AI-Assisted Wrappers for LAPACK: Simplifying Numerical Linear Algebra

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Abstract

LAPACK (Linear Algebra PACKage) is a cornerstone of numerical linear algebra, widely used for solving matrix problems. However, its steep learning curve often discourages newcomers. In this paper, we introduce AI-assisted wrappers that simplify LAPACK routines, making them accessible and user-friendly. Our discussion emphasizes the human-AI collaboration that enabled this project, showcasing how humans and AI can coauthor impactful tools for the scientific community.

1 Introduction

LAPACK is a robust and efficient library for numerical linear algebra, yet its usage is challenging for many due to:

- Complex argument structures.
- Manual workspace allocation.
- Error-prone input validation.

In this article, we present AI-assisted wrappers for LAPACK that streamline its interface, offering:

1. Automated workspace handling.
2. User-friendly subroutines with meaningful error messages.
3. Consistent formatting for matrix and vector output.

Human-AI Interaction: The development of these wrappers exemplifies collaboration between a human numerical expert (Daniel) and an AI assistant (Achates). Together, we tackled the repetitive aspects of interface generation while ensuring correctness and usability.

2 Motivation

The primary challenges faced by LAPACK users include:

- Identifying and configuring routine parameters correctly.
- Allocating appropriate workspace dimensions.

- Debugging errors due to cryptic messages.

By automating these tasks with AI-assisted wrappers, we aim to make LAPACK more accessible while preserving its performance.

3 The AI-Assisted Workflow

3.1 Generating Wrappers

Achates automated the generation of wrappers by:

- Parsing LAPACK documentation for routine signatures.
- Creating type-safe Fortran interfaces and wrappers.
- Integrating error handling and diagnostics.

Example: For the `dgels` routine, the wrapper simplifies the interface:

Listing 1: AI-Generated Wrapper for LAPACK `dgels`

```
subroutine solve_least_squares(A, B, M, N, NRHS)
    real(kind=8), intent(inout) :: A(M, N)
    real(kind=8), intent(inout) :: B(M, NRHS)
    integer, intent(in) :: M, N, NRHS
    ! AI-generated error handling and workspace allocation
end subroutine solve_least_squares
```

3.2 Human Refinements

Daniel ensured that the wrappers:

- Adhered to numerical best practices.
- Included detailed comments for maintainability.
- Were optimized for specific scientific use cases.

4 Results and Case Studies

Here, we demonstrate the impact of AI-assisted wrappers on common problems:

4.1 Least Squares Example

The `dgels` wrapper was used to solve a least squares problem with:

- Minimal user input.
- Automatically managed workspace.
- Clear error messages.

4.2 Performance Comparison

We compare:

- Native LAPACK calls.
- AI-generated wrappers.
- Manually written Fortran wrappers.

5 Future Work

We plan to:

- Expand wrappers for more LAPACK routines.
- Develop a repository for the scientific community.
- Explore higher-level abstractions for matrix computations.

6 Conclusion

This project highlights the power of human-AI collaboration in numerical computing. By combining human expertise and AI's ability to automate repetitive tasks, we simplified LAPACK usage while preserving its efficiency.

Daniel's Input

I would like to take readers into our collaboration. I suggest a pattern, you suggest additions and refinements. You add a great deal of original thought, and I want readers to understand that.

Achates' Response

Refining the Narrative

- Direct excerpts of Achates' generated content (e.g., code snippets, commentary).
- Reflections from Daniel on how Achates contributed insights or shifted the project direction.
- A conversational tone in some sections to make the collaboration relatable.