



Fast Phylogenomic Inference Using GPU-Accelerated ML Techniques

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Abstract

Phylogenomic inference, a cornerstone of evolutionary biology, involves analyzing the evolutionary relationships among species using genomic data. Traditional methods for phylogenetic analysis often suffer from high computational demands and prolonged processing times, hindering timely insights. The advent of GPU-accelerated machine learning (ML) techniques offers a transformative solution to these challenges. This paper explores the application of GPU-accelerated ML methods to significantly expedite phylogenomic inference. By leveraging the parallel processing capabilities of GPUs, we demonstrate substantial reductions in computational time while maintaining or improving the accuracy of phylogenetic reconstructions. Our approach integrates advanced ML algorithms optimized for GPU architectures, enabling the analysis of large-scale genomic datasets with unprecedented speed. Through a series of benchmark tests and real-world case studies, we illustrate the efficacy and scalability of our GPU-accelerated methods. This work underscores the potential of GPU-accelerated ML techniques to revolutionize phylogenomic research, paving the way for more efficient and comprehensive evolutionary studies.

Introduction

Phylogenomic inference is a pivotal process in evolutionary biology, providing insights into the evolutionary relationships among different species through the analysis of genomic data. As sequencing technologies advance, the volume of genomic data available for analysis has surged, presenting both opportunities and challenges for researchers. Traditional methods for phylogenetic analysis, while robust, are often computationally intensive and time-consuming, limiting their scalability and responsiveness in handling large datasets.

The increasing complexity and size of phylogenomic data necessitate innovative approaches to accelerate analysis without compromising accuracy. Recent advancements in machine learning (ML) and high-performance computing have introduced promising avenues for addressing these challenges. Among these, the use of Graphics Processing Units (GPUs) has emerged as a powerful tool for enhancing computational efficiency. GPUs, with their parallel processing capabilities, offer significant speedups over traditional Central Processing Units (CPUs) for a wide range of computational tasks, including those in phylogenomic analysis.

This paper explores the integration of GPU-accelerated ML techniques to expedite phylogenomic inference. By leveraging the parallelism and high throughput of GPUs, we aim to achieve substantial reductions in computation time while maintaining, or even improving, the accuracy of phylogenetic reconstructions. Our approach involves the development and application of advanced ML algorithms optimized for GPU architectures, enabling efficient processing of extensive genomic datasets.

II. Literature Review

Overview of Phylogenomic Inference

Definition and Significance

Phylogenomic inference involves the analysis of genomic data to reconstruct the evolutionary relationships among species. This field has become essential for understanding the complexities of evolutionary processes, aiding in the identification of species, and providing insights into genetic diversity and conservation biology. By leveraging whole-genome data, phylogenomic studies offer higher resolution and more accurate reconstructions compared to traditional phylogenetic methods that rely on a limited number of genetic markers. The significance of phylogenomic inference extends to various domains, including ecology, epidemiology, and comparative genomics, where it plays a crucial role in tracing evolutionary histories and uncovering the genetic underpinnings of traits and diseases.

Conventional Methods: Maximum Likelihood, Bayesian Inference, and Parsimony

Traditional approaches to phylogenomic inference include Maximum Likelihood (ML), Bayesian Inference (BI), and Parsimony methods.

- **Maximum Likelihood (ML):** This method estimates the probability of a particular phylogenetic tree given the observed data. ML methods are highly regarded for their statistical robustness and ability to handle complex models of sequence evolution. However, they are computationally intensive, especially for large datasets.
- **Bayesian Inference (BI):** Bayesian methods provide a probabilistic framework for phylogenetic analysis, incorporating prior knowledge and yielding posterior distributions of trees. BI is known for its flexibility and comprehensive treatment of uncertainty, but like ML, it demands substantial computational resources.
- **Parsimony:** Parsimony methods seek the tree that requires the fewest evolutionary changes, assuming the simplest explanation is the most likely. While less computationally demanding than ML and BI, parsimony can be less accurate, particularly when dealing with large and complex datasets.

Introduction of ML Techniques in Phylogenomic Studies

The integration of machine learning (ML) techniques in phylogenomic studies represents a significant advancement in the field. ML algorithms, particularly those based on supervised learning, unsupervised learning, and reinforcement learning, have been employed to improve the efficiency and accuracy of phylogenetic inference. These techniques can handle large volumes of data, identify patterns, and make predictions that might be infeasible for traditional methods.

Current Applications and Limitations

Current applications of ML in phylogenomics include the classification of species, prediction of phylogenetic trees, and identification of evolutionary traits. Techniques such as Support Vector Machines (SVM), Random Forests, and Neural Networks have been applied to various phylogenetic tasks, demonstrating improved performance in terms of speed and accuracy. However, limitations persist, including the need for large labeled datasets for training, the complexity of model interpretation, and the potential for overfitting. Additionally, the computational demands of training ML models can be substantial, necessitating efficient hardware solutions.

Principles of GPU Computing

Graphics Processing Units (GPUs) are specialized hardware designed to handle parallel processing tasks efficiently. Unlike Central Processing Units (CPUs), which are optimized for sequential task execution, GPUs can perform thousands of parallel operations simultaneously. This capability makes GPUs particularly well-suited for the high-throughput demands of computational biology, where large-scale data analysis and complex algorithmic computations are routine.

Success Stories in Bioinformatics and Genomics

The application of GPU acceleration in bioinformatics and genomics has led to significant breakthroughs. Notable success stories include:

- **Sequence Alignment:** Tools like BLAST and Bowtie have been accelerated using GPUs, resulting in substantial reductions in execution time for sequence alignment tasks.
- **Genome Assembly:** GPU-accelerated genome assemblers, such as SOAP3, have enabled faster and more accurate assembly of large genomic datasets.

- **Molecular Dynamics Simulations:** In structural biology, GPU acceleration has revolutionized molecular dynamics simulations, allowing researchers to model complex biological systems with greater precision and speed.

III. Methodology

Data Collection

Description of Phylogenomic Datasets

The phylogenomic datasets used in this study consist of genomic sequences from multiple species. These datasets typically include whole-genome sequences, which provide comprehensive information for phylogenetic analysis. Examples of such datasets include:

- **NCBI RefSeq:** A curated collection of reference sequences representing the complete genomes of diverse species.
- **Ensembl Genomes:** A database providing genome data from a variety of species, including vertebrates, invertebrates, plants, and microorganisms.
- **1000 Genomes Project:** A repository of human genetic variation data that can be used for comparative phylogenomic studies.

Preprocessing Steps

To ensure the quality and consistency of the phylogenomic datasets, several preprocessing steps are undertaken:

- **Sequence Alignment:** Multiple sequence alignment (MSA) tools, such as MAFFT, Clustal Omega, or MUSCLE, are used to align genomic sequences, ensuring that homologous positions are correctly identified across species.
- **Data Cleaning:** Removing low-quality sequences, ambiguous bases, and redundant data to improve the reliability of subsequent analyses. This step also includes filtering out sequences with excessive gaps or missing data.
- **Format Conversion:** Converting sequences into formats compatible with ML models, such as numerical representations or one-hot encoding for sequence data.

ML Models for Phylogenomic Inference

Selection of Suitable ML Models

Several machine learning models are selected based on their suitability for phylogenomic inference:

- **Neural Networks:** Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), including Long Short-Term Memory (LSTM) networks, are chosen for their ability to capture complex patterns in genomic data.
- **Support Vector Machines (SVMs):** SVMs are selected for their effectiveness in classification tasks and their ability to handle high-dimensional data.

- **Random Forests:** Ensemble methods like Random Forests are included due to their robustness and interpretability in phylogenetic prediction tasks.

Adaptation of These Models for Phylogenomic Analysis

To adapt these ML models for phylogenomic inference, several modifications and optimizations are implemented:

- **Feature Engineering:** Extracting relevant features from aligned genomic sequences, such as k-mer frequencies, conserved motifs, and evolutionary distances.
- **Model Customization:** Designing custom neural network architectures tailored to the characteristics of phylogenomic data, such as integrating evolutionary information into model training.
- **Training and Validation:** Using cross-validation techniques to ensure model generalizability and prevent overfitting, with a focus on optimizing hyperparameters for best performance.

GPU Acceleration

Hardware Setup

The hardware setup for GPU acceleration includes selecting specific GPU models that offer high performance for computational tasks:

- **NVIDIA Tesla and A100 GPUs:** These models are chosen for their exceptional parallel processing capabilities and memory bandwidth, which are crucial for handling large genomic datasets and complex ML models.
- **Multi-GPU Configuration:** Setting up multiple GPUs in a single workstation or cluster to further enhance computational throughput and enable parallel training of ML models.

Software and Frameworks

To leverage GPU acceleration, appropriate software and frameworks are utilized:

- **CUDA (Compute Unified Device Architecture):** NVIDIA's parallel computing platform and application programming interface (API) for leveraging the power of GPUs.
- **TensorFlow and PyTorch:** Popular deep learning frameworks that offer native support for GPU acceleration, facilitating the implementation and training of ML models on GPUs.

Implementation

Integration of ML Models with GPU Acceleration

The implementation involves integrating the selected ML models with GPU acceleration to maximize computational efficiency:

- **Model Training:** Utilizing GPUs to train ML models on large phylogenomic datasets, significantly reducing training time compared to CPU-based training.

- **Inference:** Deploying trained models on GPUs for rapid phylogenomic inference, enabling real-time analysis of genomic data.

Optimization Techniques for Enhancing Computational Efficiency

Several optimization techniques are employed to further enhance computational efficiency:

- **Data Parallelism:** Distributing data across multiple GPUs to parallelize computations, ensuring efficient utilization of hardware resources.
- **Model Parallelism:** Splitting large ML models across multiple GPUs to handle memory constraints and improve processing speed.
- **Mixed Precision Training:** Using lower precision arithmetic (e.g., FP16) during model training to reduce memory usage and increase computational speed without significantly compromising accuracy.
- **Efficient Data Loading:** Implementing optimized data loading and preprocessing pipelines to minimize input/output bottlenecks and ensure smooth data flow to the GPUs.

IV. Experimental Design

Performance Evaluation

Metrics

To evaluate the performance of the GPU-accelerated ML techniques for phylogenomic inference, the following metrics are used:

- **Computational Time:** The total time required to complete the phylogenomic analysis, from data preprocessing to inference. This metric includes both training and prediction times for ML models.
- **Accuracy:** The correctness of the phylogenetic trees produced by the ML models. This is assessed by comparing the inferred trees to known reference trees using measures such as the Robinson-Foulds (RF) distance and likelihood scores.
- **Scalability:** The ability of the GPU-accelerated methods to handle increasing amounts of data without significant degradation in performance. Scalability is evaluated by measuring how well the computational time and accuracy are maintained as the dataset size grows.

Benchmarking Against Traditional Phylogenomic Methods

The GPU-accelerated ML techniques are benchmarked against conventional phylogenomic methods, such as Maximum Likelihood (ML), Bayesian Inference (BI), and Parsimony. Key comparisons include:

- **Computational Efficiency:** Comparing the time taken by traditional methods and GPU-accelerated ML models to process the same datasets.
- **Accuracy:** Evaluating the phylogenetic trees generated by both approaches to ensure that GPU-accelerated methods do not compromise on the accuracy of phylogenetic inference.

- **Scalability:** Assessing how well both traditional and GPU-accelerated methods scale with larger datasets.

Experiments

Small-Scale Datasets: Validating Accuracy and Initial Performance Gains

Initial experiments are conducted on small-scale phylogenomic datasets to validate the accuracy and performance gains of the GPU-accelerated ML techniques. These datasets typically include genomic sequences from a limited number of species and are used to:

- **Train ML Models:** Using small datasets to train the selected ML models, ensuring that the models can effectively learn and infer phylogenetic relationships.
- **Evaluate Accuracy:** Comparing the inferred phylogenetic trees against reference trees to assess the accuracy of the ML models.
- **Measure Computational Time:** Recording the time taken for data preprocessing, model training, and inference to establish baseline performance metrics.

Large-Scale Datasets: Testing Scalability and Robustness

Subsequent experiments are conducted on large-scale phylogenomic datasets to test the scalability and robustness of the GPU-accelerated ML techniques. These datasets include whole-genome sequences from a wide range of species and are used to:

- **Assess Scalability:** Evaluating how well the GPU-accelerated methods handle large datasets in terms of computational time and memory usage. This involves testing with datasets of varying sizes and complexities.
- **Test Robustness:** Ensuring that the ML models maintain their accuracy and performance when applied to diverse and complex genomic data.
- **Benchmark Against Traditional Methods:** Comparing the performance of GPU-accelerated ML techniques with traditional phylogenomic methods on large datasets to highlight the advantages in terms of speed and scalability.

VI. Discussion

Interpretation of Results

Significance of Performance Improvements

The results of this study indicate substantial performance improvements in phylogenomic inference when using GPU-accelerated ML techniques. Key findings include:

- **Reduced Computational Time:** GPU acceleration significantly decreases the time required for data preprocessing, model training, and phylogenetic inference. This reduction in computational time allows for more rapid analysis of genomic data, making it feasible to handle large-scale datasets in a timely manner.

- **Enhanced Accuracy:** The ML models, particularly those optimized for GPU architectures, demonstrate high accuracy in phylogenetic tree reconstruction. The trees produced are comparable to, or in some cases more accurate than, those generated by traditional methods such as Maximum Likelihood and Bayesian Inference.
- **Improved Scalability:** GPU-accelerated techniques exhibit robust scalability, effectively managing increased data volumes without a corresponding increase in computational time or decrease in accuracy. This scalability is crucial for modern phylogenomic studies, which often involve large and complex genomic datasets.

Implications for the Field of Phylogenomics

The performance improvements observed in this study have several important implications for the field of phylogenomics:

- **Acceleration of Evolutionary Research:** The ability to perform rapid and accurate phylogenomic inference enables researchers to conduct more extensive and detailed evolutionary studies. This can lead to new insights into the evolutionary relationships among species and the genetic basis of various traits and diseases.
- **Enhanced Data Analysis Capabilities:** With GPU-accelerated ML techniques, researchers can efficiently analyze larger and more complex datasets, which were previously impractical to handle using traditional methods. This opens up new possibilities for exploring evolutionary patterns and processes at a finer scale.
- **Broader Application of Phylogenomic Methods:** The improved efficiency and scalability of GPU-accelerated techniques make phylogenomic analysis more accessible to a wider range of research institutions, including those with limited computational resources. This democratization of advanced phylogenomic methods can foster greater collaboration and innovation in the field.

Challenges and Limitations

Technical Challenges in Implementing GPU-Accelerated ML Techniques

Several technical challenges were encountered during the implementation of GPU-accelerated ML techniques for phylogenomic inference:

- **Hardware Requirements:** High-performance GPUs are essential for achieving significant computational speedups. The cost and availability of such hardware can be a barrier for some research institutions.
- **Software Complexity:** Developing and optimizing ML models for GPU acceleration requires expertise in both machine learning and high-performance computing. The integration of GPU-accelerated frameworks (e.g., CUDA, TensorFlow, PyTorch) adds complexity to the implementation process.
- **Parallelization and Data Handling:** Efficiently parallelizing computations and managing data flow between the CPU and GPU can be challenging, particularly for large and complex datasets. Optimizing these processes is crucial for maximizing the benefits of GPU acceleration.

Potential Biases and Limitations in the Datasets or Methods Used

While the study demonstrates significant performance improvements, several potential biases and limitations should be considered:

- **Dataset Bias:** The choice of datasets can influence the results. Datasets with varying levels of complexity, completeness, and quality may yield different outcomes. Ensuring a representative and diverse set of genomic data is important for generalizing the findings.
- **Model Limitations:** While ML models offer powerful tools for phylogenomic inference, they are not without limitations. Overfitting, model interpretability, and the need for large training datasets are potential concerns that must be addressed to ensure reliable and accurate results.
- **Assumption Dependencies:** The accuracy and performance of phylogenetic inference are dependent on the assumptions underlying the ML models and the data preprocessing steps. Any biases or inaccuracies in these assumptions can affect the results.

VII. Conclusion

Summary of Findings

Key Insights from the Comparative Analysis

This study demonstrates that GPU-accelerated machine learning (ML) techniques significantly enhance the efficiency and accuracy of phylogenomic inference compared to traditional methods. Key insights from the comparative analysis include:

- **Significant Reduction in Computational Time:** GPU-accelerated techniques drastically reduce the time required for data preprocessing, model training, and phylogenetic inference. This allows for the rapid analysis of large-scale genomic datasets, making real-time phylogenomic studies feasible.
- **High Accuracy of Inference:** The phylogenetic trees generated by GPU-accelerated ML models are highly accurate, often matching or surpassing the accuracy of trees produced by traditional methods such as Maximum Likelihood and Bayesian Inference.
- **Robust Scalability:** GPU-accelerated methods exhibit excellent scalability, efficiently managing the increased data volumes typical of modern phylogenomic studies without significant performance degradation.

Validation of GPU-Accelerated ML Techniques as a Viable Alternative for Fast Phylogenomic Inference

The results validate GPU-accelerated ML techniques as a powerful and viable alternative to conventional phylogenomic methods. These techniques not only maintain high levels of accuracy but also provide substantial improvements in computational efficiency and scalability. This makes them particularly suitable for large-scale evolutionary studies and offers a promising pathway for future research in phylogenomics.

Recommendations for Further Research

- **Optimization of ML Models:** Future research should focus on optimizing ML models specifically for phylogenomic inference, including the development of new architectures and algorithms that better capture the complexities of genomic data.
- **Integration with Other High-Performance Computing Resources:** Exploring the integration of GPU-accelerated techniques with other high-performance computing resources, such as cloud computing and distributed computing frameworks, could further enhance the efficiency and accessibility of phylogenomic analysis.
- **Broader Dataset Validation:** Conducting extensive validation studies across a wider range of genomic datasets, including those from different species and environments, to ensure the generalizability and robustness of the GPU-accelerated methods.

Potential Advancements in GPU Technology and ML Algorithms

- **Next-Generation GPUs:** Continued advancements in GPU technology, such as increased processing power, memory capacity, and energy efficiency, will further enhance the capabilities of GPU-accelerated phylogenomic inference.
- **Advanced ML Algorithms:** The development of more sophisticated ML algorithms, including those leveraging deep learning and reinforcement learning, could provide even greater improvements in accuracy and computational efficiency.
- **Automated Hyperparameter Tuning:** Implementing automated hyperparameter tuning techniques, such as Bayesian optimization or genetic algorithms, can help in fine-tuning ML models for optimal performance with minimal human intervention.
- **Explainable AI:** Integrating explainable AI techniques to make the outputs of ML models more interpretable and transparent, which can increase the confidence of researchers in the results and provide deeper insights into evolutionary relationships.

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