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# Low-rank Factorizations in Data Sparse Hierarchical Algorithms for Preconditioning Symmetric Positive Definite Matrices

EMMANUEL AGULLO\*, ERIC DARVE†, LUC GIRAUD‡, AND YUVAL HARNESST‡

**Abstract.** We consider the problem of choosing low-rank factorizations in data sparse matrix approximations for preconditioning large scale symmetric positive definite matrices. These approximations are memory efficient schemes that rely on hierarchical matrix partitioning and compression of certain sub-blocks of the matrix. Typically, these matrix approximations can be constructed very fast, and their matrix product can be applied rapidly as well. The common practice is to express the compressed sub-blocks by low-rank factorizations, and the main contribution of this work is the numerical and spectral analysis of SPD preconditioning schemes represented by  $2 \times 2$  block matrices, whose off-diagonal sub-blocks are low-rank approximations of the original matrix off-diagonal sub-blocks. We propose an optimal choice of low-rank approximations which minimizes the condition number of the preconditioned system, and demonstrate that the analysis can be applied to the class of hierarchically off-diagonal low-rank matrix approximations. Spectral estimates that take into account the error propagation through levels of the hierarchy which quantify the impact of the choice of low-rank compression on the global condition number are provided. The numerical results indicate that the properties of the preconditioning scheme using proper low-rank compression are superior to employing standard choices for low-rank compression. A major goal of this work is to provide an insight into how proper reweighted prior to low-rank compression influences the condition number for a simple case, which would lead to an extended analysis for more general and more efficient hierarchical matrix approximation techniques.

**Key words.** Preconditioning, Symmetric Positive Definite, Data Sparse, Hierarchical Algorithms, Low-rank Factorization, Minimal Condition Number

**AMS subject classifications.** 15A16, 15B99, 65F08, 65F30, 65F35, 65F50

**1. Introduction.** In this paper we consider preconditioning for iterative solution of large scale linear systems

$$(1) \quad Ax = b,$$

where  $A \in \mathbb{R}^{n \times n}$  is a *symmetric positive definite* (SPD) matrix. Such systems arise in a wide range of engineering applications, as means to model and understand physical phenomena. Typical example is the result of a finite element discretization of underlying differential equations of a boundary value problem. In many practical applications the matrix  $A$  becomes ill-conditioned and, thus, challenging for iterative techniques. In that case the use of preconditioned iterative methods, such as the *preconditioned conjugate gradient* (PCG) [19, 25] technique, becomes an imperative. The choice of a suitable preconditioning scheme can, often, drastically improve the convergence behavior of the iterative method and, generally, plays a vital role in the success of solving the system.

A preconditioning scheme for linear systems is, essentially, composed of linear operations or matrices that approximate  $A^{-1}$  (1), but with considerable less computational effort than explicitly inverting  $A$ . Transforming the system (1) with such a scheme is called the preconditioned system. The major concern when setting up a preconditioning scheme is to ensure that the preconditioned system has a bounded condition number, and that the number of iterations to convergence in an iterative method remains small while maintaining low associated complexity and reduced mem-

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45 ory cost. The literature on preconditioning techniques is vast, and many robust and  
 46 efficient methods have been introduced in the last 50 years. These include, among oth-  
 47 ers, incomplete factorization schemes such as ILU and Incomplete Cholesky, sparse  
 48 matrix approximations, polynomial techniques, domain decomposition methods, as  
 49 well as multigrid and algebraic multilevel iterations schemes. For a recent compre-  
 50 hensive review on this topic see [26].

51 The main contribution of this work is the numerical and spectral analysis of SPD  
 52 preconditioning schemes represented by  $2 \times 2$  block matrices, whose off-diagonal sub-  
 53 blocks are low-rank approximations of the original matrix off-diagonal sub-blocks. We  
 54 re-examine the way low-rank factorizations are obtained, by considering reweighting  
 55 of the sub-blocks prior to the low-rank compression. Reweighting can be done in  
 56 many ways, e.g., diagonal scaling, and the fundamental question that we attempt to  
 57 answer is: which reweighting is optimal with respect to the condition number of the  
 58 preconditioned system?

59 The mathematical theory for  $2 \times 2$  matrices is derived in [section 2](#). We present  
 60 an optimal 1-level preconditioning scheme using proper reweighting prior to low-rank  
 61 compression, which minimizes the spectral condition number of the preconditioned  
 62 system. Thus, a preconditioning scheme employing such low-rank factorizations is  
 63 expected to attain the same condition number with less computational resources and  
 64 associated complexity, compared to employing other standard techniques for the low-  
 65 rank factorizations. Spectral analysis shows that the scheme maps both small and  
 66 large eigenvalues of the original system exactly to 1. This feature is of great impor-  
 67 tance to Krylov subspace methods, since it is equivalent to the minimization of the  
 68 effective degree of the minimal polynomial of  $A$  that defines the maximal dimension  
 69 of the search space.

70 In [section 3](#) we propose an application of the 1-level theory for *hierarchically*  
 71 *off-diagonal low-rank* (HODLR) matrix structure, as means to demonstrate the ap-  
 72 plicability of the 1-level theory to the hierarchical multilevel case. We also provide  
 73 spectral estimates that take into account the error propagation through levels of the  
 74 hierarchy. This leads to quantification of the impact of the reweighting on the global  
 75 condition number of the preconditioned system. In essence, weighted HODLR lo-  
 76 cally minimizes the condition number at each level of the hierarchy by approximately  
 77 filtering the smallest and largest eigenvalues. Since this approach is employed hierar-  
 78 chically, it effectively creates a strong effect of global spectrum clustering.

79 The HODLR structure is a member of a wide class of hierarchical data sparse  
 80 approximations. These approximations rely on the fact that the matrix can be sub-  
 81 divided into a hierarchy of smaller block matrices, and certain sub-blocks can be effi-  
 82 ciently approximated as low-rank matrices by low-rank factorizations. The low-rank  
 83 compressions of sufficient sub-blocks leads to a dramatic reduction of the complexity  
 84 and computational cost. The best known example for such schemes is the class of hi-  
 85 erarchical matrix ( $\mathcal{H}$ -matrix) approximations [15, 17, 18, 5] which has gained growing  
 86 attention in recent years.

87 To the contrary of the more general strong hierarchical matrix structure which  
 88 allows further decomposition of the off-diagonal blocks into low-rank and full-rank  
 89 blocks, HODLR is a weak hierarchical matrix structure, which relies on a single low-  
 90 rank compression for the off-diagonal blocks. Closely related to HODLR is the *hier-*  
 91 *archically semi-separable* (HSS) [8, 28] structure, which is, in fact, a HODLR matrix  
 92 format possessing a nested off-diagonal low-rank structure.

93 Essentially, weak hierarchical methods, i.e., HODLR and HSS, are not considered  
 94 competitive with the more general strong hierarchical matrix methods, when the un-

95 derlying problem is of very large scale. However, the proposed study provides a novel  
 96 theoretical basis for optimality conditions of hierarchical preconditioning schemes.  
 97 Thus, the presented analysis can serve as starting point for a more general theory on  
 98 optimal  $\mathcal{H}$ -matrix preconditioning which is deferred to future work.

99 The weighted HODLR scheme is similar in nature to the methods proposed in  
 100 [29, 30] which propose practical HSS schemes that rely on similar ideas of reweighting  
 101 prior to compression, but without the complete numerical and spectral analysis of  
 102 this study. The costs to apply these multilevel preconditioners are about  $\mathcal{O}(n)$ , where  
 103  $n$  is the matrix size.

104 The experimental part of this work, whose goal is to demonstrate the effectiveness  
 105 of properly chosen reweighting for the low-rank approximations, is given in [section 4](#).  
 106 The section contains a detailed comparative study of HODLR preconditioning using  
 107 different methods for the low-rank compressions. As alternatives to the proper  
 108 reweighting strategy, we consider the conventional low-rank approximation in the  
 109 2-norm and the low-rank approximation with constraints [6]. The latter employs low-  
 110 rank approximations that also preserve constraints, forcing sub-blocks of the precon-  
 111 ditioning scheme to be identical to the corresponding sub-blocks of the input matrix  
 112 on predetermined subspaces. Employing the method for preconditioning SPD matrices  
 113 of discretized elliptic PDEs has been demonstrated in [7], and a similar approach  
 114 for non-symmetric sparse matrices has been recently suggested in [31].

115 The numerical results indicate, that employing proper reweighting prior to low-  
 116 rank compression, leads to a HODLR preconditioning scheme that requires far less  
 117 computational resources for the same quality of convergence performance compared  
 118 to using other low-rank compression techniques. The experiments also show, that the  
 119 HODLR preconditioning scheme with proper reweighting retains the SPD property  
 120 of the system when other standard techniques fail, and remains efficient and robust  
 121 even if low accuracy compression is employed with ranks of  $\mathcal{O}(1)$  for the low-rank  
 122 approximations of the sub-blocks. Summary and plans for future work follow in  
 123 [section 5](#).

124 **2. The Optimal One-level Preconditioning Scheme.** In this section we  
 125 introduce the optimal 1-level scheme for the preconditioning of SPD matrices. We  
 126 consider an input  $n \times n$  SPD matrix  $A$  with a  $2 \times 2$  block structure and a corresponding  
 127 1-level approximation  $K$ ,

$$128 \quad (2) \quad A = \begin{bmatrix} A_1 & M \\ M^T & A_2 \end{bmatrix}, \quad K = \begin{bmatrix} A_1 & U_1 S V_2^T \\ V_2 S U_1^T & A_2 \end{bmatrix}, \quad A_i \in \mathbb{R}^{n_i \times n_i},$$

129 where  $n = n_1 + n_2$ , and the off-diagonal blocks of  $K$  are low-rank factorizations  
 130 satisfying

$$131 \quad (3) \quad U_1 \in \mathbb{R}^{n_1 \times r}, \quad S \in \mathbb{R}^{r \times r}, \quad V_2 \in \mathbb{R}^{n_2 \times r},$$

132 with a, typically, small rank  $r$ . The matrix  $U_1$  is the *interpolation operator*, the matrix  
 133  $V_2$  is the *anterpolation operator*, and the matrix  $S$  whose rank is  $r$  is known as the  
 134 *interaction operator*. In some cases  $S$  is omitted, i.e., equivalently represented by an  
 135  $r \times r$  identity matrix.

136 We present an explicit formula for a 1-level approximation,  $K$  (2), which mini-  
 137 mizes the spectral condition number

$$138 \quad (4) \quad \text{cond}_2(R^{-T} A R^{-1}) = \|R^{-T} A R^{-1}\|_2 \cdot \|R A^{-1} R^T\|_2,$$

139 of the preconditioned system,

$$140 \quad (5) \quad R^{-T}AR^{-1}x = R^{-T}y,$$

141 for any given rank  $r = 0, 1, \dots, \min\{n_1, n_2\}$ , where  $\|\cdot\|_2$  is the 2-norm, and  $R$  denotes  
142 any square root (not necessarily principal) of  $K$  in the sense that

$$143 \quad (6) \quad K = R^T R \in \mathbb{R}^{n \times n}.$$

144 The key idea is to reweight the off-diagonal blocks prior the low-rank factorization.  
145 Proper choice of reweighting leads to a minimum spectral condition number of the  
146 preconditioned system as well as clustering of the spectrum of the preconditioned  
147 system around 1.

148 We begin in [subsection 2.1](#) by introducing the method for obtaining the minimum  
149 condition number low-rank approximation. In [subsection 2.2](#) we provide the theorem  
150 on the minimum condition number property, including a detailed description of the  
151 spectral properties of the preconditioned system. A rigorous and detailed proof of the  
152 theorem is given in [subsection 2.3](#).

153 **2.1. Explicit Formula of the Optimal One-level Scheme.** The construction  
154 of the minimum condition number 1-level preconditioner  $K$  [\(2\)](#) subject to

$$155 \quad (7) \quad \text{rk}(U_1 S V_2^T) \leq r,$$

156 is based on the following two-step method ensuring that the preconditioned matrix  
157  $R^{-T}AR^{-1}$  also inherits the SPD property of  $A$ :

158 1. Apply a two-sided block Jacobi transformation,

$$159 \quad (8) \quad \begin{bmatrix} R_1^{-T} & 0 \\ 0 & R_2^{-T} \end{bmatrix} \cdot A \cdot \begin{bmatrix} R_1^{-1} & 0 \\ 0 & R_2^{-1} \end{bmatrix} = \begin{bmatrix} I_1 & R_1^{-T} M R_2^{-1} \\ R_2^{-T} M^T R_1^{-1} & I_2 \end{bmatrix},$$

160 where  $I_i$  denotes the  $n_i \times n_i$  identity matrix, and  $R_i \in \mathbb{R}^{n_i \times n_i}$  denotes a  
161 square root of  $A_i$  i.e.,  $R_i^T R_i = A_i$ .

162 2. Extract the off-diagonal triple products [\(3\)](#) by setting,

$$163 \quad (9) \quad U_1 = R_1^T \mathcal{U}_r, \quad S = \Sigma_r = \text{diag}(\sigma_1, \dots, \sigma_r), \quad V_2 = R_2^T \mathcal{V}_r,$$

164 where  $\mathcal{U}_r$  and  $\mathcal{V}_r$  are composed of the first  $r$  left and right, respectively,  
165 singular vectors of the *singular value decomposition* (SVD),

$$166 \quad R_1^{-T} M R_2^{-1} = \mathcal{U} \Sigma \mathcal{V}^T, \quad \Sigma = \text{diag}(\sigma_1, \dots, \sigma_{\min\{n_1, n_2\}}).$$

167 The theory presented in this study implies, that in practice for a given rank bound  
168  $r \geq 0$ , any low-rank factorization,  $U_1 S V_2^T$ , satisfying

$$169 \quad \left\| R_2^{-T} M^T R_1^{-1} - R_2^{-T} U_1 S V_2^T R_1^{-1} \right\|_2 \leq \left\| R_2^{-T} M^T R_1^{-1} - \mathcal{U}_r \Sigma_r \mathcal{V}_r^T \right\|_2,$$

170 would achieve the same minimal spectral condition number. However, the truncated  
171 SVD of the reweighted off-diagonal block,  $\mathcal{U}_r \Sigma_r \mathcal{V}_r^T$ , also ensures that the spectrum of  
172 the preconditioned system is optimally clustered. This observation is discussed and  
173 explained in the next subsection.

174 **2.2. Minimal Condition Number and Spectral Analysis.** Let us now focus  
 175 on the spectral properties of the preconditioned system,  $R^{-T}AR^{-1}$ , where  $R$  is a  
 176 square root of  $K$  (2) whose off-diagonal low-rank blocks are given by (9). First, let  
 177 us consider the degenerate case  $r = 0$ . In this case  $U_1SV_2^T = 0$  and the square root  
 178 of  $K$  reduces to the following block diagonal form,

$$179 \quad (10) \quad R(r = 0) = \begin{bmatrix} R_1 & 0 \\ 0 & R_2 \end{bmatrix}.$$

180 The preconditioning scheme (5) with  $r = 0$  is, in fact, the two-sided block Jacobi (8).  
 181 There is a known result [12] showing that the two-sided block Jacobi preconditioner  
 182 (8) is optimal, in the sense that

$$183 \quad \text{cond}_2 \left( \begin{bmatrix} R_1^{-T} & 0 \\ 0 & R_2^{-T} \end{bmatrix} A \begin{bmatrix} R_1^{-1} & 0 \\ 0 & R_2^{-1} \end{bmatrix} \right) \leq \text{cond}_2 \left( \begin{bmatrix} B_1^T & 0 \\ 0 & B_2^T \end{bmatrix} A \begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix} \right),$$

184 for any non-singular  $\begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}$  with the same dimensions and partition as  $R(r = 0)$   
 185 (10). The analysis we present, thus, naturally extends this classic result.

186 The main results for the general case  $r \geq 0$  are presented in Theorem 1, whose  
 187 principal component is the spectral analysis of the preconditioned system. Our proof  
 188 shows that the spectrum of the two-sided block Jacobi preconditioned system (8)  
 189 contains (or equals to)

$$190 \quad 1 + \sigma_1, \dots, 1 + \sigma_{\min\{n_1, n_2\}}, 1 - \sigma_{\min\{n_1, n_2\}}, \dots, 1 - \sigma_1,$$

191 where  $1 - \sigma_1$  and  $1 + \sigma_1$  are the smallest and largest, respectively, eigenvalues of the  
 192 preconditioned system. Thus, the two-sided block Jacobi redistributes the spectrum of  
 193 the matrix symmetrically around 1. We show that the optimal 1-level preconditioning  
 194 scheme does the same, but also maps the largest  $r$  eigenvalues ( $1 + \sigma_1, \dots, 1 + \sigma_r$ ) and  
 195 the smallest  $r$  eigenvalues ( $1 - \sigma_r, \dots, 1 - \sigma_1$ ) of (8) exactly to 1. Hence, the spectral  
 196 condition number (4) as a function of  $r$  is

$$197 \quad \text{cond}_2 (R^{-T}AR^{-1}) = \frac{1 + \sigma_{r+1}}{1 - \sigma_{r+1}}.$$

198 An illustration of the spectral clustering done by the optimal 1-level preconditioning  
 199 scheme is displayed in Figure 1.

200 **THEOREM 1.** *Let*

$$201 \quad A = \begin{bmatrix} A_1 & M \\ M^T & A_2 \end{bmatrix}, \quad K = \begin{bmatrix} A_1 & U_1SV_2^T \\ V_2SU_1^T & A_2 \end{bmatrix},$$

202 *have the same dimensions and partition where  $A$  is SPD, and let  $R_i$  denote a square*  
 203 *root of  $A_i$ , i.e.,  $A_i = R_i^T R_i$ .*

204 *If the off-diagonal triple product approximation  $U_1SV_2^T$  satisfies*

$$205 \quad U_1 = R_1^T \mathcal{U}_r, \quad S = \Sigma_r, \quad V_2 = R_2^T \mathcal{V}_r,$$

206 *where  $\mathcal{U}_r$  and  $\mathcal{V}_r$  are composed of the first  $r$  left and right, respectively, singular vectors*  
 207 *of the SVD,*

$$208 \quad (11) \quad R_1^{-T}MR_2^{-1} = \mathcal{U}\Sigma\mathcal{V}^T, \quad \Sigma = \text{diag}(\sigma_1, \dots, \sigma_{\min\{n_1, n_2\}}),$$

209 *then:*

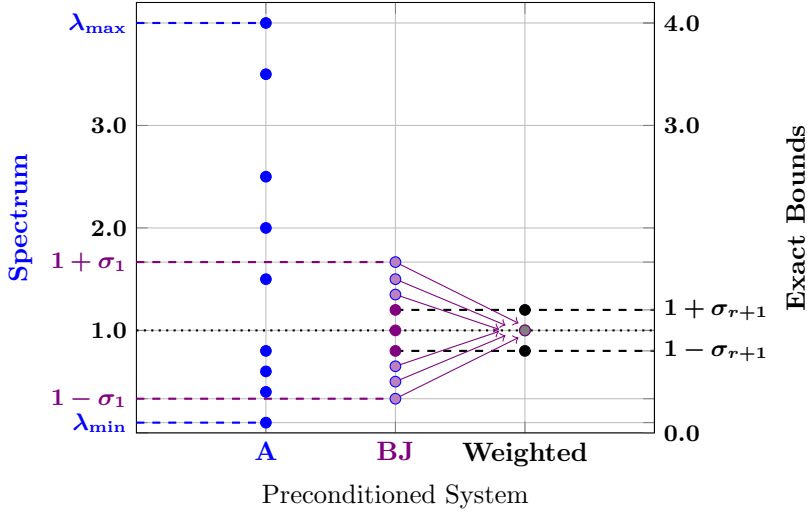


Fig. 1: **Spectrum Clustering of the Optimal 1-level Preconditioning Scheme.** The spectrum of some SPD matrix  $A$  and the transformations it goes after preconditioning by block Jacobi (BJ) and the optimal 1-level preconditioning scheme are displayed. The spectra are ordered from the left to the right starting from  $A$ , followed by BJ and end up with the optimal scheme.

- 210 1. The matrix  $K$  is SPD and possesses a square root,  $R$ , i.e.,  $K = R^T R$ .  
 211 2. For any  $r < \min\{n_1, n_2\}$  and any square root  $R$ , the spectrum of the pre-  
 212 conditioned system is contained in  $]0, 2[$  and equal to

$$213 \quad \{1 + \sigma_{r+1}, \dots, 1 + \sigma_{\min\{n_1, n_2\}}, 1, 1 - \sigma_{\min\{n_1, n_2\}}, \dots, 1 - \sigma_{r+1}\}.$$

- 214 3. Any inverse square root of  $K$ ,  $R^{-1}$ , is a minimizer of the spectral condition  
 215 number (4) in the sense that

$$216 \quad \text{cond}_2(R^{-T} A R^{-1}) \leq \text{cond}_2(\widehat{R}^{-T} A \widehat{R}^{-1}), \quad \widehat{R}^T \widehat{R} = \widehat{K},$$

217 for any SPD matrix with the same dimensions and partition as  $K$  of the form,

$$218 \quad \widehat{K} = \begin{bmatrix} A_1 & \widehat{M} \\ \widehat{M}^T & A_2 \end{bmatrix},$$

219 whose off-diagonal blocks satisfy  $\text{rk}(\widehat{M}) \leq r$ .

220 **2.3. Proof of Theorem 1.** The proof of [Theorem 1](#) regarding the spectral  
 221 properties relies on [Lemma 1](#), while the minimum condition number property is based  
 222 on the *Cauchy (eigenvalue) interlacing theorem* [23, p. 202]. The latter asserts that  
 223 the eigenvalues of any principal submatrix of a symmetric matrix interlace those of  
 224 the symmetric matrix. To be precise, if  $H \in \mathbb{R}^{n \times n}$  is a partitioned symmetric matrix  
 225 of the following form

$$226 \quad H = \begin{bmatrix} E & F \\ F^T & G \end{bmatrix},$$

227 in which  $E$  is a  $r \times r$  principal submatrix, then for each  $i = 1, \dots, r$ ,

$$228 \quad (12) \quad \lambda_i(H) \geq \lambda_i(E) \geq \lambda_{i+n-r}(H),$$

229 where the eigenvalues of the symmetric matrix  $H$  are assumed to be arranged in a  
230 decreasing order:

$$231 \quad \lambda_1(H) \geq \lambda_2(H) \geq \dots \geq \lambda_n(H).$$

232 **LEMMA 1.** *Let  $H = \begin{bmatrix} \delta I_1 & \mathcal{M} \\ \mathcal{M}^T & \delta I_2 \end{bmatrix} \in \mathbb{R}^{(n_1+n_2) \times (n_1+n_2)}$  where  $I_i$  is the  $n_i \times n_i$  identity  
233 matrix and  $\delta \in \mathbb{R}$ , and let  $\sigma_1, \dots, \sigma_{\min\{n_1, n_2\}}$  denote the singular values of  $\mathcal{M}$ .*

234 1. *If  $n_1 = n_2$  then*

$$235 \quad \text{spec}(H) = \{\delta - \sigma_1, \dots, \delta - \sigma_{n_1}, \delta + \sigma_{n_1}, \dots, \delta + \sigma_1\}.$$

236 2. *If  $n_1 \neq n_2$  then*

$$237 \quad \text{spec}(H) = \{\delta - \sigma_1, \dots, \delta - \sigma_{\min\{n_1, n_2\}}, \delta + \sigma_{\min\{n_1, n_2\}}, \dots, \delta + \sigma_1\} \cup \{\delta\},$$

238 *where the multiplicity of the eigenvalue  $\delta$  is at least  $|n_1 - n_2|$ .*

239 *Proof.* of **Lemma 1.**

240 Let us assume without the loss of generality that  $n_1 \geq n_2 = m$  and let

$$241 \quad \mathcal{M} = \mathcal{U}\Sigma\mathcal{V}^T, \quad \mathcal{U} \in \mathbb{R}^{n_1 \times n_2}, \quad \mathcal{V} \in \mathbb{R}^{n_2 \times n_2},$$

242 denote the SVD of  $\mathcal{M}$ . Let

$$243 \quad (13) \quad \mathcal{W} = \frac{1}{\sqrt{2}} \begin{bmatrix} \tilde{\mathcal{U}} & \mathcal{U} \\ \tilde{\mathcal{V}} & -\mathcal{V} \end{bmatrix} \in \mathbb{R}^{n \times n},$$

244 whose blocks are given by

$$245 \quad \tilde{\mathcal{U}} = \begin{cases} \mathcal{U} & \text{if } n_1 = n_2 \\ [u \ \sqrt{2}u^\perp] & \text{if } n_1 > n_2 \end{cases}, \quad \tilde{\mathcal{V}} = \begin{cases} \mathcal{V} & \text{if } n_1 = n_2 \\ [\mathcal{V} \ 0] & \text{if } n_1 > n_2 \end{cases},$$

246 where  $u^\perp$  is an  $n_1 \times (n_1 - n_2)$  matrix with orthonormal columns, whose range is  
247 orthogonal to the range of  $u$ ,

$$248 \quad u^T u^\perp = 0 \in \mathbb{R}^{n_2 \times (n_1 - n_2)}.$$

249 Direct calculations show that  $\mathcal{W}$  is an orthonormal matrix satisfying

$$250 \quad \mathcal{W}^T \begin{bmatrix} 0 & \mathcal{M} \\ \mathcal{M}^T & 0 \end{bmatrix} \mathcal{W} = \begin{bmatrix} \mathcal{S}_1 & 0 \\ 0 & -\mathcal{S}_2 \end{bmatrix},$$

251 where  $\mathcal{S}_i = \text{diag}[\sigma_1, \dots, \sigma_{\min\{n_1, n_2\}}, 0, \dots, 0] \in \mathbb{R}^{n_i \times n_i}$ . Thus, by the orthogonality  
252 of  $\mathcal{W}$  we obtain

$$253 \quad \mathcal{W}^T \begin{bmatrix} \delta I_1 & \mathcal{M} \\ \mathcal{M}^T & \delta I_2 \end{bmatrix} \mathcal{W} = \begin{bmatrix} \delta I_1 + \mathcal{S}_1 & 0 \\ 0 & \delta I_2 - \mathcal{S}_2 \end{bmatrix}.$$

254 Hence, the spectrum of  $H$  is given by

$$255 \quad \text{spec}(H) = \{\delta - \sigma_1, \dots, \delta - \sigma_{\min\{n_1, n_2\}}, \delta + \sigma_{\min\{n_1, n_2\}}, \dots, \delta + \sigma_1\} \cup \{\delta\},$$

256 where the multiplicity of  $\delta$  is at least  $n_1 - n_2$ . Note that in case  $n_2 > n_1$ , we can  
257 simply interchange the principal blocks of  $H$  by reordering the columns and rows of  
258  $H$ , and repeat the proof.  $\square$



259 *Proof.* of [Theorem 1](#).

260 Let  $\widehat{K}$  be a partitioned SPD matrix with the same dimensions and partition as  $K$  (2)  
261 whose off-diagonal blocks rank is bounded by  $r$ ,

$$262 \quad \widehat{K} = \begin{bmatrix} A_1 & U_1 S V_2^T \\ V_2 S U_1^T & A_2 \end{bmatrix}, \quad \text{rk}(U_1 S V_2^T) \leq r.$$

263 If  $(\lambda, \zeta) \in \mathbb{R} \times \mathbb{R}^n$  is an eigenpair of the preconditioned matrix

$$264 \quad (14) \quad \widehat{R}^{-T} A \widehat{R}^{-1}, \quad \widehat{K} = \widehat{R}^T \widehat{R},$$

265 then by employing the change of variables,  $\zeta = \widehat{R} \xi$ , we obtain

$$266 \quad \widehat{R}^{-T} A \widehat{R}^{-1} \zeta = \lambda \zeta \Leftrightarrow \widehat{R}^{-T} A \xi = \lambda \widehat{R} \xi \Leftrightarrow \widehat{R}^{-1} \widehat{R}^{-T} A \xi = \lambda \xi.$$

267 Since  $\widehat{R}^{-1} \widehat{R}^{-T} = \widehat{K}^{-1}$ , we conclude that regardless to the particular choice of square  
268 root,  $\widehat{R}$ , the spectrum of the preconditioned system (14) remains unchanged.

269 Let  $R_i \in \mathbb{R}^{n_i \times n_i}$  denote a, generally, non-symmetric square root of  $A_i$ . By direct  
270 calculations we obtain

$$271 \quad (15) \quad \begin{bmatrix} R_1^{-T} & 0 \\ 0 & R_2^{-T} \end{bmatrix} A \begin{bmatrix} R_1^{-1} & 0 \\ 0 & R_2^{-1} \end{bmatrix} = \begin{bmatrix} I_1 & R_1^{-T} M R_2^{-1} \\ R_2^{-T} M^T R_1^{-1} & I_2 \end{bmatrix},$$

272 and by [Lemma 1](#), the spectrum of (15) is contained in (or equal to)

$$273 \quad \{1 + \sigma_1, \dots, 1 + \sigma_{\min\{n_1, n_2\}}, 1, 1 - \sigma_{\min\{n_1, n_2\}}, \dots, 1 - \sigma_1\},$$

274 where  $\sigma_i$  are the singular values of  $R_1^{-T} M R_2^{-1}$ . Since  $R_i$  are non-singular, the pre-  
275 conditioned matrix (15) is SPD. Hence, we have

$$276 \quad 1 - \sigma_1 > 0 \quad \Rightarrow \quad \text{spec} \left( \begin{bmatrix} I_1 & R_1^{-T} M R_2^{-1} \\ R_2^{-T} M^T R_1^{-1} & I_2 \end{bmatrix} \right) \subset ]0, 2[.$$

277 Consider the specific choice of inverse square root of  $\widehat{K}$ ,

$$278 \quad \widehat{R}^{-1} = \begin{bmatrix} R_1^{-1} & 0 \\ 0 & R_2^{-1} \end{bmatrix} \widehat{\mathcal{W}} \widehat{\mathcal{D}}^{-1/2} \widehat{\mathcal{W}}^T, \quad \widehat{\mathcal{D}} = \begin{bmatrix} I_1 + \widehat{\mathcal{S}}_{1,r} & 0 \\ 0 & I_2 - \widehat{\mathcal{S}}_{2,r} \end{bmatrix}.$$

279 The matrix  $\widehat{\mathcal{W}}$  is orthogonal of the same form as (13) in the proof of [Lemma 1](#)  
280 with respect to (15), and  $\widehat{\mathcal{S}}_{i,r} = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in \mathbb{R}^{n_i \times n_i}$  where  $\sigma_i$  are the  
281 singular values of  $R_1^{-T} U_1 S V_2^T R_2^{-1}$ . Setting the choice  $\widehat{R}^{-1}$  into (4) and employing  
282 the fact that the 2-norm is invariant under unitary transformations, we obtain

$$283 \quad \text{cond}_2(\widehat{R}^{-T} A \widehat{R}^{-1}) = \left\| \widehat{\mathcal{D}}^{-1/2} H \widehat{\mathcal{D}}^{-1/2} \right\|_2 \left\| \widehat{\mathcal{D}}^{1/2} H^{-1} \widehat{\mathcal{D}}^{1/2} \right\|_2,$$

284 where  $H$  is an SPD matrix given by

$$285 \quad H = \widehat{\mathcal{W}}^T \mathcal{W} \mathcal{D} \mathcal{W}^T \widehat{\mathcal{W}}, \quad \mathcal{D} = \begin{bmatrix} I_1 + \mathcal{S}_{1,m} & 0 \\ 0 & I_2 - \mathcal{S}_{2,m} \end{bmatrix}.$$

286 The matrices  $\mathcal{W}$  (13) and  $\mathcal{S}_{i,m}$  are defined and constructed in the proof of [Lemma 1](#).  
287 Note that like  $\widehat{\mathcal{W}}$ , the matrix  $\mathcal{W}$  is orthogonal. Hence, the product  $\mathcal{W}^T \widehat{\mathcal{W}}$  is also an  
288 orthogonal matrix.

289 Our definitions so far indicate that the following diagonal matrices,

$$290 \quad \underline{\mathcal{D}} = \begin{bmatrix} I_1 & 0 \\ 0 & (I_2 - \widehat{\mathcal{S}}_{2,r}) \end{bmatrix}, \quad \overline{\mathcal{D}} = \begin{bmatrix} (I_1 + \widehat{\mathcal{S}}_{1,r}) & 0 \\ 0 & I_2 \end{bmatrix}.$$

291 bound the diagonal matrix  $\widehat{\mathcal{D}}$

$$292 \quad \underline{\mathcal{D}} \leq \widehat{\mathcal{D}} \leq \overline{\mathcal{D}}$$

293 in the sense that  $(\widehat{\mathcal{D}} - \underline{\mathcal{D}})$  and  $(\overline{\mathcal{D}} - \widehat{\mathcal{D}})$  are non-negative definite. Thus, applying

294 the change of variables  $\xi = \widehat{\mathcal{D}}^{-1/2}x$  and exploiting the properties of the Rayleigh  
295 quotient, we can write

$$296 \quad \left\| \widehat{\mathcal{D}}^{-1/2}H\widehat{\mathcal{D}}^{-1/2} \right\|_2 = \max_{x \neq 0} \frac{x^T \widehat{\mathcal{D}}^{-1/2}H\widehat{\mathcal{D}}^{-1/2}x}{x^T x} = \max_{\xi \neq 0} \frac{\xi^T H \xi}{\xi^T \widehat{\mathcal{D}} \xi}$$

$$297 \quad (16) \quad \geq \max_{\xi \neq 0} \frac{\xi^T H \xi}{\xi^T \overline{\mathcal{D}} \xi} = \max_{y \neq 0} \frac{y^T \overline{\mathcal{D}}^{-1/2}H\overline{\mathcal{D}}^{-1/2}y}{y^T y} = \left\| \overline{\mathcal{D}}^{-1/2}H\overline{\mathcal{D}}^{-1/2} \right\|_2,$$

299 where  $y = \overline{\mathcal{D}}^{-1/2}\xi$ . Using the same arguments it can also be shown that

$$300 \quad \left\| \widehat{\mathcal{D}}^{1/2}H^{-1}\widehat{\mathcal{D}}^{1/2} \right\|_2 \geq \left\| \underline{\mathcal{D}}^{1/2}H^{-1}\underline{\mathcal{D}}^{1/2} \right\|_2.$$

301 Let  $Z = \text{span}\{e_{r+1}, \dots, e_n\}$  where  $e_i$  denotes the  $i$ -th canonical basis vector, and  
302 let  $P_Z$  denote the orthogonal projection matrix on  $Z$ . The structure of  $\overline{\mathcal{D}}$  implies

$$303 \quad \left\| \overline{\mathcal{D}}^{-1/2}H\overline{\mathcal{D}}^{-1/2} \right\|_2 \geq \max_{P_Z y \neq 0} \frac{(P_Z y)^T \overline{\mathcal{D}}^{-1/2}H\overline{\mathcal{D}}^{-1/2}P_Z y}{(P_Z y)^T P_Z y} = \max_{P_Z y \neq 0} \frac{(P_Z y)^T H P_Z y}{(P_Z y)^T P_Z y}.$$

304 Essentially,  $P_Z^T H P_Z$  represents an  $(n-r) \times (n-r)$  principal block of a unitarily  
305 equivalent matrix of  $H$  whose eigenvalues are identical to  $H$ . Thus, by the Cauchy  
306 interlacing theorem (12),

$$307 \quad \left\| \overline{\mathcal{D}}^{-1/2}H\overline{\mathcal{D}}^{-1/2} \right\|_2 \geq \lambda_{r+1}(H) = 1 + \sigma_{r+1}.$$

308 Applying similar arguments it can also be shown that

$$309 \quad \left\| \underline{\mathcal{D}}^{1/2}H^{-1}\underline{\mathcal{D}}^{1/2} \right\|_2 \geq \lambda_{r+1}(H^{-1}) = \frac{1}{1 - \sigma_{r+1}},$$

310 which leads to the following lower bound on the spectral condition number,

$$311 \quad \text{cond}_2(R^{-T}AR^{-1}) \geq \frac{1 + \sigma_{r+1}}{1 - \sigma_{r+1}}.$$

312 Finally, let us consider the specific choice  $U_1 S V_2^T = R_1^T \mathcal{U}_r \Sigma \mathcal{V}_r^T R_2$  where  $\mathcal{U}_r$  and  
313  $\mathcal{V}_r$  are composed of the first  $r$  columns of  $\mathcal{U}$  and  $\mathcal{V}$ , respectively, in the SVD of  
314  $R_1^{-T} M R_2^{-1}$ . Consequently, we have  $\sigma_i = \sigma_i$ ,  $i = 1, \dots, r$ . Thus, setting accordingly  
315  $\widehat{\mathcal{W}} = \mathcal{W}$  and  $\widehat{R} = R$  we obtain by direct calculations:

$$316 \quad \text{cond}_2(R^{-T}AR^{-1}) = \left\| R^{-T}AR^{-1} \right\|_2 \left\| RA^{-1}R^T \right\|_2 = \frac{1 + \sigma_{r+1}}{1 - \sigma_{r+1}},$$

317 and the proof is complete.  $\square$

318 **3. The Multilevel Weighted HODLR Preconditioning Scheme.** In this  
 319 section we introduce the multilevel HODLR preconditioning scheme for SPD matrices.  
 320 The method is based on the theory presented in [section 2](#) and relaxation of the original  
 321 problem. The motivation is twofold. First we demonstrate that the 1-level analysis  
 322 can be extended to a multilevel preconditioning scheme. Second, we provide spectral  
 323 bounds on the eigenvalues of the preconditioned system which give account for error  
 324 propagation through the levels of the hierarchy.

325 In [subsection 3.1](#) we give a brief review of the HODLR matrix structure which  
 326 will be employed throughout the remainder of this paper. We focus on the symmetric  
 327 case, since this work is concerned with the preconditioning of SPD matrices. In  
 328 [subsection 3.2](#) we introduce the preconditioning scheme, which is based on hierarchical  
 329 construction and fast application of the inverse square roots,  $R^{-1}$  and  $R^{-T}$ . In  
 330 [subsection 3.3](#) we briefly consider the associated memory and the computational costs  
 331 of constructing and applying the scheme. An in-depth spectral analysis is presented  
 332 in [subsection 3.4](#). Our analysis provides estimates of the spectral bounds of the  
 333 preconditioned system at each level, that take into account the approximation error  
 334 at the lower levels of the hierarchy. These bounds are, however, of qualitative nature  
 335 as they reflect a possible worst case scenario which is not likely to occur in practice.  
 336 A rigorous and detailed proof of the theory is given in [subsection 3.5](#).

337 **3.1. Symmetric HODLR Matrix Structure.** A symmetric HODLR matrix,  
 338  $K \in \mathbb{R}^{n \times n}$ , can be described in the following recursive manner,

$$339 \quad (17) \quad K = K_1^{(0)}, \quad K_k^{(\ell)} = \begin{bmatrix} K_{2k-1}^{(\ell+1)} & U_{2k-1}^{(\ell+1)} S_k^{(\ell)} V_{2k}^{(\ell+1)T} \\ V_{2k}^{(\ell+1)} S_k^{(\ell)} U_{2k-1}^{(\ell+1)T} & K_{2k}^{(\ell+1)} \end{bmatrix} \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}},$$

340 for  $\ell = 0, 1, \dots, L-1$  and  $k = 1, 2, \dots, 2^\ell$ , where  $\ell$  is the level of  $K_k^{(\ell)}$  in the hierarchy.  
 341 The triple products,  $U_{2k-1}^{(\ell+1)} S_k^{(\ell)} V_{2k}^{(\ell+1)T}$ , represent low-rank blocks in the sense that

$$342 \quad (18) \quad U_{2k-1}^{(\ell+1)} \in \mathbb{R}^{n_{2k-1}^{(\ell+1)} \times r_k^{(\ell)}}, \quad V_{2k}^{(\ell+1)} \in \mathbb{R}^{n_{2k}^{(\ell+1)} \times r_k^{(\ell)}}, \quad S_k^{(\ell)} \in \mathbb{R}^{r_k^{(\ell)} \times r_k^{(\ell)}},$$

343 where  $r_k^{(\ell)}$  is the rank of the corresponding off-diagonal block of  $K$ . Typically,  
 344  $r_k^{(\ell)} \ll n_{2k-1}^{(\ell+1)}, n_{2k}^{(\ell+1)}$ . An illustration of the hierarchical structure of  $K$  is displayed in  
 345 [Figure 2](#).

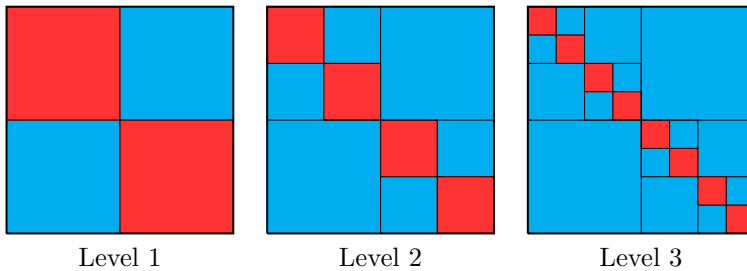


Fig. 2: **The HODLR Structure.** The first 3 levels,  $\ell = 1, 2, 3$ , of the HODLR structure are illustrated: at each level the blue color blocks are the low-rank off-diagonal blocks and the red blocks are the HODLR principal submatrices.

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The common practice is to set the HODLR matrix as an approximation of a given matrix,  $A \in \mathbb{R}^{n \times n}$ . The low-rank off-diagonal blocks of  $K$  satisfy

$$(19) \quad \left\| M_k^{(\ell)} - U_{2k-1}^{(\ell+1)} S_k^{(\ell)} V_{2k}^{(\ell+1)T} \right\|_2 \leq \tau_k^{(\ell)} \cdot \left\| M_k^{(\ell)} \right\|_2,$$

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where  $M_k^{(\ell)}$  denotes the corresponding off-diagonal block of  $A$  and  $\tau_k^{(\ell)} > 0$  is a chosen tolerance. Typically, a prior reordering of the matrix rows and columns is needed to confirm that  $r_k^{(\ell)}$  are, indeed, low.

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For obtaining low-rank approximations satisfying (19), the low-rank *singular value decomposition* (SVD) [14] which originated in [11] is, generally, considered the best choice, since it is optimal with respect to any unitarily invariant norm (2-norm, Frobenius). The computational cost required to obtain the SVD of  $M_k^{(\ell)}$  is relatively expensive necessitating an  $\mathcal{O}(m^3)$  operations, where  $m = n_k^{(\ell)}/2$ . For this reason a variety of fast approximation algorithms attempting to efficiently obtain a low-rank approximation close enough to the low-rank SVD have been proposed. These include, among others, the rank revealing LU [22], rank revealing QR [16], randomized algorithms [13, 20, 27], adaptive cross approximation [24] and boundary distance low-rank [2]. For more details see a review on this topic in [2].

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### 3.2. Recursive Formula of the Multilevel Preconditioning Scheme.

By our definitions (17) the principal blocks of  $K$  and the corresponding blocks of  $A$  are described by

$$(20) \quad K_k^{(\ell)} = \begin{bmatrix} K_{2k-1}^{(\ell+1)} & U_{2k-1}^{(\ell+1)} S_k^{(\ell)} V_{2k}^{(\ell+1)T} \\ V_{2k}^{(\ell+1)} S_k^{(\ell)} U_{2k-1}^{(\ell+1)T} & K_{2k}^{(\ell+1)} \end{bmatrix}, A_k^{(\ell)} = \begin{bmatrix} A_{2k-1}^{(\ell+1)} & M_k^{(\ell)} \\ M_k^{(\ell)T} & A_{2k}^{(\ell+1)} \end{bmatrix},$$

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where  $K_k^{(\ell)}, A_k^{(\ell)} \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}}$ , and the rank of each off-diagonal triple product approximation satisfies

$$(21) \quad \text{rk} \left( U_{2k-1}^{(\ell+1)} S_k^{(\ell)} V_{2k}^{(\ell+1)T} \right) \leq r_k^{(\ell)}.$$

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The key idea we propose is to construct each  $K_k^{(\ell)}$  as an optimal 1-level preconditioning scheme of the matrix

$$B_k^{(\ell)} = \begin{bmatrix} K_{2k-1}^{(\ell+1)} & M_k^{(\ell)} \\ M_k^{(\ell)T} & K_{2k}^{(\ell+1)} \end{bmatrix} \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}},$$

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which is obtained by replacing the principal blocks of  $A_k^{(\ell)}$  with the corresponding principal blocks of  $K_k^{(\ell)}$ . This is a relaxation of the original problem, which facilitates a fast construction method. The resulting preconditioned global system condition number is no longer ensured to be minimal. However, the numerical results in section 4 indicate that the proposed approach is highly robust and, in general, attains superior condition number compared to HODLR approximations using other low-rank approximation schemes.

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Before proceeding we introduce some necessary notations. Let  $R_k^{(\ell)} \in \mathbb{R}^{n_k^{(\ell)} \times n_k^{(\ell)}}$  denote the square root of  $K_k^{(\ell)}$  in the sense that  $K_k^{(\ell)} = R_k^{(\ell)T} R_k^{(\ell)}$ . Let  $\mathcal{U}_{k,r}^{(\ell)} \in$

382  $\mathbb{R}^{n_{2k-1}^{(\ell+1)} \times r_k^{(\ell)}}$  and  $\mathcal{V}_{k,r}^{(\ell)} \in \mathbb{R}^{n_{2k}^{(\ell+1)} \times r_k^{(\ell)}}$  be two thin matrices with orthogonal columns  
 383 composed of the first  $r_k^{(\ell)}$  left and right, respectively, singular vectors of the SVD,

$$384 \quad (22) \quad R_{2k-1}^{(\ell+1)-T} M_k^{(\ell)} R_{2k}^{(\ell+1)-1} = U_k^{(\ell)} \Sigma_k^{(\ell)} \mathcal{V}_k^{(\ell)T},$$

385 where  $\Sigma_{k,r}^{(\ell)} \in \mathbb{R}^{r_k^{(\ell)} \times r_k^{(\ell)}}$  is the principal submatrix of

$$386 \quad \Sigma_k^{(\ell)} = \text{diag}(\sigma_{k,1}^{(\ell)}, \dots, \sigma_{k, \min\{n_{2k-1}^{(\ell+1)}, n_{2k}^{(\ell+1)}\}}^{(\ell)}).$$

387 For brevity and clarity we will abuse the notation and employ  $U = U_{k,r}^{(\ell)}$  and  
 388  $\mathcal{V} = \mathcal{V}_{k,r}^{(\ell)}$ . The proof of [Theorem 1](#) implies that the following recursive formulas for a  
 389 fast application of the inverse square roots hold,

$$390 \quad R_k^{(\ell)-T} = \left( I + \frac{1}{2} \begin{bmatrix} \mathcal{U}_r & \mathcal{U}_r \\ \mathcal{V}_r & -\mathcal{V}_r \end{bmatrix} \begin{bmatrix} \mathcal{S}_r^+ - I & 0 \\ 0 & \mathcal{S}_r^- - I \end{bmatrix} \begin{bmatrix} \mathcal{U}_r^T & \mathcal{V}_r^T \\ \mathcal{U}_r^T & -\mathcal{V}_r^T \end{bmatrix} \right) \begin{bmatrix} R_{2k-1}^{(\ell+1)} & 0 \\ 0 & R_{2k}^{(\ell+1)} \end{bmatrix}^{-T},$$

391 and

$$392 \quad R_k^{(\ell)-1} = \begin{bmatrix} R_{2k-1}^{(\ell+1)} & 0 \\ 0 & R_{2k}^{(\ell+1)} \end{bmatrix}^{-1} \left( I + \frac{1}{2} \begin{bmatrix} \mathcal{U}_r & \mathcal{U}_r \\ \mathcal{V}_r & -\mathcal{V}_r \end{bmatrix} \begin{bmatrix} \mathcal{S}_r^+ - I & 0 \\ 0 & \mathcal{S}_r^- - I \end{bmatrix} \begin{bmatrix} \mathcal{U}_r^T & \mathcal{V}_r^T \\ \mathcal{U}_r^T & -\mathcal{V}_r^T \end{bmatrix} \right),$$

393 where  $\mathcal{S}_r^\pm = (I \pm \Sigma_{k,r}^{(\ell)})^{-\frac{1}{2}}$ . These formulas can be verified by writing the product  
 394  $R_k^{(\ell)-T} K_k^{(\ell)} R_k^{(\ell)-1}$  which, indeed, equals to the identity matrix, assuming  $K_k^{(\ell)}$  is SPD.

395 **3.3. Utilization and Construction of the Preconditioning Scheme.** The  
 396 recursive representations of  $R_k^{(\ell)-1}$  and  $R_k^{(\ell)-T}$  indicate that both matrices, essentially,  
 397 posses HODLR structure. Thus,  $R_k^{(\ell)-1}$  and  $R_k^{(\ell)-T}$  can be applied relatively fast in  
 398 matrix product operations. In the case that a constant average rank,  $r^{(\ell)} = \mathcal{O}(r)$ , is  
 399 taken for the off-diagonal blocks, the recursive representations implies the following  
 400 relation

$$401 \quad (23) \quad \mathcal{C}^{(\ell)}(m, n, r) = 2\mathcal{C}^{(\ell+1)}(m, n, r) + \mathcal{O}\left(m \cdot \frac{n}{2^\ell} \cdot r\right),$$

402 where  $\mathcal{C}^{(\ell)}(m, n, r)$  denotes the computational cost of the operation  $R_k^{(\ell)-T} \cdot F_k^{(\ell)}$  at  
 403 level  $\ell$ ,  $F_k^{(\ell)} \in \mathbb{R}^{n_k^{(\ell)} \times m}$ , and  $n_k^{(\ell)} = n^{(\ell)} = n/2^\ell$  is assumed. The first contribution in  
 404 [\(23\)](#) stems from the recursive calls of the inverse square roots of the diagonal blocks.  
 405 The second contribution is associated with the cost of the matrix product operations.  
 406 Expanding [\(23\)](#) into a sum yields the total computational cost estimate,

$$407 \quad \mathcal{C}^{(0)}(m, n, r) = \sum_{\ell=0}^{\log\left(\frac{n}{r}\right)} \mathcal{O}(m \cdot rn) = \mathcal{O}(m \cdot rn \log(n)),$$

408 where the depth of the hierarchy is set by  $n = 2^L r$ . Similarly, the cost of storing  
 409  $R_k^{(0)-1}$  and  $R_k^{(0)-T}$  is equal to  $\mathcal{O}(rn \log n)$  in the case where the average rank per  
 410 level,  $r^{(\ell)}$ , is of  $\mathcal{O}(r)$ . See [\[2\]](#) for further details. As noted in the introduction if the  
 411 HODLR scheme is generalized to HSS the costs to apply the preconditioner reduce to  
 412 about  $\mathcal{O}(n)$ , see [\[30\]](#) for further details.

413 Constructing the preconditioner is accomplished by performing a single pass over  
 414 the hierarchy from bottom to top. At each level  $\ell$  we compute the low-rank factor-  
 415 izations of the triple products

$$416 \quad (24) \quad R_{2k-1}^{(\ell+1)-T} M_k^{(\ell)} R_{2k}^{(\ell+1)-1}$$

417 where  $k = 1, 2, \dots, 2^\ell$ . Obtaining the low-rank factorization is performed by the  
 418 following procedure:

- 419 • Capture the range of (24) in a matrix  $Q_L^{(k,\ell)}$  whose columns are orthonormal,

$$420 \quad \left( I - Q_L^{(k,\ell)} Q_L^{(k,\ell)T} \right) \cdot R_{2k-1}^{(\ell+1)-T} M_k^{(\ell)} R_{2k}^{(\ell+1)-1} \approx \mathbf{0}, \quad Q_L^{(k,\ell)T} Q_L^{(k,\ell)} = I.$$

- 421 • Capture the range of the transpose of (24) in a matrix  $Q_R^{(k,\ell)}$  whose columns  
 422 are orthonormal,

$$423 \quad \left( I - Q_R^{(k,\ell)} Q_R^{(k,\ell)T} \right) \cdot R_{2k}^{(\ell+1)-T} M_k^{(\ell)T} R_{2k-1}^{(\ell+1)-1} \approx \mathbf{0}, \quad Q_R^{(k,\ell)T} Q_R^{(k,\ell)} = I.$$

- 424 • Compute the rank  $r^{(k,\ell)}$  truncated SVD of the reduced matrix,

$$425 \quad Q_L^{(k,\ell)T} \cdot R_{2k-1}^{(\ell+1)-T} M_k^{(\ell)} R_{2k}^{(\ell+1)-1} \cdot Q_R^{(k,\ell)} \approx U_{k,r}^{(\ell)} \Sigma_{k,r}^{(\ell)} V_{k,r}^{(\ell)}$$

- 426 • Reconstruct the WSVD left and right singular vectors matrices,

$$427 \quad \mathcal{U}_{k,r}^{(\ell)} = Q_L \cdot U_{k,r}, \quad \mathcal{V}_{k,r}^{(\ell)} = Q_R \cdot V_{k,r}.$$

428 If the effective rank of (24) is small, e.g.  $\mathcal{O}(1)$ , we can capture the range matrices,  
 429  $Q_L^{(k,\ell)}$  and  $Q_R^{(k,\ell)}$ , quickly by applying (24) and its transpose on a small set of random-  
 430 ized column vectors. See [21] for more details. However, if the effective rank of (24)  
 431 is not small, the procedure can become costly.

432 **3.4. Spectral Estimates and Error Propagation.** Let us now focus on the  
 433 spectral properties of the preconditioned submatrices,  $R_k^{(\ell)-T} A_k^{(\ell)} R_k^{(\ell)-1}$ , where  $R_k^{(\ell)}$   
 434 is the square root of the principal submatrix  $K_k^{(\ell)}$ . The submatrix  $A_k^{(\ell)}$  is given in  
 435 (20). Clearly the important case is  $\ell = 0$ , since we are ultimately interested in  
 436 preconditioning the input matrix,  $A = A_1^{(0)}$ .

437 For brevity and clarity we will abuse the notation and employ the following rep-  
 438 resentations in the spirit of section 2,

$$439 \quad K_k^{(\ell)} = \begin{bmatrix} K_1 & U_1 S V_2^T \\ V_2 S U_1^T & K_2 \end{bmatrix}, \quad A_k^{(\ell)} = \begin{bmatrix} A_1 & M \\ M^T & A_2 \end{bmatrix}, \quad R_i^T R_i = K_i \quad (i = 1, 2).$$

440 Note that  $R_i$  represents an approximate square root of  $A_i$ , as opposed to the exact  
 441 square root that was assumed in section 2. We make the fundamental assumption  
 442 that we have at our disposal spectral bounds estimates,

$$443 \quad (25) \quad \alpha_i \leq \lambda_{\min} (R_i^{-T} A_i R_i^{-1}) \leq \lambda_{\max} (R_i^{-T} A_i R_i^{-1}) \leq \beta_i \quad (i = 1, 2).$$

444 The lower-level bounds,  $\alpha_i$  and  $\beta_i$  ( $i = 1, 2$ ), can be obtained numerically, or possibly  
 445 estimated analytically by the theory presented in this subsection. Note that in the  
 446 case  $\ell = L - 1$  we have  $\alpha_i = 1 = \beta_i$ , and in the case  $\ell = L - 2$  we have from section 2  
 447 the exact bounds

$$448 \quad \alpha_i = \lambda_{\min} (R_i^{-T} A_i R_i^{-1}) = 1 - \sigma_{2k-2+i,r}^{(L-1)} \in (0, 1],$$

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$$\beta_i = \lambda_{\max} \left( R_i^{-T} A_i R_i^{-1} \right) = 1 + \sigma_{2k-2+i,r}^{(L-1)} \in [1, 2).$$

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The main result of the current subsection is presented in [Theorem 2](#). The theorem provides a description of the behavior of the current-level spectral bounds,

453 (26)

$$\alpha \leq \lambda_{\min} \left( R_k^{(\ell)-T} A_k^{(\ell)} R_k^{(\ell)-1} \right) \leq \lambda_{\max} \left( R_k^{(\ell)-T} A_k^{(\ell)} R_k^{(\ell)-1} \right) \leq \beta,$$

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as a function of the lower-level bounds [\(25\)](#) and the rank of the off-diagonal blocks,  $r = r_k^{(\ell)}$ . The definition of the bounds  $\alpha$  and  $\beta$  [\(26\)](#) is based on variational formulation and provided in [Lemma 2](#). The analysis requires sufficient (but not necessary) conditions on the given lower-level bounds,  $\alpha_i$  and  $\beta_i$  ( $i = 1, 2$ ). We show that the proposed HODLR preconditioning scheme, essentially, maps both the  $r$  largest and the  $r$  smallest eigenvalues to a closed segment containing 1. When this segment is small, the preconditioner retains optimality or near optimality. We also show that the sensitivity of the spectral bounds to the inaccuracies  $K_i \neq A_i$  ( $i = 1, 2$ ) is governed by the *Cauchy-Bunyakowski-Schwarz* (CBS) constant [\[3, 4\]](#).

463

**THEOREM 2.** *Let*

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$$A = \begin{bmatrix} A_1 & M \\ M^T & A_2 \end{bmatrix}, \quad K = \begin{bmatrix} K_1 & U_1 S V_2^T \\ V_2 S U_1^T & K_2 \end{bmatrix},$$

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*be symmetric matrices of the same dimensions and partition where  $A$  is SPD. Assume that the off-diagonal triple product approximation  $U_1 S V_2^T$  satisfy*

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$$U_1 = R_1^T \mathcal{U}_r, \quad S = \Sigma_r, \quad V_2 = R_2^T \mathcal{V}_r,$$

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*where  $\mathcal{U}_r$  and  $\mathcal{V}_r$  are composed of the first  $r$  left and right, respectively, singular vectors of the SVD,*

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$$R_1^{-T} M R_2^{-1} = \mathcal{U} \Sigma \mathcal{V}^T, \quad \Sigma = \text{diag}(\sigma_1, \dots, \sigma_{\min\{n_1, n_2\}}),$$

471

*and  $R_i^T R_i = K_i$  ( $i = 1, 2$ ).*

472

*Assuming there exist real positive constants,*

473 (27)

$$0 < \alpha_1, \alpha_2 \leq 1 \leq \beta_1, \beta_2,$$

474 *such that*

475 (28)

$$0 < \alpha_i x_i^T K_i x_i \leq x_i^T A_i x_i \leq \beta_i x_i^T K_i x_i \quad \forall x_i \in \mathbb{R}^{n_i},$$

476

*we have the following spectral estimates:*

477

1. *If  $\sigma_1 < \sqrt{\alpha_1 \alpha_2}$  then*

478 (29)

$$\alpha = \min \left\{ \alpha_{1,2}^{\text{avg}} - \sqrt{\sigma_{r+1}^2 + (\alpha_{1,2}^{\text{dif}})^2}, \quad \frac{\alpha_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} - \delta_{\alpha}^{1,2} \right\},$$

479

*where*

480

$$\alpha_{1,2}^{\text{avg}} = \frac{\alpha_1 + \alpha_2}{2}, \quad \alpha_{1,2}^{\text{dif}} = \frac{\alpha_1 - \alpha_2}{2}, \quad (\alpha = \alpha \text{ or } \beta),$$

481

*and*

482

$$\delta_{\alpha}^{1,2} = \sqrt{\frac{1}{4} \left| \frac{\alpha_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} - \frac{\alpha_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} \right|^2 + \frac{(\alpha_{1,2}^{\text{dif}})^2}{1 - \sigma_1^2}} - \frac{1}{2} \left| \frac{\alpha_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} - \frac{\alpha_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} \right|},$$

483

*is a positive lower spectral bound of the preconditioned system,*

484

$$0 < \alpha \leq \lambda \left( R^{-T} A R^{-1} \right), \quad K = R^T R.$$

485 2. If  $\sigma_1 < 1$  then

486 (30) 
$$\beta = \max \left\{ \beta_{1,2}^{\text{avg}} + \sqrt{\sigma_{r+1}^2 + (\beta_{1,2}^{\text{dif}})^2}, \frac{\beta_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} + \delta_\beta^{1,2} \right\},$$

487 where

488 
$$\beta_{1,2}^{\text{avg}} = \frac{\beta_1 + \beta_2}{2}, \quad \beta_{1,2}^{\text{dif}} = \frac{\beta_1 - \beta_2}{2}, \quad (\beta = \alpha \text{ or } \beta),$$

489 and

490 
$$\delta_\beta^{1,2} = \sqrt{\frac{1}{4} \left| \frac{\beta_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} - \frac{\beta_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} \right|^2 + \frac{(\beta_{1,2}^{\text{dif}})^2}{1 - \sigma_1^2} - \frac{1}{2} \left| \frac{\beta_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} - \frac{\beta_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} \right|}.$$

491 is an upper spectral bound of the preconditioned system,

492 
$$0 < \lambda(R^{-T}AR^{-1}) \leq \beta, \quad K = R^T R.$$

493 **REMARKS.** The justification for (27) is a consequence of [Theorem 2](#), which shows  
 494 that  $\alpha$  (29) and  $\beta$  (30) are monotonically non-increasing and non-decreasing as func-  
 495 tions of the level, respectively. This observation is also supported by numerical evi-  
 496 dence in [section 4](#). If  $\sqrt{\alpha_1 \alpha_2} \leq \sigma_1 < 1$ , then the preconditioned system remains SPD.  
 497 However, the theory presented here can not predict the positive value of the lower  
 498 spectral bound,  $\alpha$  (29).

499 From [Theorem 2](#) we observe that each estimated bound,  $\alpha$  or  $\beta$ , is a minimum  
 500 or a maximum, respectively, of two competing terms: the first depends on the largest  
 501 singular value,  $\sigma_1$ , and the second is a function of the truncation error,  $\sigma_{r+1}$ . In fact,  
 502 when the truncation error becomes sufficiently small it does not affect the values of  
 503 the bounds, which are governed solely by the terms depending on the largest singular  
 504 value. Thus in this case, improving the approximation by increasing the rank  $r$  does  
 505 not improve the corresponding condition number estimate,  $\beta/\alpha$ . An illustration of  
 506 this observation is given in [Figure 3](#).

507 The last observation as displayed in [Figure 3](#) indicates that the value of  $\sigma_1$  is cen-  
 508 tral to the estimation of the spectral bounds, and effectively dominates the condition  
 509 number of the preconditioned system. In this sense  $\sigma_1$  reflects the sensitivity of the  
 510 condition number of  $R_k^{(\ell)-T} A_k^{(\ell)} R_k^{(\ell)-1}$  to the lower level inaccuracies. It can be shown  
 511 that  $\sigma_1$  is the so-called *Cauchy-Bunyakowski-Schwarz* (CBS) constants of the matrix  
 512  $K$ , which is defined by

513 (31) 
$$\sigma_1 = \sup_{x_1, x_2 \neq 0} \frac{x_1^T M x_2}{\sqrt{x_1^T K_1 x_1} \sqrt{x_2^T K_2 x_2}} \geq 0.$$

514 Definition (31) originated from the theory of *Algebraic Multilevel Iterations Methods*  
 515 [3, 4], and coincides with the *principal angle* (cosine of the smallest angle) between the  
 516 column space of  $[I_1 \ 0]^T$  and the column space of  $[0 \ I_2]^T$  with respect to the inner  
 517 product  $\langle x, y \rangle_A = y^T A x$ . Thus,  $\sigma_1$  represents the local contribution of the upper  
 518 level to the overall condition number. Using (31) with assumption (27) leads to the  
 519 following relation

520 
$$\frac{1}{\sqrt{\beta_1 \beta_2}} \leq \frac{\sigma_1}{\sigma_1^{\text{exact}}} \leq \frac{1}{\sqrt{\alpha_1 \alpha_2}},$$

521 where  $\sigma_1^{\text{exact}}$  is the corresponding CBS constant of  $A$ . The important conclusion here  
 522 is that  $\sigma_1$  and  $\sigma_1^{\text{exact}}$  are correlated where  $\sigma_1^{\text{exact}}$  is intrinsically predetermined by the



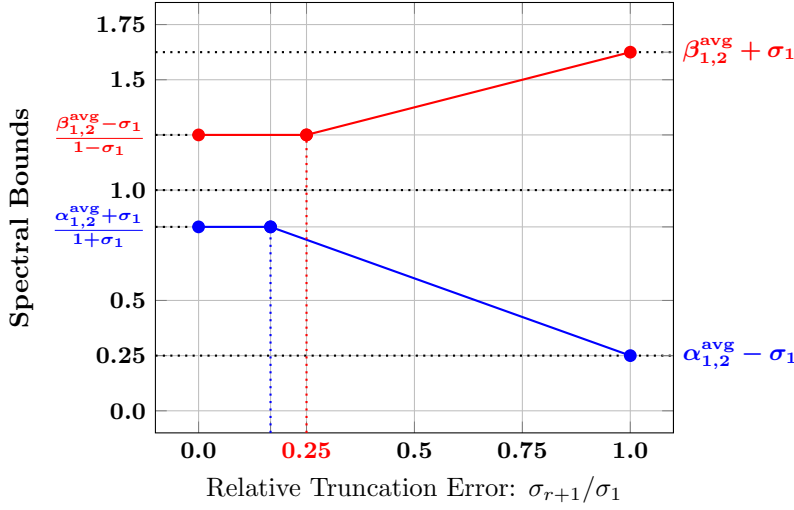


Fig. 3: **Spectral Bounds.** A typical behavior of the spectral bounds displayed for the case  $\alpha_1 = \alpha_2$  and  $\beta_1 = \beta_2$ . The lower bound  $\alpha$  (29) vs.  $\sigma_{r+1}/\sigma_1$  is plotted in blue, and the upper bound  $\beta$  (30) vs.  $\sigma_{r+1}/\sigma_1$  is plotted in red.

523 given matrix,  $A$ , and the chosen partition. If  $K$  is close to  $A$  then we can expect  $\sigma_1$   
 524 to be close to  $\sigma_1^{\text{exact}}$ , and in this case we have little influence over its value.

525 Regarding the spectrum of the preconditioned system, the interpretation of **The-**  
 526 **orem 2** is similar to the interpretation of **Theorem 1**. From the proof it can be inferred  
 527 that two-sided block Jacobi (i.e., the case  $r = 0$ ) effectively maps the spectra of the  
 528 bounding preconditioned systems to two segments centered around  $\alpha_{1,2}^{\text{avg}}$  and  $\beta_{1,2}^{\text{avg}}$ ,

$$529 \quad \left[ \alpha_{1,2}^{\text{avg}} - \sqrt{\sigma_1^2 + (\alpha_{1,2}^{\text{dif}})^2}, \quad \alpha_{1,2}^{\text{avg}} + \sqrt{\sigma_1^2 + (\alpha_{1,2}^{\text{dif}})^2} \right],$$

$$530$$

$$531 \quad \left[ \beta_{1,2}^{\text{avg}} - \sqrt{\sigma_1^2 + (\beta_{1,2}^{\text{dif}})^2}, \quad \beta_{1,2}^{\text{avg}} + \sqrt{\sigma_1^2 + (\beta_{1,2}^{\text{dif}})^2} \right].$$

532 The multilevel Weighted HODLR preconditioning scheme does the same, but also  
 533 maps the largest and smallest eigenvalues to the segments

$$534 \quad (32) \quad \left[ \frac{\sigma_1 + \alpha_{1,2}^{\text{avg}}}{1 + \sigma_1} - \delta_{\alpha}^{1,2}, \quad \frac{\sigma_1 - \alpha_{1,2}^{\text{avg}}}{1 - \sigma_1} + \delta_{\alpha}^{1,2} \right],$$

535

$$536 \quad (33) \quad \left[ \frac{\beta_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1} - \delta_{\beta}^{1,2}, \quad \frac{\beta_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1} + \delta_{\beta}^{1,2} \right],$$

537 respectively. Thus, assuming the segments (32) and (33) are small, a significant  
 538 improvement in the condition number as well as the clustering of the spectrum of the  
 539 original preconditioned system is expected. An illustration is given in **Figure 4**. The  
 540 figure is similar to **Figure 1** where the main difference is that the weighted HODLR  
 541 preconditioning scheme now maps the extreme eigenvalues to an interval containing  
 542 1 and not exactly to 1.

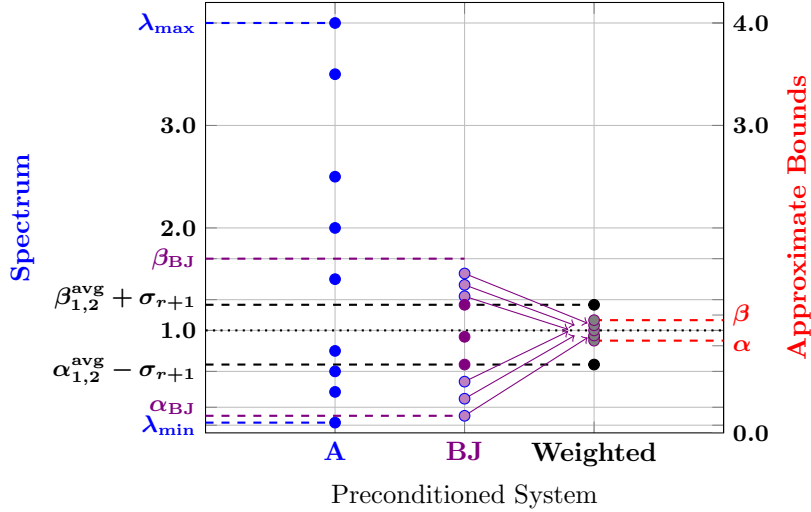


Fig. 4: **Spectrum Clustering for the Multilevel Weighted HODLR Preconditioning Scheme.** The spectrum of some SPD matrix  $A$  and the transformation it goes after preconditioning by block Jacobi (BJ) and the multilevel weighted HODLR preconditioning scheme are displayed. The spectra are ordered from the left to the right starting from  $A$ , followed by Block Jacobi (BJ) and ends up with the multilevel weighted HODLR scheme. The spectral bounds  $\alpha$  (29) and  $\beta$  (30) are marked on the right  $y$ -axis, while the spectral bounds for the block Jacobi case  $\alpha_{\text{BJ}} = \alpha(r = 0)$  and  $\beta_{\text{BJ}} = \beta(r = 0)$  are marked on the left  $y$ -axis.

543 **3.5. Proof of Theorem 2.** The proof of Theorem 2 is based on Lemma 2 which  
 544 provides the definition of the bounds  $\alpha$  (29) and  $\beta$  (30), and on the technical result  
 545 presented in Lemma 3.

546 LEMMA 2. *Let*

547 
$$A = \begin{bmatrix} A_1 & M \\ M^T & A_2 \end{bmatrix}, \quad K = \begin{bmatrix} K_1 & U_1 S V_2^T \\ V_2 S U_1^T & K_2 \end{bmatrix},$$

548 *and the associated lower-level bounds*

549 (34) 
$$0 < \alpha_1, \alpha_2 \leq 1 \leq \beta_1, \beta_2,$$

550 *satisfy the assumptions of Theorem 2.*

551 *Let us define*

552 (35) 
$$\underline{K} = \begin{bmatrix} \alpha_1 K_1 & M \\ M^T & \alpha_2 K_2 \end{bmatrix}, \quad \overline{K} = \begin{bmatrix} \beta_1 K_1 & M \\ M^T & \beta_2 K_2 \end{bmatrix}.$$

553 *Then we have:*

554 1. *The matrices  $\underline{K}, \overline{K}$  are SPD iff*

555 
$$\sigma_1 < \sqrt{\alpha_1 \alpha_2}, \quad \sigma_1 < \sqrt{\beta_1 \beta_2},$$

556 *respectively, where  $\sigma_1$  is the largest singular of  $R_1^{-T} M R_2^{-1}$ .*

2. If  $\underline{K}$ ,  $\overline{K}$  are SPD, there exist two positive constants,  $\alpha$  and  $\beta$ , such that

$$(36) \quad \alpha = \min_{x \neq 0} \frac{x^T \underline{K} x}{x^T \overline{K} x} \leq \lambda_{\min}(\widehat{B}^T A \widehat{B}) \leq \lambda_{\max}(\widehat{B}^T A \widehat{B}) \leq \max_{x \neq 0} \frac{x^T \overline{K} x}{x^T \underline{K} x} = \beta.$$

*Proof.* of Lemma 2.

To show the first part of the lemma we consider a general matrix of the form

$$H = \begin{bmatrix} \delta_1 K_1 & M \\ M^T & \delta_2 K_2 \end{bmatrix}, \quad \delta_1, \delta_2 > 0.$$

Let us apply the following two-sided transformations

$$\widehat{H} = \begin{bmatrix} \frac{1}{\sqrt{\delta_1}} R_1^{-T} & 0 \\ 0 & \frac{1}{\sqrt{\delta_2}} R_2^{-T} \end{bmatrix} H \begin{bmatrix} \frac{1}{\sqrt{\delta_1}} R_1^{-1} & 0 \\ 0 & \frac{1}{\sqrt{\delta_2}} R_2^{-1} \end{bmatrix} = \begin{bmatrix} I & \frac{1}{\sqrt{\delta_1 \delta_2}} \mathcal{M} \\ \frac{1}{\sqrt{\delta_1 \delta_2}} \mathcal{M}^T & I \end{bmatrix},$$

where  $\mathcal{M} = R_1^{-T} M R_2^{-1}$ . The matrix  $\widehat{H}$  is SPD iff  $H$  is SPD as well. Thus, by Lemma 1 the matrix  $H$  is SPD iff  $1 - \sigma_1 / \sqrt{\delta_1 \delta_2} > 0$ , and the conditions ensuring  $\underline{K}$ ,  $K$ , and  $\overline{K}$  are SPD immediately follow.

For the second part of the lemma it is sufficient to assume that  $\underline{K}$  is SPD which, by the first part, ensures that  $K$  and  $\overline{K}$  are SPD as well. Accordingly, we obtain the following inequalities

$$\frac{x^T K x}{x^T \underline{K} x} \leq \frac{x^T K x}{x^T A x} \leq \frac{x^T K x}{x^T \overline{K} x} \quad \forall x \neq 0.$$

The Lagrangian stationary points of each generalized Rayleigh quotient in the inequalities above constitute the spectrum of each preconditioned system. Thus, the proof is complete.  $\square$

LEMMA 3. Let  $H = \begin{bmatrix} \mathcal{D}^{(1)} & \mathcal{D}^{(2)} \\ \mathcal{D}^{(2)} & \mathcal{D}^{(3)} \end{bmatrix} \in \mathbb{R}^{2r \times 2r}$ , where  $\mathcal{D}^{(i)}$  ( $i = 1, 2, 3$ ) are diagonal matrices,

$$\mathcal{D}^{(i)} = \text{diag}(d_1^{(i)}, \dots, d_r^{(i)}).$$

If  $d_j^{(2)} \neq 0$  for all  $j = 1, 2, \dots, r$ , then

$$\text{spec}(H) = \{\lambda_j^-\}_{j=1}^m \cup \{\lambda_j^+\}_{j=1}^m, \quad \lambda_j^\pm = \frac{d_j^{(1)} + d_j^{(3)}}{2} \pm \sqrt{\left(\frac{d_j^{(1)} - d_j^{(3)}}{2}\right)^2 + \left(d_j^{(2)}\right)^2},$$

where  $\text{spec}(H)$  denotes the spectrum of the symmetric matrix  $H$ .

*Proof.* of Lemma 3.

From the given structure of  $H$  it is clear that  $\lambda \in \mathbb{R}$  is an eigenvalue of  $H$  iff for some  $j = 1, 2, \dots, m$  the vectors  $(d_j^{(1)} - \lambda, d_j^{(2)})$  and  $(d_j^{(2)}, d_j^{(3)} - \lambda)$  are linearly dependent. Since we have assumed  $d_j^{(2)} \neq 0$ , we have that  $(d_j^{(1)} - \lambda, d_j^{(2)})$  and  $(d_j^{(2)}, d_j^{(3)} - \lambda)$  are linearly dependent iff

$$\frac{d_j^{(1)} - \lambda}{d_j^{(2)}} = \frac{d_j^{(2)}}{d_j^{(3)} - \lambda} \Leftrightarrow (d_j^{(1)} - \lambda)(d_j^{(3)} - \lambda) - (d_j^{(2)})^2 = 0.$$

The solution to the quadratic equation above is

$$\lambda = \lambda_j^\pm = \frac{d_j^{(1)} + d_j^{(3)}}{2} \pm \sqrt{\left(\frac{d_j^{(1)} - d_j^{(3)}}{2}\right)^2 + \left(d_j^{(2)}\right)^2},$$

and the proof is complete.  $\square$

589 *Proof.* of [Theorem 2](#).

590 Considering the conditions of [Theorem 2](#) we have by [Lemma 2](#) that the spectral  
591 bounds,  $\alpha$  and  $\beta$ , satisfying

$$592 \quad 0 < \alpha = \min_{x \neq 0} \frac{x^T \underline{K} x}{x^T K x} \leq \lambda_{\min}(R^{-T} A R^{-1}) \leq \lambda_{\max}(R^{-T} A R^{-1}) \leq \max_{x \neq 0} \frac{x^T \overline{K} x}{x^T K x} = \beta,$$

593 exist where  $\underline{K}$  and  $\overline{K}$  are defined in [Lemma 2](#).

594 To find the exact values of  $\alpha$  and  $\beta$ , we consider a generalized Rayleigh quotient

$$595 \quad Q(x) = \frac{x^T H x}{x^T K x}, \quad H = \begin{bmatrix} \delta_1 K_1 & M \\ M^T & \delta_2 K_2 \end{bmatrix},$$

596 whose range is strictly positive. Thus,  $Q(x)$  represents either  $x^T \underline{K} x / x^T K x$  or  $x^T \overline{K} x$ .

597 We apply the change of variables,  $x = \begin{bmatrix} R_1^{-T} & 0 \\ 0 & R_2^{-1} \end{bmatrix} \xi$ , and obtain the following equivalent  
598 representation

$$599 \quad Q(x) = \frac{\xi^T \widehat{H} \xi}{\xi^T \widehat{K} \xi}, \quad \widehat{H} = \begin{bmatrix} \delta_1 I_1 & \mathcal{M} \\ \mathcal{M}^T & \delta_2 I_2 \end{bmatrix}, \quad \widehat{K} = \begin{bmatrix} I_1 & \mathcal{M}_r \\ \mathcal{M}_r^T & I_2 \end{bmatrix},$$

600 where  $\mathcal{M} = R_1^{-T} M R_2^{-1}$  and  $\mathcal{M}_r = U_r \Sigma_r \mathcal{V}_r^T$  is the  $r$ -rank weighted SVD approxima-  
601 tion of  $\mathcal{M}$ .

602 Let  $w_i$  denote the  $i$ -th column of the orthogonal matrix  $\mathcal{W}$  ([13](#)) as defined in  
603 [Lemma 1](#). Then we have:

- 604 1.  $\widehat{K} w_i = (1 + \sigma_1) w_i$ ,  $i = 1, 2, \dots, r$ .
- 605 2.  $\widehat{K} w_{n_1+i} = (1 - \sigma_1) w_{n_1+i}$ ,  $i = 1, 2, \dots, r$ .
- 606 3.  $\widehat{K} w_j = w_j$ ,  $j \neq 1, \dots, r, n_1 + 1, \dots, n_1 + r$ .

607 and similarly for  $\widehat{H}$ , it can be verified that:

- 608 1.  $\widehat{H} w_i = (\delta_{1,2}^{\text{avg}} + \sigma_1) w_i + \delta_{1,2}^{\text{dif}} w_{n_1+i}$ ,  $i = 1, 2, \dots, \min\{n_1, n_2\}$ .
- 609 2.  $\widehat{H} w_{n_1+i} = (\delta_{1,2}^{\text{avg}} - \sigma_1) w_{n_1+i} + \delta_{1,2}^{\text{dif}} w_i$ ,  $i = 1, 2, \dots, \min\{n_1, n_2\}$ .
- 610 3.  $\widehat{H} w_j = w_j$ ,  $j \neq 1, \dots, \min\{n_1, n_2\}, n_1 + 1, \dots, n_1 + \min\{n_1, n_2\}$ .

611 where  $\delta_{1,2}^{\text{avg}} = (\delta_1 + \delta_2)/2$  and  $\delta_{1,2}^{\text{dif}} = (\delta_1 - \delta_2)/2$ . Clearly, both  $\widehat{K}$  and  $\widehat{H}$  are invari-  
612 ant over the subspaces  $Z = \text{span}\{w_1, \dots, w_r, w_{n_1+1}, \dots, w_{n_1+r}\}$  and its orthogonal  
613 complement,  $Z^\perp$ . Hence, by the properties of the generalized Rayleigh quotient we  
614 have:

$$615 \quad \max_{x \neq 0} Q(x) = \max \left\{ \max_{\xi \in Z \setminus \{0\}} Q(x), \max_{\xi \in Z^\perp \setminus \{0\}} Q(x) \right\},$$

616 and

$$617 \quad \min_{x \neq 0} Q(x) = \min \left\{ \min_{\xi \in Z \setminus \{0\}} Q(x), \min_{\xi \in Z^\perp \setminus \{0\}} Q(x) \right\}.$$

618 By our results so far, if  $x = \xi \in Z^\perp$  then  $Q(x) = \xi^T \widehat{H} \xi / \xi^T \xi$ . Let us apply the  
619 change of variables of the form  $\xi = C \zeta \in Z^\perp$ , given explicitly by

$$620 \quad \xi = \zeta_1 w_{r+1} + \dots + \zeta_{n_1-r} w_{n_1} + \zeta_{n_1-r+1} w_{n_1+r+1} + \dots + \zeta_{n_1+n_2-2r} w_{n_1+n_2},$$

621 where  $\zeta_i$  is the  $i$ -th coordinate of  $\zeta$  and as before  $w_i$  denotes the  $i$ -th column in the  
622 orthogonal matrix  $\mathcal{W}$  ([13](#)). Then, for any  $\xi \in Z^\perp$  we obtain

$$623 \quad Q(x) = \frac{\zeta^T \widehat{H}_{Z^\perp} \zeta}{\zeta^T \zeta}, \quad \widehat{H}_{Z^\perp} = \begin{bmatrix} \mathcal{D}_{Z^\perp}^{(1)} & \mathcal{D}_{Z^\perp}^{(2)} \\ \mathcal{D}_{Z^\perp}^{(2)T} & \mathcal{D}_{Z^\perp}^{(3)} \end{bmatrix},$$

624 where  $\mathcal{D}_{Z^\perp}^{(2)} = \delta_{1,2}^{\text{dif}} I_{n_1, n_2}$  and

$$625 \quad \mathcal{D}_{Z^\perp}^{(1)} = \begin{cases} \text{diag}(\delta_{1,2}^{\text{avg}} + \sigma_{r+1}, \dots, \delta_{1,2}^{\text{avg}} + \sigma_{n_1}) & \text{if } n_1 \leq n_2 \quad , \\ \text{diag}(\delta_{1,2}^{\text{avg}} + \sigma_{r+1}, \dots, \delta_{1,2}^{\text{avg}} + \sigma_{n_1}, \delta_1, \dots, \delta_1) & \text{if } n_1 > n_2 \quad . \end{cases}$$

626

$$627 \quad \mathcal{D}_{Z^\perp}^{(3)} = \begin{cases} \text{diag}(\delta_{1,2}^{\text{avg}} - \sigma_{r+1}, \dots, \delta_{1,2}^{\text{avg}} - \sigma_{n_2}) & \text{if } n_2 \leq n_1 \quad , \\ \text{diag}(\delta_{1,2}^{\text{avg}} - \sigma_{r+1}, \dots, \delta_{1,2}^{\text{avg}} - \sigma_{n_2}, \delta_2, \dots, \delta_2) & \text{if } n_2 > n_1 \quad . \end{cases}$$

628 Now, by [Lemma 3](#), we obtain that the spectrum of  $\widehat{H}_{Z^\perp}$  contains the sets

$$629 \quad \left\{ \delta_{1,2}^{\text{avg}} + \sqrt{\sigma_{r+1}^2 + (\delta_{1,2}^{\text{dif}})^2}, \dots, \delta_{1,2}^{\text{avg}} + \sqrt{\sigma_{\min\{n_1, n_2\}}^2 + (\delta_{1,2}^{\text{dif}})^2} \right\},$$

630

$$631 \quad \left\{ \delta_{1,2}^{\text{avg}} - \sqrt{\sigma_{\min\{n_1, n_2\}}^2 + (\delta_{1,2}^{\text{dif}})^2}, \dots, \delta_{1,2}^{\text{avg}} - \sqrt{\sigma_{r+1}^2 + (\delta_{1,2}^{\text{dif}})^2} \right\}.$$

632 Hence, we conclude that

$$633 \quad \min_{\xi \in Z^\perp \setminus \{0\}} Q(x) = \delta_{1,2}^{\text{avg}} - \sqrt{\sigma_{r+1}^2 + (\delta_{1,2}^{\text{dif}})^2},$$

634

$$635 \quad \max_{\xi \in Z^\perp \setminus \{0\}} Q(x) = \delta_{1,2}^{\text{avg}} + \sqrt{\sigma_{r+1}^2 + (\delta_{1,2}^{\text{dif}})^2}.$$

636 For the case  $\xi \in Z$  let us apply the change of variables of the form  $\xi = C\psi \in Z$ ,  
637 given explicitly by

$$638 \quad \xi = \psi_1 w_1 + \dots + \psi_r w_r + \psi_{r+1} w_{n_1+1} + \dots + \psi_{2r} w_{n_1+r},$$

639 where  $\psi_i$  is the  $i$ -th coordinate of  $\psi$  and as before  $w_i$  denotes the  $i$ -th column in the  
640 orthogonal matrix  $\mathcal{W}$  [\(13\)](#). Then, for any  $\xi \in Z$  we obtain

$$641 \quad Q(x) = \frac{\psi^T \widehat{H}_Z \psi}{\psi^T \psi}, \quad \widehat{H}_Z = \begin{bmatrix} \mathcal{D}_Z^{(1)} & \mathcal{D}_Z^{(2)} \\ \mathcal{D}_Z^{(2)} & \mathcal{D}_Z^{(3)} \end{bmatrix},$$

642

$$643 \quad \mathcal{D}_Z^{(1)} = \text{diag} \left( \frac{\delta_{1,2}^{\text{avg}} + \sigma_1}{1 + \sigma_1}, \dots, \frac{\delta_{1,2}^{\text{avg}} + \sigma_r}{1 + \sigma_r} \right),$$

644

$$645 \quad \mathcal{D}_Z^{(2)} = \text{diag} \left( \frac{\delta_{1,2}^{\text{dif}}}{\sqrt{1 - \sigma_1^2}}, \dots, \frac{\delta_{1,2}^{\text{dif}}}{\sqrt{1 - \sigma_r^2}} \right),$$

646

$$647 \quad \mathcal{D}_Z^{(3)} = \text{diag} \left( \frac{\delta_{1,2}^{\text{avg}} - \sigma_1}{1 - \sigma_1}, \dots, \frac{\delta_{1,2}^{\text{avg}} - \sigma_r}{1 - \sigma_r} \right).$$

648 Applying once more the outcome of [Lemma 3](#) we have that the spectrum of  $\widehat{H}_Z$  is  
649 composed of the following values

$$650 \quad \frac{1}{2} \left( \frac{\delta_{1,2}^{\text{avg}} + \sigma_i}{1 + \sigma_i} + \frac{\delta_{1,2}^{\text{avg}} - \sigma_i}{1 - \sigma_i} \right) \pm \sqrt{\frac{1}{4} \left( \frac{\delta_{1,2}^{\text{avg}} + \sigma_i}{1 + \sigma_i} + \frac{\delta_{1,2}^{\text{avg}} - \sigma_i}{1 - \sigma_i} \right)^2 + \frac{(\delta_{1,2}^{\text{dif}})^2}{1 - \sigma_i^2}},$$

651 where  $i = 1, 2, \dots, r$  and the proof is complete.  $\square$

652 **4. Numerical Study.** This section contains the experimental part of this work.

653 The main goal is to demonstrate the effect of different low-rank approximations (18)  
 654 for the off-diagonal blocks on the preconditioned system using HODLR. We perform  
 655 a comparative study and consider the following low-rank techniques:

- 656 • **R-HODLR:** the off-diagonal low-rank factorizations are obtained in the stand-  
 657 dard or regular approach using truncated SVD.
- 658 • **C-HODLR:** the off-diagonal low-rank factorizations are obtained using trunc-  
 659 ated SVD with additional imposed constraints as described in [6].
- 660 • **W-HODLR:** the off-diagonal low-rank factorizations are obtained using the  
 661 weighted HODLR preconditioning scheme for the multi-level case. The con-  
 662 struction and application of the scheme follows the outlined procedure in  
 663 subsection 3.3.

664 Employing SVD is done for convenience and uniformity of the comparison, and can  
 665 be replaced, in practice, by other more efficient low-rank approximation techniques.

666 Subsection 4.1 describes the computational setting, and presents a pair of severely  
 667 ill-conditioned sparse systems which have been used in the numerical simulations. An-  
 668 other simplified numerical example along a more detailed analysis can be found in [1].  
 669 In subsection 4.2 we describe the numerical results of the PCG approximation using  
 670 HODLR preconditioning. The results indicate that the weighted low-rank factoriza-  
 671 tion scheme proves to be superior to other standard techniques.

672 **4.1. Sparse Matrices and Computational Setting.** In the presented numer-

673 ical study we have explored and analyzed the PCG solution for the following sparse  
 674 matrices, which have been picked from the SuiteSparse matrix collection [10].

- 675 • **bcsstk16:**  $4,884 \times 4,884$ , SPD, spectral condition number  $\approx 4.94 \cdot 10^9$ .
- 676 • **bcsstk15:**  $3,948 \times 3,948$ , SPD, spectral condition number  $\approx 6.53 \cdot 10^9$ .

677 For constructing the HODLR preconditioning schemes we interpret each matrix  
 678 as a discrete graph and apply a balanced partitioning using successive bisections. We  
 679 employ SCOTCH [9] for each bisection dividing a given vertex set into two distinct sets  
 680 of approximately equal size whose cut is minimal, i.e., the number of edges running  
 681 between the separated subsets is as small as possible. The process starts with the  
 682 entire set of vertices, and then applied recursively on each separated subset until  
 683 reaching the predetermined bottom level of the hierarchy,  $L$ .

684 Construction of the preconditioning schemes and the iterative solution of the  
 685 preconditioned system has been implemented with a Fortran90 code. In all the sim-  
 686 ulations we have employed the following selections:

- 687 •  $L = \lceil \log_2(n/100) \rceil$  for an  $n \times n$  matrix as the lowest level of the hierarchy,  
 688 which forces the size of the smallest blocks in the partition under 100.
- 689 • Constant off-diagonal block ranks over all levels of the hierarchy with the  
 690 following  $\mathcal{O}(1)$  values:

$$(37) \quad r_k^{(\ell)} = 0, 5, 10, 15, 20, 25, \quad \ell = 0, 1, \dots, L, \quad k = 1, \dots, 2^\ell.$$

692 Note that  $r_k^{(\ell)} \equiv 0$  reduces the preconditioning scheme to *block Jacobi* (BJ), regardless  
 693 of the specific low-rank factorization technique.

694 The construction of the low-rank factorizations (24) follows the path outlined in  
 695 subsection 3.3. We have produced fast low-rank factorizations by first removing all  
 696 the zero rows and columns of the sparse block  $M_k^{(\ell)}$  (20), and then computing the  
 697 low-rank factorization (24) on the reduced block. For the sparse case, this procedure  
 698 is, typically, equivalent in terms of complexity to the randomized technique [21].

699 **4.2. Numerical Results and Analysis.** This subsection contains the numeri-  
 700 cal results of PCG solution for the chosen sparse systems, using R-HODLR, C-HODLR  
 701 and W-HODLR preconditioning schemes. For both matrices, bcsstk16 and bcsstk15,  
 702 we have set the right-hand side to  $b = 1$ , and the iterative approximation was stopped  
 703 at the first occurrence of

$$704 \quad \|Ax_{(i)} - b\|_2 \leq 10^{-8} \|b\|_2 ,$$

705 where  $i = 1, 2, \dots$  is the iteration step index and  $x_{(i)}$  denotes the approximate solution  
 706 at step  $i$ . The results indicate that in all the test cases, the W-HODLR scheme  
 707 outperforms the other techniques, and retain good properties even when low accuracy  
 708 for the off-diagonal blocks approximations is employed.

709 **Figure 5** contains plots of the PCG convergence history profiles for bcsstk16.  
 710 All plots in this case indicate that increasing the constant rank (37), improves the  
 711 approximation quality, and achieves faster convergence rate. It is also evident that R-  
 712 HODLR and C-HODLR achieve similar convergence with the same memory resources,  
 713 while W-HODLR converges faster with the same memory resources. **Figure 6** con-  
 714 tains plots of the PCG convergence history profiles for bcsstk15. The results show  
 715 that R-HODLR and C-HODLR fail to converge in 1000 PCG iterations. In fact,  
 716 setting constant rank 0, i.e., Block Jacobi, performs better than using these schemes  
 717 with a constant rank greater than zero. This occurs because the use of naive approxi-  
 718 mations for the off-diagonal blocks makes the problem even more ill-conditioned. The  
 719 W-HODLR scheme, however, converges with excellent convergence rates, where the  
 720 convergence rate improves when the constant rank (37) is increased.

721 **5. Summary and Future Work.** In this work we have addressed the problem  
 722 of choosing low-rank factorizations in fast hierarchical algorithms for preconditioning  
 723 SPD matrices.

724 We have presented a mathematical analysis for obtaining low-rank factorizations,  
 725 that minimize the spectral condition number of the preconditioned system for the 1-  
 726 level ( $2 \times 2$ ) case. The key idea was to properly reweight the blocks prior the low-rank  
 727 factorization, which leads to a minimum spectral condition number.

728 The presented theory has been extended to HODLR preconditioning schemes,  
 729 including analysis of the spectral properties and bounds that take into account the  
 730 error propagation through the levels of the hierarchy.

731 The numerical experiments indicate, that employing proper reweighting for the  
 732 off-diagonal blocks prior to low-rank compression, leads to a HODLR preconditioning  
 733 scheme that requires far less computational resources for the same quality of perfor-  
 734 mance of convergence than using the other low-rank compression techniques.

735 As noted in the introduction a major goal of this work is to provide an analysis  
 736 of optimal choice of low-rank approximations for a simple case; i.e., HODLR, which  
 737 could lead to an extended analysis for the strong hierarchical case. This point will be  
 738 explored and pursued in a future study.

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 740 valuable remarks, questions and comments that enabled us to substantially improve  
 741 this paper.

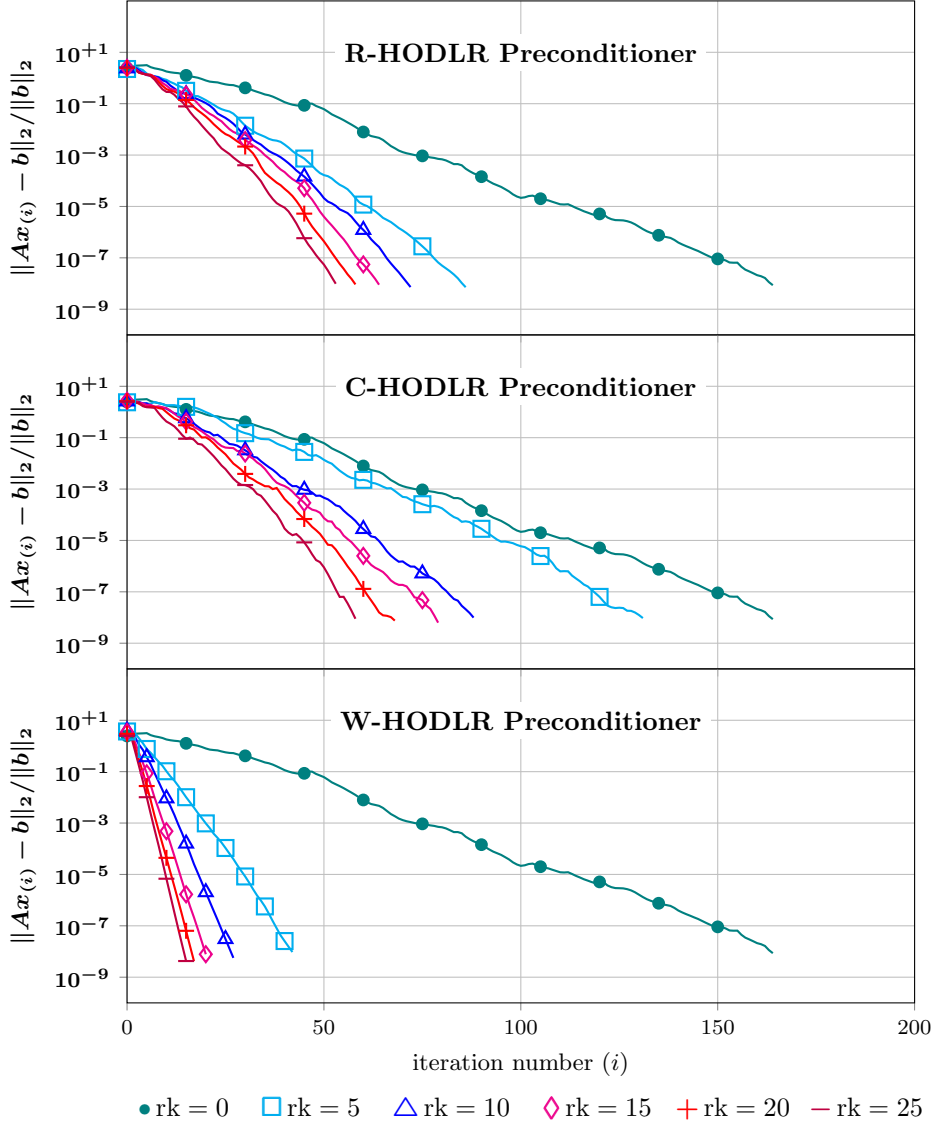


Fig. 5: **PCG Convergence History: 'bcstkt16'**. Three plots showing PCG convergence history profiles, i.e., the values  $\|Ax_{(i)} - b\|_2 / \|b\|_2$  as a function of the iteration number  $i$ , for each preconditioning scheme. Each plot displays various profiles, where each profile corresponds to a different constant rank value (37) of the approximations for the off-diagonal blocks by low-rank factorizations.



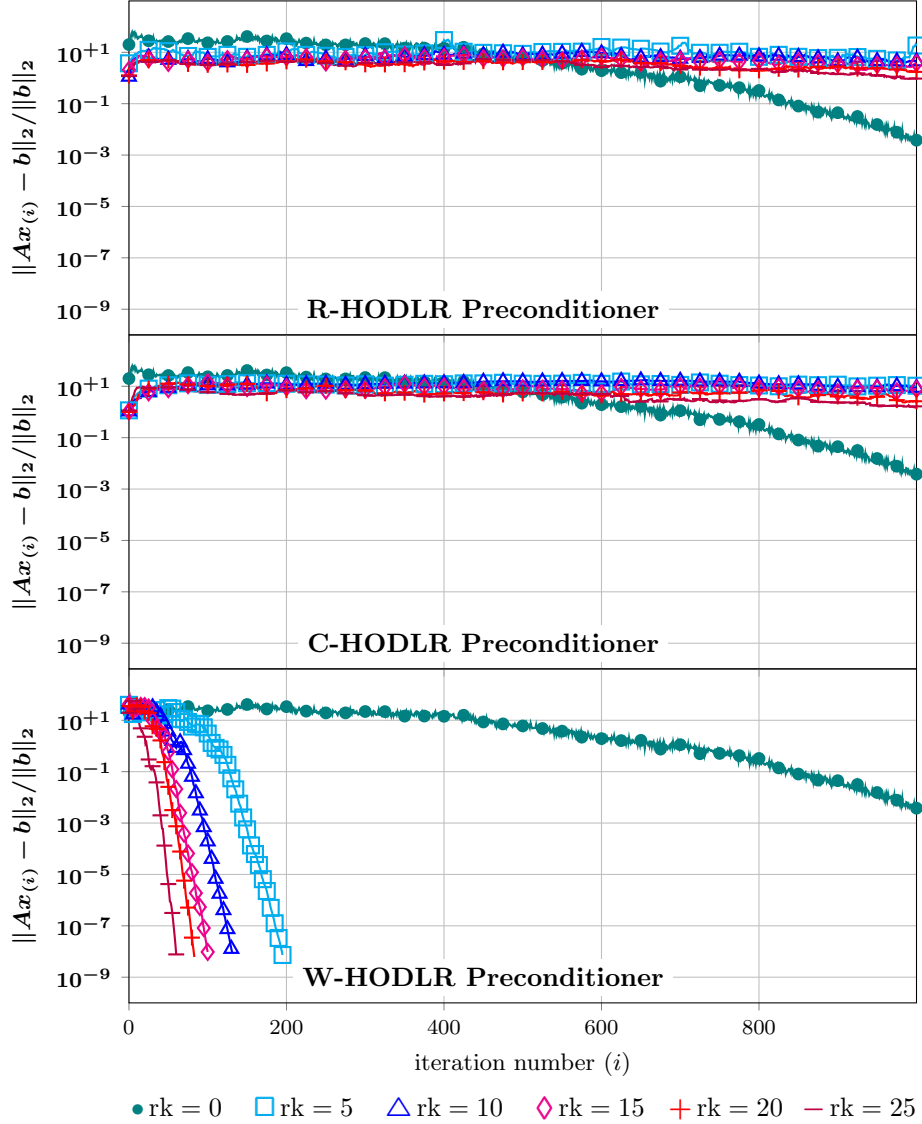


Fig. 6: **PCG Convergence History: 'bcstkt15'**. Three plots showing PCG convergence history profiles, i.e., the values  $\|Ax_{(i)} - b\|_2 / \|b\|_2$  as a function of the iteration number  $i$ , for each preconditioning scheme. Each plot displays various profiles, where each profile corresponds to a different constant rank value (37) of the approximations for the off-diagonal blocks by low-rank factorizations.

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