Fast randomized linear algebra for electronic structure computations

Linear algebra is at the heart of many problems arising in modern applications. For instance, applications coming from quantum chemistry involve matrices that describe configurations and interactions of atomic particles. As a consequence of the enormous number of particles, those matrices are extremely large (e.g., $10^{20} \times 10^{20}$) and the use standard approaches to finite-dimensional eigenproblems or linear systems are far from reasonable. As running case study, we consider the computation of the ground state energy of a quantum mechanical system; this energy corresponds to the smallest eigenvalue of the Schrödinger-Hamiltonian operator

$$\mathcal{H}v = -\frac{1}{2} \Delta v + Uv,$$

where $\Delta$ is the Laplace operator and $U$ is a potential.

Recently, it has been proposed a general framework called Fast Randomized Iteration (FRI) \[1\] for running iterative schemes — based on matrix-vector operations — in case the problem size allows only to manipulate sparse vectors (i.e., containing many zero entries). The considered benchmark algorithm is the power method for computing eigenpairs $(\lambda, v)$:

$$Av = \lambda v.$$

The main idea is to start with a sparse initial guess $x$ and, at every iteration, enhance the sparsity of the outcome of $Ax$ by means of a randomized thresholding. In case of a non sparse $A \in \mathbb{C}^{n \times n}$ another randomized compression technique is applied on each row of $A$ in order to make the cost per iteration independent on $n$.

From the convergence point of view, the authors show that, under some assumptions on the compression technique and on the operator, the iterates have finite variance and the correspondent iterates of the deterministic power method as expected values. Therefore, the averages of the estimated eigenvalue and of the inner products of the (sparse) estimates of the eigenvector should converge to the exact quantities.

The project offer a balance between theory (linear algebra and probability theory or statistics), algorithmic developments, and implementation. The main goals of the project are:

- understand the interplay between the convergence properties and the assumptions on the randomized thresholding scheme,
- implement and test methods based on FRI for solving eigenvalue problems and linear systems.

Further investigations — depending on the development of the project — might concern

- a deeper understanding of the quantum chemistry application (still on the linear algebra side) that could lead to other extremely large scale problems,
- the use of data-sparse vectors (in place of sparse) such as Kronecker product of smaller vectors and alternative thresholding techniques (e.g. low-rank truncation).

Requirements

- Basic programming skills in Matlab (Julia or Python are also an option)
- Basic knowledge of linear algebra and probability theory

References


A talk (35 min) and corresponding slides about [1] can be found here: \url{http://www.birs.ca/events/2018/5-day-workshops/18w5023/videos/watch/201811131705-Weare.html}

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