Randomized matrix decompositions for faster scientific computing

Traditional numerical methods based on expensive matrix factorizations struggle with the scale of modern scientific applications. For example, kernel-based algorithms take a data set of size \( N \), form the kernel matrix of size \( N \times N \), and then perform an eigendecomposition or inversion at a cost of \( O(N^3) \) operations. For data sets of size \( N \geq 10^5 \), kernel learning is too expensive, straining the limits of personal workstations and even dedicated computing clusters. Randomized iterative methods have emerged as faster alternatives to the classical approaches. These algorithms combine random exploration of matrix structures with information about which structures are most important, leading to significant speed-ups.

In this talk, I review recent developments concerning two randomized algorithms. The first is "randomized block Krylov iteration", which uses an array of random Gaussian test vectors to probe a large data matrix in order to provide a randomized principal component analysis. Remarkably, this approach works well even when the matrix of interest is not low-rank. The second algorithm is "randomly pivoted Cholesky decomposition", which iteratively samples columns from a positive semidefinite matrix using a novelty metric and reconstructs the matrix from the randomly selected columns. Ultimately, both algorithms furnish a randomized approximation of an \( N \times N \) matrix with a reduced rank \( k \ll N \), which enables fast inversion or singular value decomposition at a cost of \( O(Nk^2) \) operations. The speed-up factor from \( N^3 \) to \( Nk^2 \) operations can be 3 million. The newest algorithms achieve this speed-up factor while guaranteeing performance across a broad range of input matrices.

Refreshments served at 3:30pm 4th floor Lounge – Amos Eaton
Biographical Sketch

Robert Webber is a postdoctoral scholar in Caltech's Department of Computing & Mathematical Sciences, hosted by Joel Tropp. He is interested in randomized numerical methods and their applications to data science and scientific computing. Specifically, Webber’s work focuses on:

- **Randomized algorithms**: developing and analyzing large-scale iterative methods that leverage randomness to overcome the limitations of traditional algorithms.
- **Interdisciplinary applications**: applying randomized algorithms to tackle problems in chemistry, astronomy, and geophysics through collaborations with domain experts.

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