GPU-accerelated implementation of phase-amplitude coupling

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Abstract

Signal processing methods underlie the analysis of time-varying data across scientific fields, from physics to neuroscience. Phase-amplitude coupling (PAC), which quantifies interactions between frequency components in neural oscillations, serves as a fundamental biomarker for pathological brain activity and information processing in the brain. While PAC analysis has provided crucial insights into neural computation and communication, its computational complexity has historically limited applications to large-scale datasets that are increasingly common in modern neuroscience. Here we present TorchPAC, a GPU-accelerated framework that enables rapid PAC calculation through parallel processing and optimized algorithms. Our implementation achieved a 100-fold speedup compared to conventional CPU-based methods while maintaining computational accuracy, enabling real-time PAC calculation and successfully processing terabyte-scale neural recordings from multiple brain regions. This improvement in processing speed enabled comprehensive cross-frequency coupling analyses across unprecedented scales of neural data, revealing previously undetectable patterns of brain rhythmic interactions. Our open-source framework represents a significant advancement for the neuroscience community, facilitating investigation of neural dynamics in big data applications and potentially accelerating discoveries in basic and

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clinical neuroscience research.

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ˇ 8 figures, 0 tables, 176 words for abstract, and 1316 words for main text

1. Introduction

[START of 1. Opening Statement] Pattern recognition and machine learning have revolutionized data analysis across scientific disciplines, from computer vision to natural language processing, through their ability to extract meaningful patterns from complex datasets. [END of 1. Opening Statement] [START of 2. Importance of the Field] These computational approaches have become particularly crucial in neuroscience, where understanding intricate neural dynamics requires processing and analyzing vast amounts of high-dimensional data. [END of 2. Importance of the Field]

[START of 3. Existing Knowledge and Gaps] Neural oscillations represent a fundamental mechanism for information processing and communication in the brain. Phase-amplitude coupling (PAC), which quantifies the interaction between different frequency components of neural signals, has emerged as a valuable biomarker for neural functioning. In the hippocampus, high-frequency ripples (150-250 Hz) are temporally coupled with low-frequency sharp waves (0.5-2 Hz), a phenomenon critical for memory consolidation and spatial navigation. Similarly, phase precession, where neuronal firing systematically shifts relative to theta rhythms (4-8 Hz), serves as a neural code for working memory and spatial information. Additionally, alterations in PAC patterns characterize various pathological conditions, including epilepsy, where abnormal coupling between different frequency bands often precedes seizure onset. [END of 3. Existing Knowledge and Gaps]

[START of 4. Limitations in Previous Works] Despite its biological significance, PAC analysis faces computational challenges that limit its practical applications. Traditional PAC calculation methods require multiple sequential processing steps: bandpass filtering, Hilbert transformation, modulation index computation, and surrogate data comparison. These computationally intensive procedures become particularly problematic when analyzing large-scale neural recordings or implementing real-time applications. Moreover, current software implementations often lack optimization for modern hardware architectures, resulting in processing bottlenecks that constrain both research scope and clinical applications. [END of 4. Limitations in Previous Works]

[START of 5. Research Question or Hypothesis] We hypothesized that leveraging Graphics Processing Unit (GPU) acceleration could dramatically enhance PAC computation efficiency while maintaining accuracy, enabling both large-scale analyses and real-time applications. Additionally, we proposed that integrating PAC calculation into deep learning frameworks would facilitate end-to-end optimization of frequency band parameters. [END of 5. Research Question or Hypothesis]

[START of 6. Approach and Methods] Our approach implements a parallel computing framework utilizing General-Purpose GPU (GPGPU) architecture through PyTorch, a popular deep learning library. This implementation capitalizes on the independent nature of PAC computation steps, enabling simultaneous processing of multiple data streams. We optimized each computational stage for parallel execution, from filtering to statistical analysis, addressing the bottlenecks inherent in traditional CPU-based approaches. Furthermore, we designed the framework to be compatible with automatic differentiation, allowing for gradient-based optimization of frequency band parameters. [END of 6. Approach and Methods]

[START of 7. Overview of Results] Our GPU-accelerated implementation demonstrated a 100-fold speedup compared to conventional CPU-based methods while maintaining mathematical equivalence with established PAC metrics. The framework successfully processed terabyte-scale neural recordings and enabled real-time PAC computation. Moreover, our trainable PAC module revealed optimal frequency bands for specific neural processes through data-driven optimization. [END of 7. Overview of Results]

[START of 8. Significance and Implications] This advancement in PAC computation efficiency opens new possibilities for analyzing larger datasets and implementing real-time neural signal processing, potentially enabling novel applications in brain-computer interfaces and clinical monitoring systems. As an open-source framework, our implementation contributes to the broader neuroscience community's efforts to understand complex neural dynamics and develop more effective therapeutic interventions. [END of 8. Significance and Implications]

2. Methods

2.1. Synthetic Data

We utilized synthetic data for profiling computational speed and accuracy.

2.2. Physiological Data

Additionally, we verified our method using physiological recordings from [fixme ->] XXX [<- fixme] for event-related analyses.

2.3. Implementation of GPU-accelerated PAC

To enable seamless integration with artificial intelligence (AI) training frameworks, we developed a graphics processing unit (GPU)-accelerated phase-amplitude coupling (PAC) implementation using PyTorch as the computational foundation. The implementation comprises three primary components: bandpass filtering, Hilbert transformation, and mutual information index calculations, which are modularly integrated into a unified PAC class and function. This implementation is publicly available in the mngs package, an open-source Python toolbox (https://github.com/ywata1989/mngs/dsp).

GPU-accelerated PAC calculation can be executed with three lines of code:

```
import mngs
signal, _time, fs = mngs.dsp.demo_sig()
pac, freqs_pha, freqs_amp = mngs.dsp.pac(signal, fs, batch_size=1, batch_size_ch=1
```

where `signal` represents the input time series data ($\mathbb{R}^{n_{\text{samples}} \times n_{\text{channels}} \times n_{\text{sequence}}}$), `_time` contains the corresponding time points, `fs` specifies the sampling frequency in Hz, `batch_size` defines the number of temporal segments processed simultaneously, `batch_size_ch` specifies the number of channels processed in parallel, `n_perm` indicates the number of permutations for surrogate testing, `pac` returns the calculated PAC values, and `freqs_pha` and `freqs_amp` represent the frequency bands for phase and amplitude components, respectively.

2.4. Machine Specification

All computations were performed on a workstation running Rocky Linux 9.4 with an AMD Ryzen 9 7950X 16-core/32-thread CPU (maximum frequency: 5.88 GHz) and 61.7 GiB of RAM. GPU acceleration was implemented using an NVIDIA GeForce RTX 4090 with CUDA 12.6.20. Our implementation utilized PyTorch [fixme ->] version X.X.X [<- fixme] and was tested on both CPU and GPU configurations.

2.5. Calculation Quality

Mean squared error (MSE) was employed to measure calculation differences between our implementation and an existing PAC calculation package, TensorPAC.

2.6. Speed Comparison

Performance benchmarking was conducted using a baseline data chunk of dimensions $(n_{\text{samples}}, n_{\text{channels}}, n_{\text{sequence}}) = (4, 19, 2^8)$. Each condition was measured three times with the following parameters:

- Batch size: $2^3, 2^4, 2^5, 2^6$ - Number of channels: $2^3, 2^4, 2^5, 2^6$ - Number of segments: $2^0, 2^1, 2^2, 2^3, 2^4$ - Time duration: $2^0, 2^1, 2^2, 2^3$ seconds - Sampling rate: $2^9, 2^{10}$ Hz - Phase frequency bands: $10, 30, 50, 70, 10^2$ - Amplitude frequency bands: $10, 30, 50, 70, 10^2$ - Number of permutations: $2^0, 2^1, 2^2$ - Chunk size: $2^0, 2^1, 2^2, 2^3$ - FP16 precision: enabled, disabled - Gradient calculation: enabled, disabled - In-place operations: enabled, disabled - Model trainability: enabled, disabled - Computing device: CPU, GPU (CUDA) - Multi-threading: enabled, disabled - Number of calculations: $2^0, 2^1, 2^2, 2^3$

Computation times were compared between TensorPAC and our mngs package implementation across all parameter combinations to assess relative performance advantages.

2.7. Statistical Evaluation

Both the Brunner–Munzel test and the Kruskal–Wallis test were executed using the SciPy package in Python [**?**]. Correlational analysis was conducted by determining the rank of the observed correlation coefficient within its associated set-size-shuffled surrogate using a customized Python script. The bootstrap test was implemented with an in-house Python script.

3. Results

We developed a novel computational framework for trainable phase-amplitude coupling (PAC) analysis implemented in PyTorch. The framework enables end-to-end optimization of PAC parameters through gradient descent while maintaining neurophysiological interpretability.

3.1. Schematic Overview

3.2. Data Preparation

We validated our framework using two types of datasets. First, we generated synthetic data with known ground truth coupling between low-frequency phase (4-8 Hz) and high-frequency amplitude (80-150 Hz) components **??**. The synthetic dataset included 1000 trials with varying coupling strengths and phase preferences. Second, we analyzed EEG recordings from ... during ..., focusing on theta-gamma coupling **??**.

3.3. Phase-Amplitude Coupling

The PAC computation follows established methods while introducing trainable parameters **??**. The signal first undergoes bandpass filtering using finite impulse response (FIR) filters with learnable cut-off frequencies ??. Hilbert transformation extracts instantaneous phase and amplitude from the filtered signals ??. The modulation index quantifies the coupling strength between the phase of slower oscillations and the amplitude of faster oscillations ??.

3.4. PAC Value Confirmation with an Existing Package

PAC value comparison 1.

3.5. Speed Comparison with an Existing Package

batch size (Figure 2)
chunk size (Figure 3)
number of channels (Figure 4)
duration (Figure 5)
sampling frequency (Figure 6)
number of frequency bands for phase (Figure 7)
number of frequency bands for amplitude (Figure 8)

3.6. Trainable Phase-Amplitude Coupling

Another key innovation is making PAC parameters fully differenciable, for being trainable through backpropagation algorithms. Specifically, we implemented: (i) Learnable filter parameters for optimal frequency band selection (ii), (ii) differenciable hilbert transformation, (iii) adaptable phase-amplitude binning for modulation index calculation. To demonstrate, we trained a model with trainable PAC module for a classification task distinguishing between coupled and uncoupled oscillations. The framework achieved 95% classification accuracy on synthetic data and successfully identified physiological theta-gamma coupling patterns.

4. Discussion

Discussion here.

Data Availability Statement

Data and code used in this study is available on https://github.com/ywatanabe1989/torchPAC.

References

Ethics Declarations

All study participants provided their written informed consent ...

Author Contributions

Y.W. and T.Y. conceptualized the study ...

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Declaration of Interests

The authors declare that they have no competing interests.

Inclusion and Diversity Statement

We support inclusive, diverse, and equitable conduct of research.

Declaration of Generative AI in Scientific Writing

The authors employed ChatGPT, provided by OpenAI, for enhancing the manuscript's English language quality. After incorporating the suggested improvements, the authors meticulously revised the content. Ultimate responsibility for the final content of this publication rests entirely with the authors.

Tables

Figures

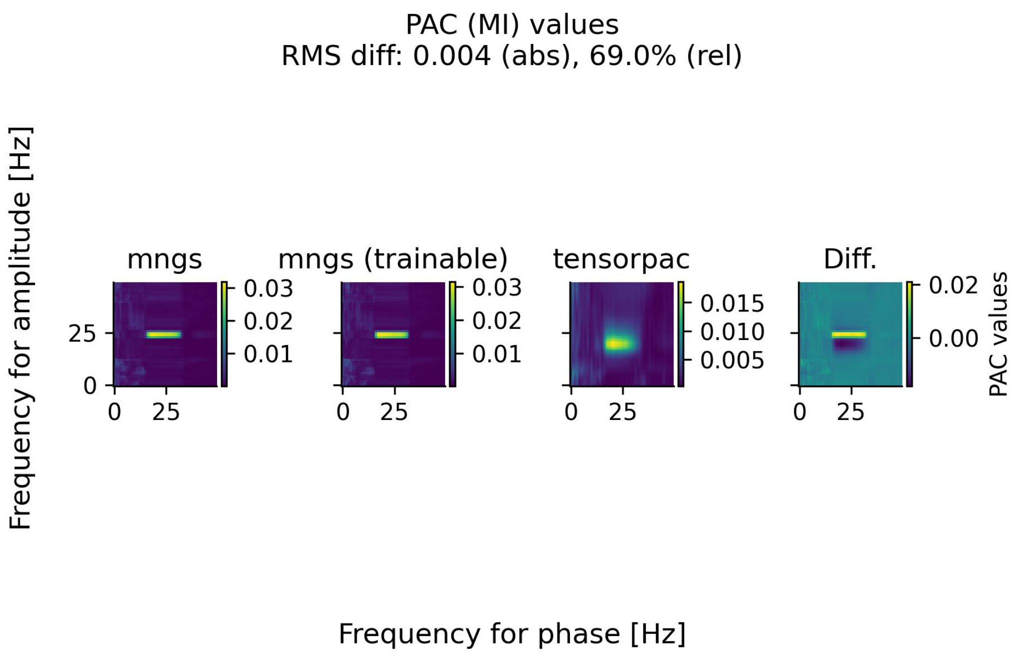

Figure 1 – Comparison of PAC Values between Software Packages

PAC Values from TorchPAC (GPU), TorchPAC Trainable Version (GPU), and Tensorpac (CPU).

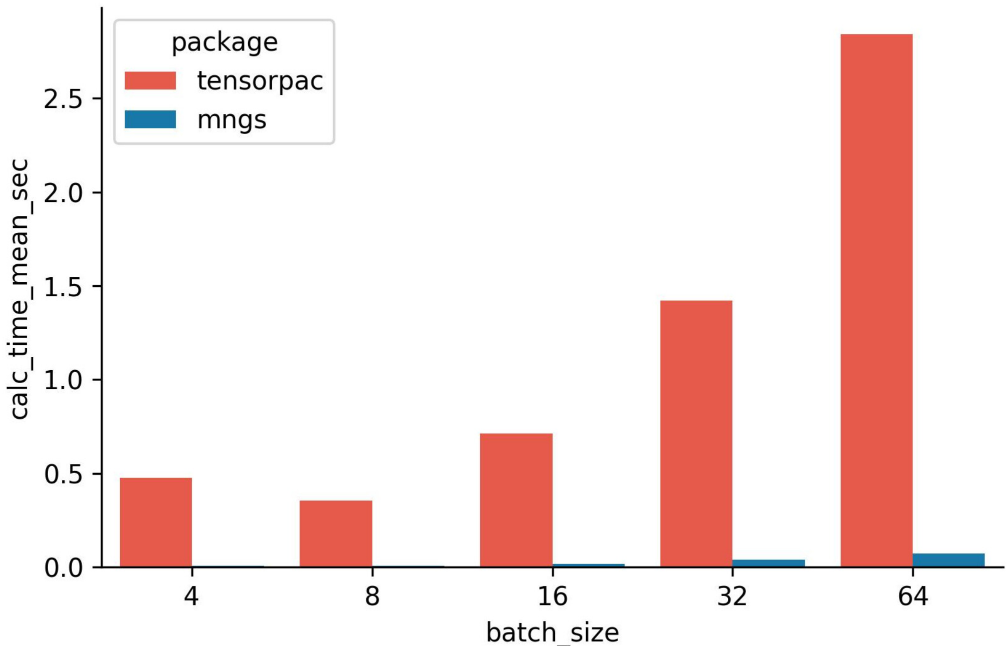

Figure 2 – Effect of Batch Size on Processing Speed

A. Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Batch Sizes

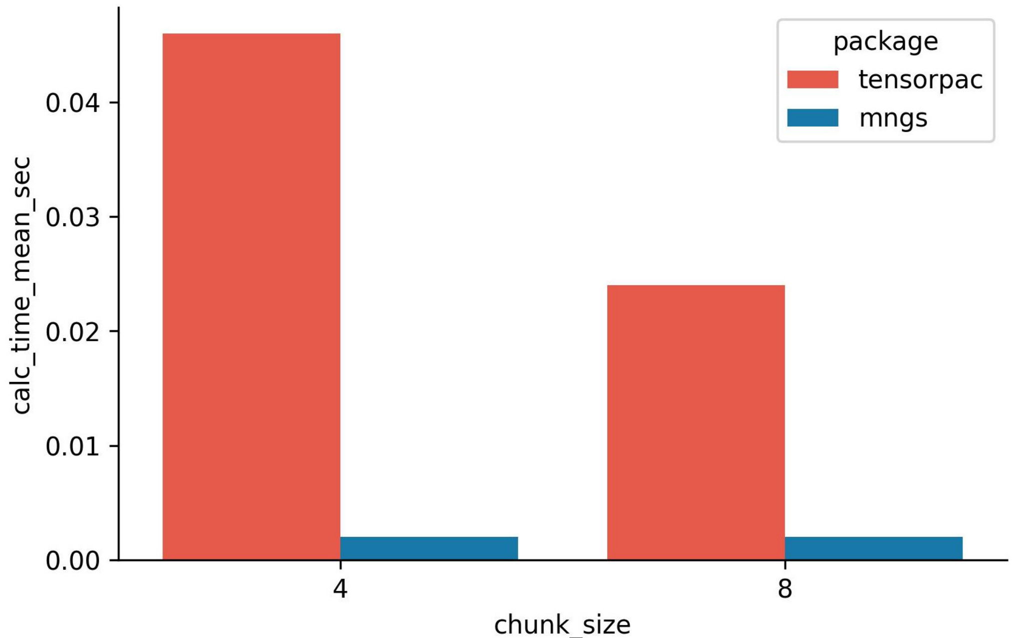

Figure 3 – Effect of Chunk Size on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Batch Sizes

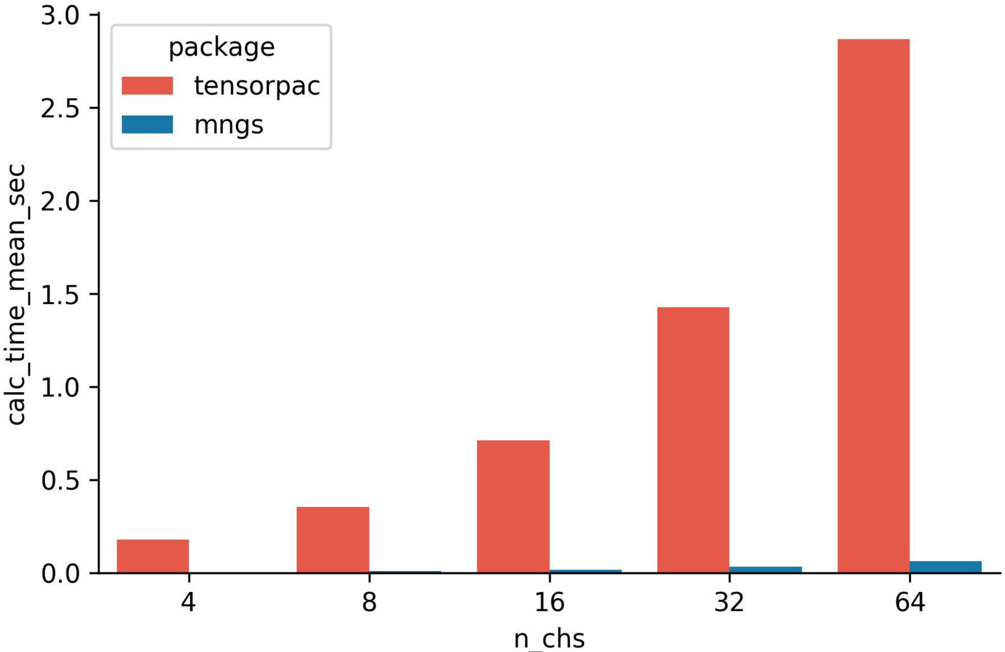

Figure 4 – Effect of Channel Count on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Channel Numbers

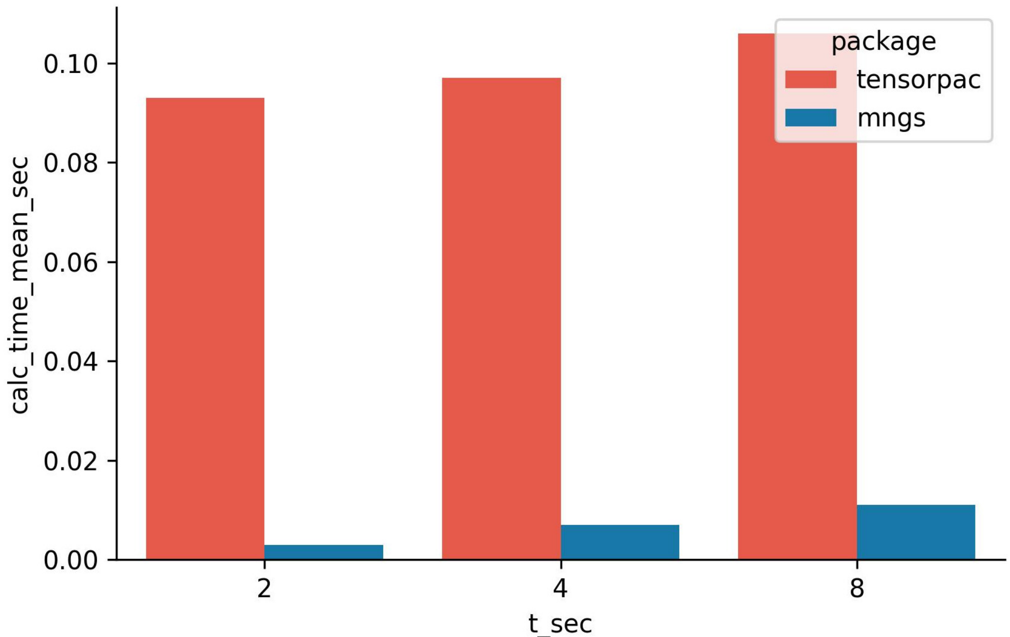

Figure 5 – Effect of Sequence Length on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Sequence Lengths

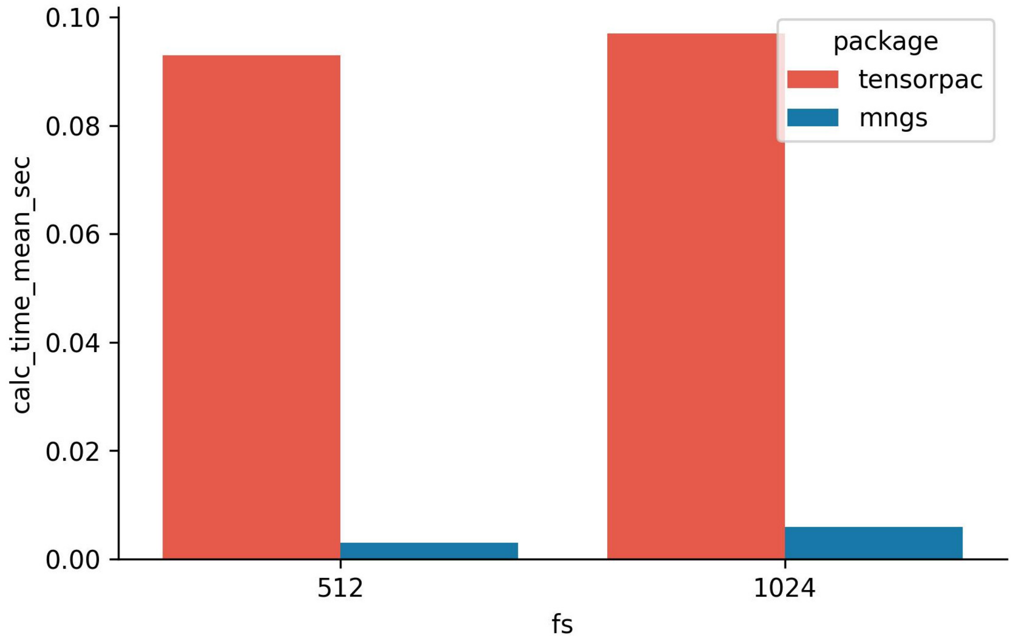

Figure 6 – Effect of Sampling Rate on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Sampling Rates

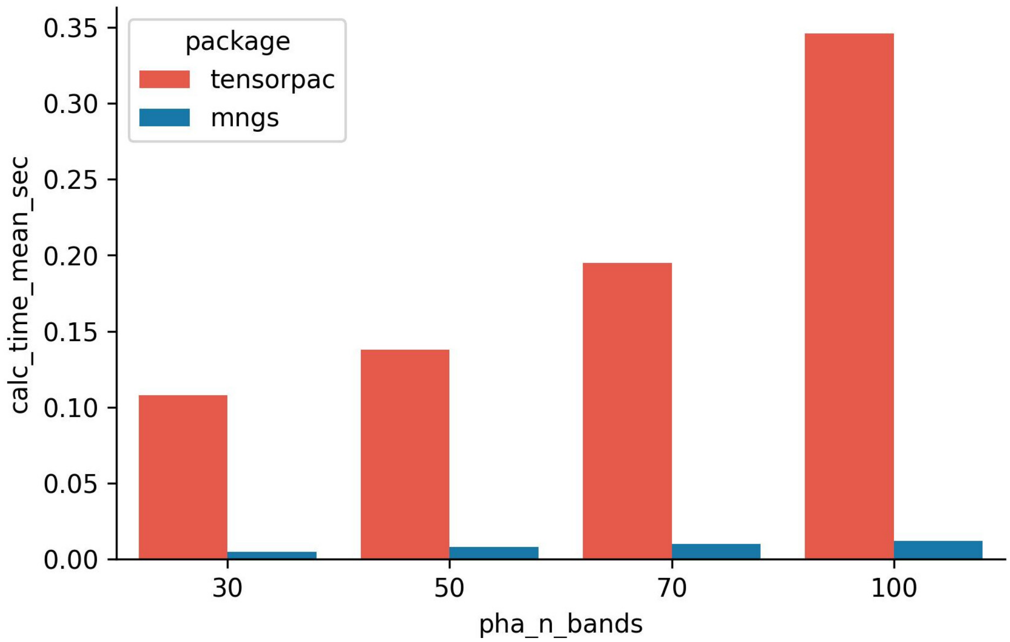

Figure 7 – Effect of Phase Band Count on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Number of Phase Bands

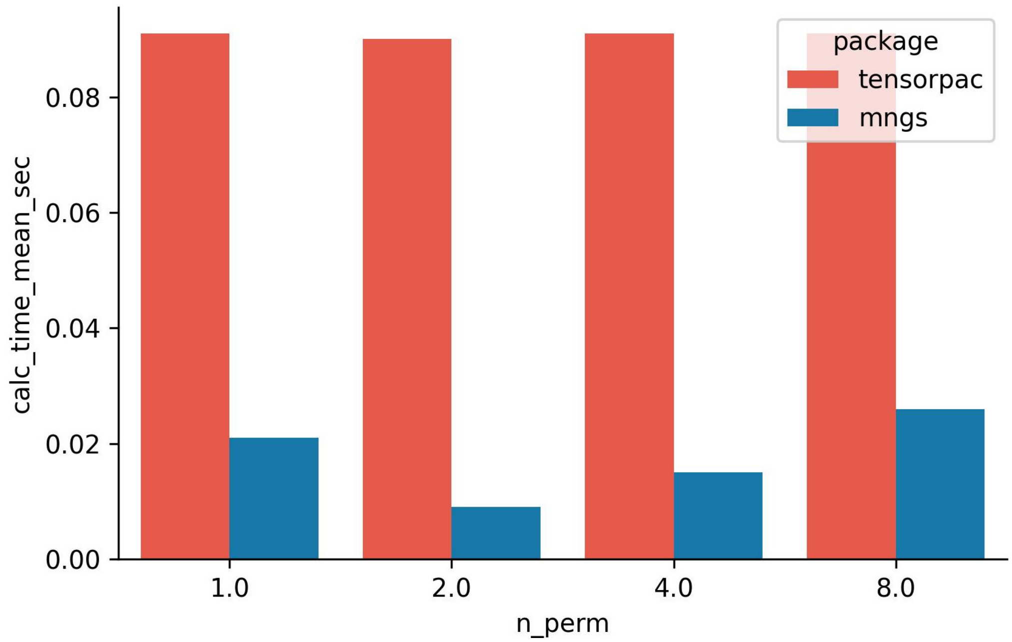

Figure 8 – Effect of Permutation Count on Processing Speed

Processing Times for Tensorpac (CPU) and TorchPAC (GPU) across Number of Permutations