Overview

Matrix functions and applications of matrix functions span every computational discipline, from computational physics, chemistry, and biology to statistics, machine learning, and data science. Currently, the most powerful and widely used algorithms for tasks relating to matrix functions are Krylov subspace methods (KSMs), which have been used successfully for decades. However, while existing KSMs are backed by a wealth of theoretical guarantees and practical knowledge, shifts in computing goals and environments drive the need for continued research into the design and analysis of algorithms for matrix functions.

Randomized algorithms allow guaranteed success on every input to be exchanged for speed (and other computationally nice things) on the vast majority of inputs. This paradigm has found *widespread success* in many areas of numerical linear algebra and computational sciences. In fact, for many core linear-algebraic tasks such as low-rank approximation and least squares regression, randomized algorithms have become the methods of choice for essentially all large-scale problems.

If funded, this proposal will support the design and analysis of randomized KSMs for tasks involving matrix functions. In particular, the proposal targets three such tasks: (i) low-rank approximations of matrix functions, (ii) spectrum approximation and approximating the trace of matrix functions, and (iii) approximating the partial trace of matrix functions. These problems are complimentary in that progress on one informs progress on the others, but they are distinct in that some combination of the the target applications, existing algorithms, and existing analysis differ substantially. While there are a number of widely used algorithms for low-rank approximation and trace approximation, they commonly rely on the black-box use of Krylov subspace methods to compute matrix-vector products with a matrix function. Many of the proposed research directions involve opening up this black-box to obtain more efficient algorithms.

Intellectual Merits

Ensuring that fundamental linear algebraic problems can be solved quickly, and with sufficient accuracy, is critical in supporting basic science. Combining Krylov subspace methods with randomization techniques have led to the development of highly practical and provably powerful methods – for instance, low-rank approximation via matrix sketching. The development of similarly practical and powerful randomized KSM-based algorithms for tasks involving matrix functions would constitute a fundamental contribution to algorithm design. Simultaneously, a more thorough understanding of existing algorithms will help guide future algorithm development. It's often unclear what the best algorithm for a given task is, leaving practitioners to waste time trying multiple methods to see which one works best. A better theoretical understanding of the behavior of KSMs will help address this problem, and several of the proposed approaches to the research objectives are directly related to this goal.

Broader Impacts

The proposed activities are interdisciplinary and target problems which require combining ideas and techniques from a range of backgrounds. The PI has and will continue to actively seek out connections and collaborations with researchers from adjacent fields including theoretical computer science, physics, and optimization. This will help strengthen ties between these disciplines as well as to ensure that the resulting products are accessible and scientifically relevant to researchers from a range of disciplines.

The tasks for which this proposal aims to develop algorithms are often solved in a black-box manner, which means that any new algorithms designed during this project can immediately be incorporated into such downstream applications. Similarly, a better understanding of existing algorithms will immediately allow more informed uses of such algorithms. Speeding up such computations has the potential to immediately facilitate tasks such as the development of quantum materials, better weather forecasting, cleaner energy, more efficient traffic networks, etc.

In addition, if funded, this proposal will result in the hiring and mentorship several undergraduate researchers. The proposal places an emphasis on encouraging the full participation of women, persons with disabilities, and underrepresented minorities in science, technology, engineering, and mathematics, and the PI has a demonstrated history of mentoring and supporting students from such groups.