

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.

Recently, algorithms for solving linear systems based on randomized gradient estimates have emerged from the computer science and optimization communities. These algorithms have promising theoretical properties; for example, on certain types of linear systems of equations, they enjoy provably faster runtime guarantees than KSMs. However, compared to KSMs, these stochastic gradient methods are less easily adapted to problems involving matrix functions beyond the matrix inverse, and they are less amenable to parallelization and other hardware-based optimizations.

In this proposal, the PI seeks a mathematical science postdoctoral research fellowship (MSPRF) to conduct research and organize conference and seminar sessions on algorithms for fundamental linear algebraic tasks related to matrix functions. The proposed research objectives focus on combining the power of recent randomization techniques from theoretical computer science and optimization with the practicality of KSMs to design and analyze algorithms for solving linear systems and algorithms for computing general matrix functions and the product of matrix functions with vectors.

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 solving linear systems and computing matrix functions and products of matrix functions would constitute a fundamental contribution to algorithm design. Simultaneously, a better 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. As such the PI, whose background is in numerical linear algebra, has selected a sponsoring scientist from optimization and co-mentor from theoretical computer science. 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. Speeding up these computations has the potential to immediately facilitate tasks such as the development of better weather forecasting, cleaner energy, and more efficient traffic networks.

A MSPRF will also enable the PI to continue working towards building a more equitable and inclusive scientific community. Specifically, funding will afford the PI the time necessary to organize conference sessions and seminars whose participants are reflective of broader society and whose content is reflective of the societal goal of increased equity. During their PhD the PI has already organized several conference sessions and seminars which made significant strides towards these goals. The PI has also helped organize and served on many student panels related to grad student wellbeing, including panels on mental health and department climate, further demonstrating a commitment to community outreach.