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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 HARNESS†‡

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 2×2 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 2×2 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 2×2 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 2×2 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:*

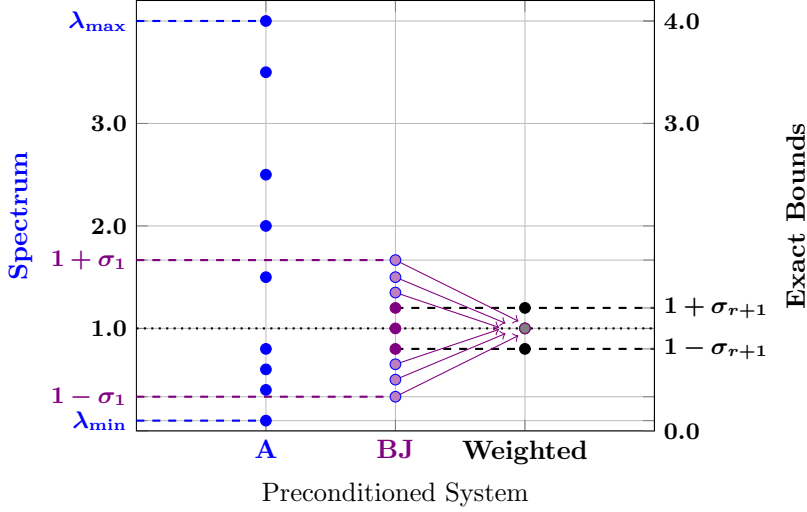


Fig. 1: **Spectrum Clustering of the Optimal 1-level Preconditioning Scheme.** The spectrum of some SPD matrix A and the transformations it goes after preconditioning by block Jacobi (BJ) and the optimal 1-level preconditioning scheme are displayed. The spectra are ordered from the left to the right 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 δ 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 δ 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 σ_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 σ_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 $\widehat{\mathcal{R}} = R$ 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 ℓ 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](#).

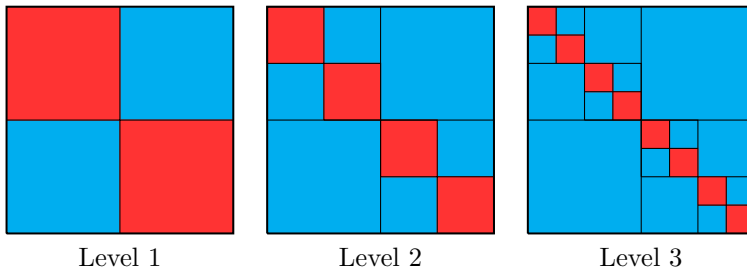


Fig. 2: **The HODLR Structure.** The first 3 levels, $\ell = 1, 2, 3$, of the HODLR structure are illustrated: at each level the blue color blocks are the low-rank off-diagonal blocks and the red blocks are the HODLR principal submatrices.

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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 ℓ , $F_k^{(\ell)} \in \mathbb{R}^{n_k^{(\ell)} \times m}$, 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 ℓ 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, α_i and β_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

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

449

450

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

451

452

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 α and β [\(26\)](#) is based on variational formulation and provided in [Lemma 2](#). The analysis requires sufficient (but not necessary) conditions on the given lower-level bounds, α_i and β_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

467

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

468

469

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

470

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

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

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

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 α (29) and β (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, α (29).

499 From [Theorem 2](#) we observe that each estimated bound, α or β , is a minimum
 500 or a maximum, respectively, of two competing terms: the first depends on the largest
 501 singular value, σ_1 , and the second is a function of the truncation error, σ_{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, β/α . 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 σ_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 σ_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 σ_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, σ_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 σ_1^{exact} is the corresponding CBS constant of A . The important conclusion here
 522 is that σ_1 and σ_1^{exact} are correlated where σ_1^{exact} is intrinsically predetermined by the

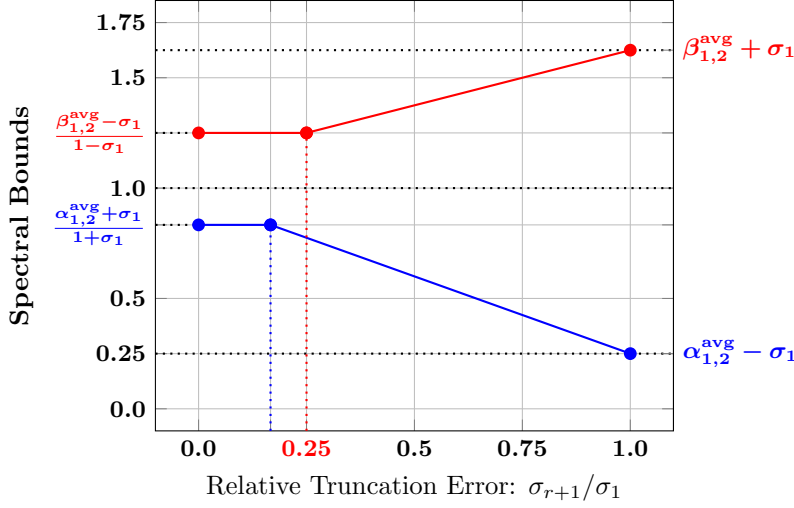


Fig. 3: **Spectral Bounds.** A typical behavior of the spectral bounds displayed for the case $\alpha_1 = \alpha_2$ and $\beta_1 = \beta_2$. The lower bound α (29) vs. σ_{r+1}/σ_1 is plotted in blue, and the upper bound β (30) vs. σ_{r+1}/σ_1 is plotted in red.

523 given matrix, A , and the chosen partition. If K is close to A then we can expect σ_1
 524 to be close to σ_1^{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.

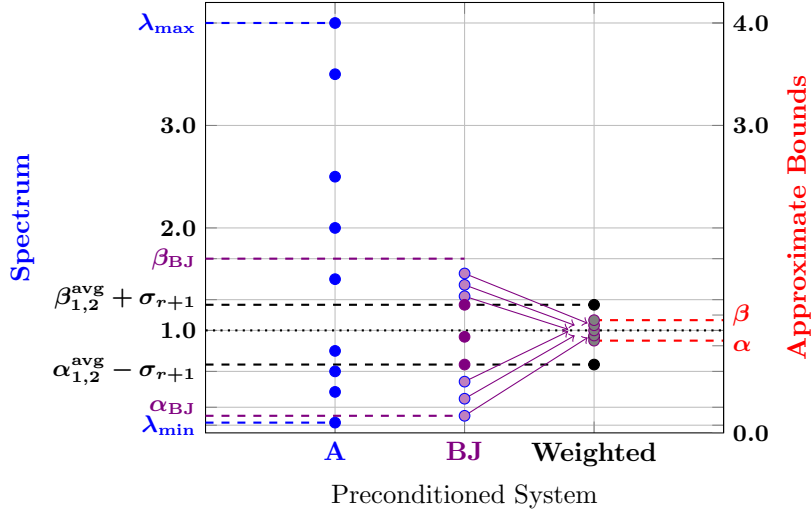


Fig. 4: **Spectrum Clustering for the Multilevel Weighted HODLR Preconditioning Scheme.** The spectrum of some SPD matrix A and the transformation it goes after preconditioning by block Jacobi (BJ) and the multilevel weighted HODLR preconditioning scheme are displayed. The spectra are ordered from the left to the right starting from A , followed by Block Jacobi (BJ) and ends up with the multilevel weighted HODLR scheme. The spectral bounds α (29) and β (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 α (29) and β (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 σ_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, α and β , 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

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

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, α and β , 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 α and β , 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 ζ_i is the i -th coordinate of ζ 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

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

626

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

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 ψ_i is the i -th coordinate of ψ 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 ard 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:

$$691 \quad (37) \quad r_k^{(\ell)} = 0, 5, 10, 15, 20, 25, \quad \ell = 0, 1, \dots, L, \quad k = 1, \dots, 2^\ell.$$

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 numerical
 700 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 (2×2) 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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 741 this paper.

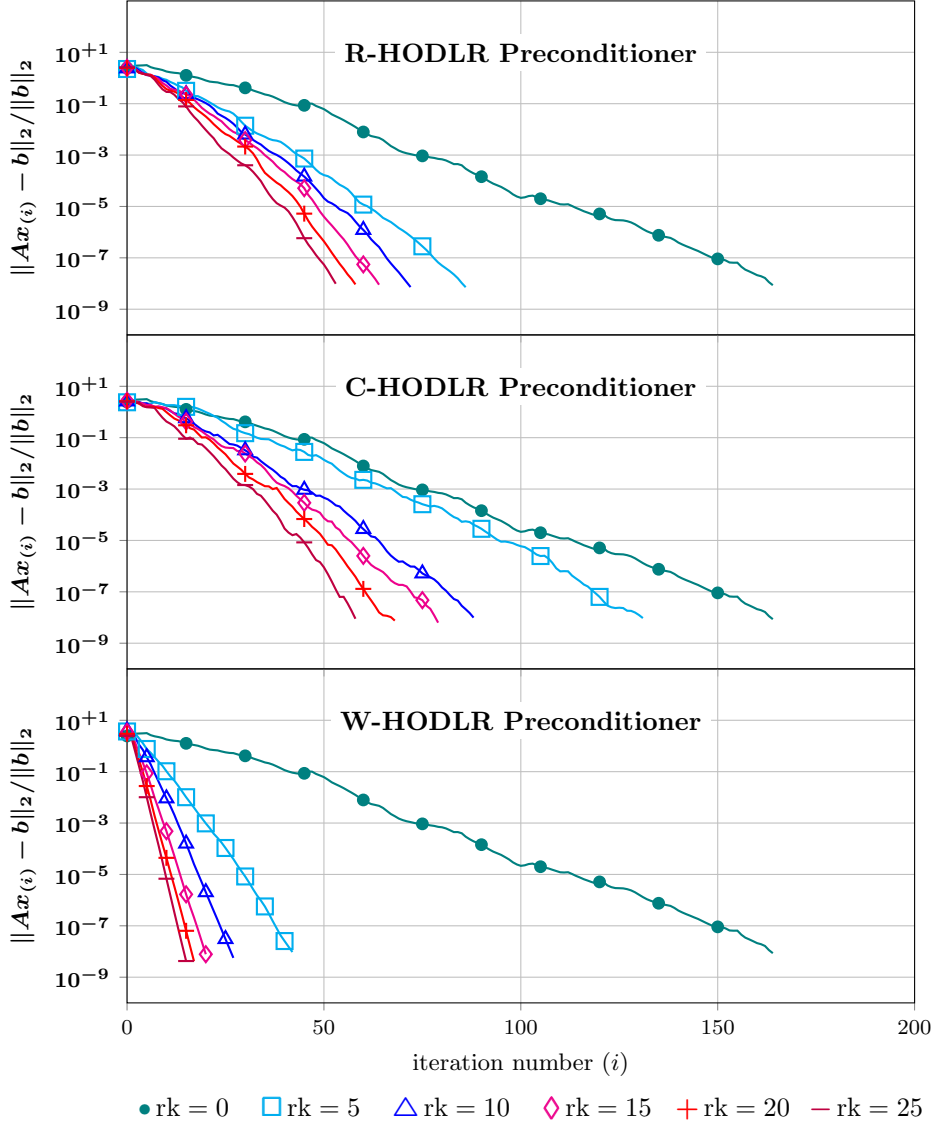


Fig. 5: **PCG Convergence History: 'bcstkt16'**. Three plots showing PCG convergence history profiles, i.e., the values $\|Ax_{(i)} - b\|_2 / \|b\|_2$ as a function of the iteration number i , for each preconditioning scheme. Each plot displays various profiles, where each profile corresponds to a different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

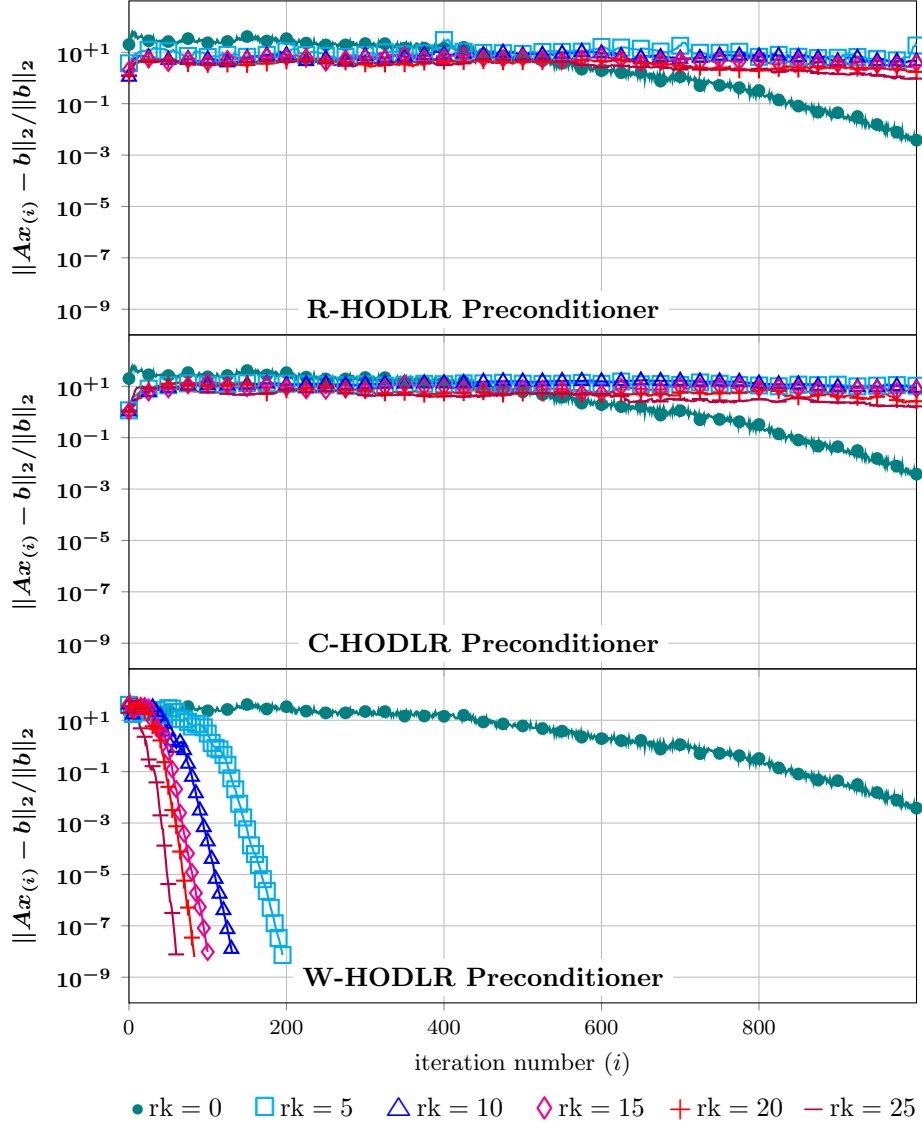


Fig. 6: **PCG Convergence History: 'bcstk15'**. Three plots showing PCG convergence history profiles, i.e., the values $\|Ax_{(i)} - b\|_2 / \|b\|_2$ as a function of the iteration number i , for each preconditioning scheme. Each plot displays various profiles, where each profile corresponds to a different constant rank value (37) of the approximations for the off-diagonal blocks by low-rank factorizations.

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REFERENCES

- 743 [1] E. AGULLO, E. DARVE, L. GIRAUD, AND Y. HARNESS, *Nearly optimal fast preconditioning*
744 *of symmetric positive definite matrices*, Research Report RR-8984, Inria Bordeaux Sud-
745 Ouest, Nov. 2016.
- 746 [2] A. AMINFAR, S. AMBIKASARAN, AND E. DARVE, *A fast block low-rank dense solver with appli-*
747 *cations to finite-element matrices*, Journal of Computational Physics, 304 (2016), pp. 170
748 – 188.
- 749 [3] O. AXELSSON AND P. S. VASSILEVSKI, *Algebraic multilevel preconditioning methods. I*, Nu-
750 *merische Mathematik*, 56 (1989), pp. 157–177.
- 751 [4] O. AXELSSON AND P. S. VASSILEVSKI, *Algebraic Multilevel Preconditioning Methods, II*, SIAM
752 *Journal on Numerical Analysis*, 27 (1990), pp. 1569–1590.
- 753 [5] M. BEBENDORF, *Hierarchical Matrices: A Means to Efficiently Solve Elliptic Boundary Value*
754 *Problems*, Springer Berlin Heidelberg, 2008.
- 755 [6] M. BEBENDORF, M. BOLLHÖFER, AND M. BRATSCH, *Hierarchical matrix approximation with*
756 *blockwise constraints*, BIT Numerical Mathematics, 53 (2013), pp. 311–339.
- 757 [7] M. BEBENDORF, M. BOLLHÖFER, AND M. BRATSCH, *On the spectral equivalence of hierarchi-*
758 *cal matrix preconditioners for elliptic problems*, Mathematics of Computation, 85 (2016),
759 pp. 2839–2861.
- 760 [8] S. CHANDRASEKARAN, M. GU, AND T. PALS, *A Fast ULV Decomposition Solver for Hierarchi-*
761 *cally Semiseparable Representations*, SIAM Journal on Matrix Analysis and Applications,
762 28 (2006), pp. 603–622.
- 763 [9] C. CHEVALIER AND F. PELLEGRINI, *PT-Scotch: A tool for efficient parallel graph ordering*,
764 *Parallel Computing*, 34 (2008), pp. 318 – 331. Parallel Matrix Algorithms and Applications.
- 765 [10] T. A. DAVIS AND Y. HU, *The University of Florida Sparse Matrix Collection*, ACM Trans.
766 *Math. Softw.*, 38 (2011), pp. 1:1–1:25.
- 767 [11] C. ECKART AND G. YOUNG, *The approximation of one matrix by another of lower rank*, Psy-
768 *chometrika*, 1 (1936), pp. 211–218.
- 769 [12] L. ELSNER, *A note on optimal block-scaling of matrices*, Numerische Mathematik, 44 (1984),
770 pp. 127–128.
- 771 [13] A. FRIEZE, R. KANNAN, AND S. VEMPALA, *Fast Monte-carlo Algorithms for Finding Low-rank*
772 *Approximations*, J. ACM, 51 (2004), pp. 1025–1041.
- 773 [14] G. H. GOLUB AND C. F. V. LOAN, *Matrix computations, Forth Edition*, Johns Hopkins Uni-
774 *versity Press*, 2013.
- 775 [15] L. GRASEDYCK AND W. HACKBUSCH, *Construction and Arithmetics of H-Matrices*, Springer
776 *Journal of Computing*, 70 (2003), pp. 295–334.
- 777 [16] M. GU AND S. C. EISENSTAT, *Efficient Algorithms for Computing a Strong Rank-Revealing QR*
778 *Factorization*, SIAM Journal on Scientific Computing, 17 (1996), pp. 848–869.
- 779 [17] W. HACKBUSCH, *A Sparse Matrix Arithmetic Based on H-Matrices. Part I: Introduction to*
780 *H-Matrices*, Computing, 62 (1999), pp. 89–108.
- 781 [18] W. HACKBUSCH AND B. N. KHOROMSKIJ, *A Sparse H-Matrix Arithmetic. Part II: Application*
782 *to Multi-Dimensional Problems*, Computing, 64 (2000), pp. 21–47.
- 783 [19] M. R. HESTENES AND E. STIEFEL, *Methods of conjugate gradients for solving linear systems*,
784 *Journal of Research of the National Bureau of Standards*, 49 (1952).
- 785 [20] E. LIBERTY, F. WOOLFE, P.-G. MARTINSSON, V. ROKHLIN, AND M. TYGERT, *Randomized algo-*
786 *rithms for the low-rank approximation of matrices*, Proceedings of the National Academy
787 of Sciences, 104 (2007), pp. 20167–20172.
- 788 [21] P. G. MARTINSSON, *A Fast Randomized Algorithm for Computing a Hierarchically Semisepa-*
789 *rable Representation of a Matrix*, SIAM Journal on Matrix Analysis and Applications, 32
790 (2011), pp. 1251–1274.
- 791 [22] L. MIRANIAN AND M. GU, *Strong rank revealing LU factorizations*, Linear Algebra and its
792 *Applications*, 367 (2003), pp. 1 – 16.
- 793 [23] B. PARLETT, *The Symmetric Eigenvalue Problem*, Society for Industrial and Applied Mathe-
794 *matics*, 1998.
- 795 [24] S. RJASANOW, *Adaptive cross approximation of dense matrices*, in Int. Association Boundary
796 *Element Methods Conf., IABEM, 2002*, pp. 28–30.
- 797 [25] Y. SAAD, *Iterative Methods for Sparse Linear Systems, Second Edition*, Siam, 2003.
- 798 [26] A. J. WATHEN, *Preconditioning*, Acta Numerica, 24 (2015), pp. 329–376.
- 799 [27] F. WOOLFE, E. LIBERTY, V. ROKHLIN, AND M. TYGERT, *A fast randomized algorithm for the*
800 *approximation of matrices*, Applied and Computational Harmonic Analysis, 25 (2008),
801 pp. 335 – 366.
- 802 [28] J. XIA, S. CHANDRASEKARAN, M. GU, AND X. S. LI, *Fast algorithms for hierarchically semisep-*

- 803 *arable matrices*, Numerical Linear Algebra with Applications, 17 (2010), pp. 953–976.
804 [29] J. XIA AND M. GU, *Robust Approximate Cholesky Factorization of Rank-Structured Symmetric*
805 *Positive Definite Matrices*, SIAM Journal on Matrix Analysis and Applications, 31 (2010),
806 pp. 2899–2920.
807 [30] J. XIA AND Z. XIN, *Effective and Robust Preconditioning of General SPD Matrices via Struc-*
808 *tured Incomplete Factorization*, SIAM Journal on Matrix Analysis and Applications, 38
809 (2017), pp. 1298–1322.
810 [31] K. YANG, H. POURANSARI, AND E. DARVE, *Sparse Hierarchical Solvers with Guaranteed Con-*
811 *vergence*, ArXiv e-prints, (2016), [arXiv:1611.03189](https://arxiv.org/abs/1611.03189).