CSIAM Trans. Appl. Math.
doi: 10.4208/csiam-am.2021.nla.02

Vol. **2**, No. 2, pp. 263-296
June 2021

Multi-Layer Hierarchical Structures

Jianlin Xia*

Department of Mathematics, Purdue University, West Lafayette, IN 47907, USA.

Received 10 July 2020; Accepted 5 October 2020

Abstract. In structured matrix computations, existing rank structures such as hierarchically semiseparable (HSS) forms admit fast and stable factorizations. However, for discretized problems, such forms are restricted to 1D cases. In this work, we propose a framework to break such a 1D barrier. We study the feasibility of designing multi-layer hierarchically semiseparable (MHS) structures for the approximation of dense matrices arising from multi-dimensional discretized problems such as certain integral operators. The MHS framework extends HSS forms to higher dimensions via the integration of multiple layers of structures, i.e., structures within the dense generator representations of HSS forms. Specifically, in the 2D case, we lay theoretical foundations and justify the existence of MHS structures based on the fast multipole method (FMM) and algebraic techniques such as representative subset selection. Rigorous numerical rank bounds and conditions for the structures are given. Representative subsets of points and a multi-layer tree are used to intuitively illustrate the structures. The MHS framework makes it convenient to explore multidimensional FMM structures. MHS representations are suitable for stable direct factorizations and can take advantage of existing methods and analysis well developed for simple HSS methods. Numerical tests for some discretized operators show that the appropriate inner-layer numerical ranks are significantly smaller than the off-diagonal numerical ranks used in standard HSS approximations.

AMS subject classifications: 15A23, 65F05, 65F30

Key words: MHS structure, numerical rank, representative subset, inner-layer structure, generator, fast multipole method.

1 Introduction

Rank structured matrices have been widely used for the fast direct solution of some integral and differential equations, especially elliptic problems. See [1,5,8,9,12,15,29,32,37,38,41] for a partial list of references. A basic idea of these methods is to approximate certain dense (intermediate) matrices or fill-in by rank structured forms. Such dense

*Corresponding author. *Email address:* `xiaj@purdue.edu` (J. Xia)

matrices include discretized integral operators, inverses of discretized PDEs, and Schur complements in the direct factorizations of some sparse matrices. PDE/integral equation theories together with linear algebra techniques have been used to show the existence of the rank structures. That is, appropriate off-diagonal blocks of these dense matrices have small numerical ranks.

Several rank structured representations have been designed for the approximation of these dense matrices. Among the most widely used ones are hierarchical structured representations such as $\mathcal{H}$ [4], $\mathcal{H}^2$ [5], and hierarchically semiseparable (HSS) matrices [8,42]. $\mathcal{H}/\mathcal{H}^2$ matrices and matrices based on the fast multipole method (FMM) are applicable to 2D and 3D cases. However, factorizations of such matrices usually involve recursion or inversion [6, 15] and their numerical behaviors such as stability are unclear. The HSS form mainly aims at 1D cases, and is essentially a special $\mathcal{H}^2$ form that explores the weak admissibility [19]. It is based on simple domain bisections and is thus easier to implement and analyze. It is also widely accessible to the general scientific computing community. In particular, efficient, stable, and scalable HSS operations (especially ULV-type factorizations [8, 42]) are available. Moreover, the hierarchical approximation accuracy and backward stability of HSS methods are well studied [33, 34]. For more general sparse problems, the applicability of HSS matrices can be extended via the integration into sparse matrix techniques such as nested dissection [11] and the multifrontal method [10].

Existing HSS-based structured direct solvers work well for 1D discretized integral equations and 2D discretized elliptic PDEs. However, the efficiency is usually less satisfactory for higher dimensions. It is possible to still approximate the dense matrices corresponding to two dimensions by HSS forms. Although this simplifies the implementation, the performance of the relevant matrix operations is far from optimal for large sizes due to the large off-diagonal numerical ranks.

In some recent studies, additional structures within some HSS approximations have been explored. In fact, it has been noticed that, in some applications, the dense blocks (called generators) that define the HSS forms are also structured [9, 18, 39, 43, 45]. By taking advantage of such structures, it is possible to design multi-dimensional structured algorithms for dense discretized matrices just based on simple HSS methods. For example, in a fast selected inversion algorithm [44], some diagonal and off-diagonal blocks of the inverse of a sparse matrix are approximated by HSS and low-rank forms, respectively. For some 2D discretized integral operators, the method in [9] exploits the inner structures with the aid of some integral equation techniques.

In this work, we lay theoretical foundations for a multi-layer hierarchically semiseparable (MHS) structure for multiple dimensions and design an MHS representation. We show the feasibility of using MHS forms to approximate some dense discretized matrices. We exploit multiple layers of hierarchial or tree structures under the general FMM framework. For some discretized matrices on 2D domains, if HSS forms are used for the approximation, we show that the dense generators have inner HSS or low-rank structures similarly to the work in [9]. Unlike the method in [9], we consider general FMM inter-