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New Algebraic Fast Algorithms for N-Body Problems in Two and Three Dimensions

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Abstract. We present two new algebraic multilevel hierarchical matrix algorithms to perform fast matrix-vector product (MVP) for N-body problems in d dimensions, namely efficient $\mathcal{H}_*^2$ (fully nested algorithm, i.e., $\mathcal{H}^2$ matrix algorithm) and $(\mathcal{H}^2+\mathcal{H})_*$ (semi-nested algorithm, i.e., cross of $\mathcal{H}^2$ and $\mathcal{H}$ matrix algorithms). The efficient $\mathcal{H}_*^2$ and $(\mathcal{H}^2+\mathcal{H})_*$ hierarchical representations are based on our recently introduced weak admissibility condition in higher dimensions (Khan et al., J. Comput. Phys. 2024), where the admissible clusters are the far-field and the vertex-sharing clusters. Due to the use of nested form of the bases, the proposed hierarchical matrix algorithms are more efficient than the non-nested algorithms ($\mathcal{H}$ matrix algorithms). We rely on purely algebraic low-rank approximation techniques (e.g., ACA (Bebendorf et al., Computing 2003) and NCA (Bebendorf et al., Numer. Math. 2012; Gujjula and Ambikasaran, arXiv:2203.14832 2022; Zhao et al., IEEE Trans. Microw. Theory Tech. 2019)) and develop both algorithms in a black-box (kernel-independent) fashion. The initialization time of the proposed algorithms scales quasi-linearly, i.e., complexity $\mathcal{O}(N\log^{\alpha}(N))$, $\alpha \geq 0$ and small. Using the proposed hierarchical representations, one can perform the MVP that scales at most quasi-linearly. Another noteworthy contribution of this article is that we perform a comparative study of the proposed algorithms with different algebraic (NCA or ACA-based compression) fast MVP algorithms (e.g., $\mathcal{H}^2$, $\mathcal{H}$, etc.) in 2D and 3D ($d=2,3$). The fast algorithms are tested on various kernel matrices and applied to get fast iterative solutions of a dense linear system arising from the discretized integral equations and radial basis function interpolation. The article also discusses the scalability of the algorithms and provides various benchmarks. Notably, all the algorithms are developed in a similar fashion in `C++` and tested within the same environment, allowing for meaningful comparisons. The numerical results demonstrate that the proposed algorithms are competitive to the NCA-based standard $\mathcal{H}^2$ matrix algorithm (where the admissible clusters are the far-field clusters) with respect to the memory and time. The `C++` implementation of the proposed algorithms is available at `https://github.com/riteshkhan/H2weak/`.

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1 Introduction

Kernel matrices are frequently encountered in many fields such as PDEs [17,23,27], Gaussian processes [29], machine learning [16,33], inverse problems [31], etc. These kernel matrices are usually large and dense. A direct evaluation of the product of a $N\times N$ kernel matrix with vector is prohibitive as its time and space complexity scale as $\mathcal{O}(N^2)$. However, these matrices possess block low-rank structures, which can be leveraged to store and perform matrix operations. The literature on the block low-rank matrices is vast, and we do not intend to review it here. Instead, we refer to a few selected articles [9,11,22,35] and the books by Hackbusch [20] and Bebendorf [4].

In the past decades, various algorithms have been developed to perform the matrix-vector product efficiently. One of the first works in this area was the Barnes-Hut algorithm [3] or Tree code, which reduces the matrix-vector product complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(N\log(N))$. Greengard and Rokhlin [17, 18] propose the fast multipole method, which further reduces the matrix-vector product cost to $\mathcal{O}(N)$. After that, various FMM-like kernel-independent algorithms [34] were proposed, primarily based on analytic expansions. Hackbusch and collaborators [8,9] are the pioneers in interpreting certain sub-blocks (sub-matrices) of the matrices arising from N-body problems as low-rank and provide an important theoretical framework. In [8, 9, 15], they discuss the standard (or strong) admissibility condition, i.e., where the separation distance between two clusters exceeds the diameter of either cluster. It is to be noted that the FMM (equivalent to $\mathcal{H}^2$ matrix with standard admissibility) and the Tree code (equivalent to $\mathcal{H}$ matrix with standard admissibility) are based on the standard or strong admissibility condition. In their subsequent work [21], they introduce the notion of weak admissibility condition for one-dimensional problems. This article shows that the rank of interaction between the neighboring intervals in 1D does not scale as a positive power of N, and consequently, the neighboring or non-overlapping intervals are admissible. HODLR [1,2], HSS [11,32] and HBS [14] matrices belong to the category of $\mathcal{H}$ matrix based on this weak admissibility condition. However, the work [21] does not discuss the notion of weak admissibility condition in higher dimensions. A straightforward extension of this idea, i.e., compressing all the non-self interactions, does not result in a quasi-linear matrix-vector product algorithm in d dimensions ($d>1$) since the rank of the nearby clusters grows as $\mathcal{O}(N^{(d-1)/d}\log(N))$ [23,25].

In our recent work [25], we have shown that the rank of the far-field and the vertex-sharing interactions do not scale with any positive power of N. Hence, admissibility of the far-field and the vertex-sharing clusters could be a way to extend the notion of weak