrow A[mid + j + 1]$ ;
10:  end
11:   $i \leftarrow 0, j \leftarrow 0$ ;
12:   $k \leftarrow start$ ;
13:  while  $i < n_1$  AND  $j < n_2$  do
14:    if  $A_L[i] \leq A_R[j]$  then
15:       $A[k] \leftarrow A_L[i]$ ;
16:       $i \leftarrow i + 1$ ;
17:    end
18:    else
19:       $A[k] \leftarrow A_R[j]$ ;
20:       $j \leftarrow j + 1$ ;
21:    end
22:     $k \leftarrow k + 1$ ;
23:  end
24: Function MergeSort( $A, start, end$ ):
25:   if  $start < end$  then
26:      $mid \leftarrow \lfloor \frac{start+end}{2} \rfloor$ ;
27:     MergeSort( $A, start, mid$ );
28:     MergeSort( $A, mid + 1, end$ );
29:     Merge( $A, start, mid, end$ );
30:   end
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- 1) Initially, data is exchanged along edges  $E_0$ , which connect nodes differing by the first bit.
- 2) In the subsequent step, data is exchanged along edges  $E_1$  and  $E_0$ .
- 3) This is followed by exchanges over edges  $E_2, E_1$  and  $E_0$ , and so on, continuing up to  $E_{d-1}$ .
- 4) Finally, exchanges are performed over all edges  $E_{d-1}, E_{d-2}, \dots, E_0$ , incorporating all dimensions.

Each step progressively sorts the data by higher dimensions, leveraging the hypercube's connectivity to distribute the sorting workload efficiently across multiple processors. This approach ensures that the data becomes sorted in parallel, taking full advantage of the hypercube's architecture.

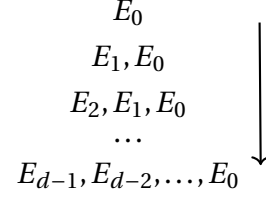


Fig. 1. Bitonic Sorting Paradigm execution schema

3) *Bitonic Sorting Paradigm Implementation:* Based on the Bitonic Sorting Paradigm, the implementation can be summarized as follows:

- 1) Divide the dataset into  $P$  equal parts, assigning one part to each processor.
- 2) Use the Merge Sort routine to sort each subset locally on its respective processor.
- 3) Employ the Bitonic Sorting Paradigm on a virtual hypercube with  $\log_2(P)$  dimensions. During each stage:
  - Merge sorted sequences from adjacent processors, where one processor merges sequences from the lower index and the other from the higher index.
  - Continue merging until each processor's sequence reaches the middle point.

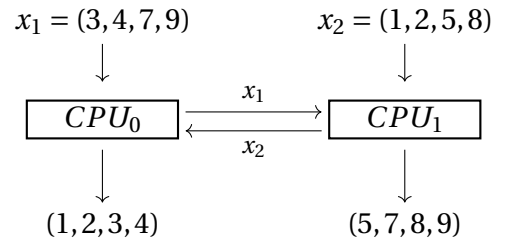


Fig. 2. Bitonic Merging on 2 processors

This approach minimizes inter-processor communication while maximizing parallelism. It is worth noting that the sorting routine used in the initial phase can be tailored to the specific

processor type, ensuring compatibility without disrupting the overall computational framework.

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**Algorithm 2:** Bitonic Sort

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**Input:** Array  $A$ , Processor Set  $P$

**Output:** Sorted array  $A$

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1: Function BitonicSort( $A, P$ ):
    // Scatter  $A$  across  $P$ 
    processors
2:    $A_0, A_1, \dots, A_{P-1}$ ;
    // Execute in parallel on each
    processor  $p \in \{0, \dots, P-1\}$ 
3:   MergeSort( $A_p, 0, |A_p|-1$ );
4:   for  $l \leftarrow 0$  to  $(\log_2 P) - 1$  do
5:     for  $i \leftarrow l$  to  $0$  step  $-1$  do
6:        $pal \leftarrow \text{partner}(p, i, l)$ ;
7:        $A_r \leftarrow \text{data\_from}(pal)$ ;
        // Exchange data between  $p$ 
        and  $pal$ 
8:       if  $p$  merges from low index
        then
9:         MergeLow( $A_p, A_r$ );
10:      end
11:      else
12:        MergeHigh( $A_p, A_r$ );
13:      end
14:    end
15:  end
    // Gather  $A_p$  from each
    processor  $p$ 
16:   $A \leftarrow A_0 \cup A_1 \cup \dots \cup A_{P-1}$ ;

```

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## II. INTENDED EXPERIMENTS

The sequential MergeSort algorithm is implemented in C, while the BitonicSort algorithm is executed using MPI. The code and all implementation details are available on **GitHub**.

For simplicity, the algorithm is tested on datasets whose sizes are powers of two, with the number of processors also being a power of two. This simplification can be mitigated using padding strategies, which become less significant as the dataset size increases. Thus, this approach remains relevant and effective for larger datasets. The tests include 10 measurements of both computation and communication time

for each input size, with the datasets generated randomly for each measurement. Below are the input sizes used:

| Instance Size |            |
|---------------|------------|
| Power of 2    | Decimal    |
| $2^{25}$      | 33554432   |
| $2^{26}$      | 67108864   |
| $2^{27}$      | 134217728  |
| $2^{28}$      | 268435456  |
| $2^{29}$      | 536870912  |
| $2^{30}$      | 1073741824 |

All tests were performed on the **CAPRI** High-Performance Computing (HPC) system, owned by the University of Padova. CAPRI is designed to provide computational power for testing innovative algorithms across various research fields. It is equipped with the following hardware:

- 16 Intel(R) Xeon(R) Gold 6130 @ 2.10GHz CPUs
- 6 TB of RAM
- 2 NVIDIA Tesla P100 16GB GPUs
- 40 TB of disk space

The objective of these tests is to verify that the parallelization approach improves computing time while keeping communication time as a low percentage of the overall execution time.

To evaluate this, the sequential MergeSort was run for each input size 10 times, and the average computation time for each size is referred to as  $T_{Seq}$ . Subsequently, the BitonicSort algorithm was executed on 2 to 32 processors, with the number of processors being powers of 2. For each configuration, the average computation time was measured similarly to the sequential tests, and the speedup

$$S(P) = \frac{T_{Seq}}{T(P)}$$

was analyzed, where  $T(P)$  is the execution time of the algorithm on  $P$  processors. Finally, the Computing-over-Communication Ratio (CCR) was evaluated, defined as

$$CCR(P) = \frac{T_{Calc}(P)}{T_{Tot}(P)}$$

where  $T_{Calc}(P)$  is the time devoted to computation, and  $T_{Tot}(P)$  is the total execution time of the algorithm.