BEST KRONECKER PRODUCT APPROXIMATION OF THE BLURRING OPERATOR IN THREE DIMENSIONAL IMAGE RESTORATION PROBLEMS*

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Abstract. In this paper, we propose a method to find the best Kronecker product approximation of the blurring operator which arises in three dimensional image restoration problems. We show that this problem can be reduced to a well known rank-1 approximation of the scaled three dimensional point spread function (PSF) array, which is much smaller. This approximation can be used as a preconditioner in solving image restoration problems with iterative methods. The comparison of the approximation by the new scaled PSF array and approximation by the original PSF array that is used in [J. G. Nagy and M. E. Kilmer, *IEEE Trans. Image Process.*, 15 (2006), pp. 604–613], confirms the performance of the new proposed approximation.

Key words. image restoration, Kronecker product approximation, tensor decomposition, tensor best rank-1 approximation, preconditioner

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1. Introduction. Image restoration is the process of reconstructing a true image of a scene from its blurred and noisy measurement. Mathematically, space-invariant image restoration can be modeled as

$$(1.1) \quad y(s) = \int h(s-t)x(t)dt + e(s), \quad s, t \in \mathbb{R}^d, \quad d = 1, 2, 3,$$

where x and y are functions that represent true and noisy blurred (observed) images, respectively, and e denotes additive noise in the process [8]. Also $h(s-t)$ is a function that specifies how the points in the image are blurred and will be called a point spread function (PSF). The discrete version of the blurring procedure can be written as

$$(1.2) \quad \mathbf{b} = A\mathbf{x}, \quad \mathbf{b} = \mathbf{y} + \mathbf{e},$$

where A is the blurring matrix [8]. This is a discrete ill-posed problem and the solution is very sensitive to the noise in the right-hand side of (1.2) [20]. The structure of the blurring matrix A depends on the assumptions made on the pixels outside the image that affect the blurring process [8]. Since we do not know the real values of these pixels, in image restoration artificial boundary conditions (BC) are usually imposed. In the literature, zero, periodic, reflective, and antireflective are the most well known BCs [9, 8, 16, 2]. Corresponding to these different boundary conditions, the blurring matrix has multilevel Toeplitz, Circulant, and Toeplitz plus Hankel structures, respectively.

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The structure of the blurring matrix A also depends on the PSF array. When the PSF array is separable (i.e., it has rank-1), the blurring process in different modes of the image are independent and the blurring matrix A is the Kronecker product of the blurring matrices of these modes. This type of linear system of equations can be solved easily [8].

When the PSF array is not separable, using iterative methods to solve the large linear system (1.2) is the best choice. Since the blurring matrix A has special structure (Toeplitz, Toeplitz plus Hankel, etc.), matrix-vector multiplications can be carried out very fast [8, 15, 3]. Thus, each step of an iterative method can be implemented efficiently. However, it is often the case that it is necessary to use some suitable approximation of A as a preconditioner to improve the rate of convergence [6, 7, 18].

Various circulant approximations of matrix A have been proposed; see, for example, [7]. In [18] an incomplete Lanczos process was used to find a preconditioner for ill-posed problems. Using Kronecker product approximation of the blurring matrix as a preconditioner is another approach that has been studied in some papers [9, 13, 17, 12]. This is equivalent to approximating the PSF array with a separable one. Finding the best Kronecker product approximation of general block matrices has been discussed by Van Loan and Pitsianis [19], and Kamm and Nagy in [9] addressed this issue for two dimensional (2-D) image restoration problems with zero BC. They showed that this problem is equivalent to finding the best rank-1 approximation of the scaled PSF array with a size much smaller than that of the blurring matrix. In recent years, this approach has been applied for other boundary conditions, too [13, 17, 10].

In this paper, we introduce the best Kronecker product approximation of a three level banded block Toeplitz matrix that occurs in three dimensional (3-D) image restoration problems. In fact, this is an extension of the result of [9] to 3-D problems. The Kronecker product approximation of the blurring matrix was used as a preconditioner for 3-D image restoration for the first time in [12], but the optimality of the approximation was not discussed. Based on the results of the 2-D case, one can predict that the best Kronecker product approximation in the 3-D case can be obtained by using the best rank-1 approximation of a scaled PSF array (order-3 tensor). In this paper we prove, using tensor concepts, that the optimal Kronecker product approximation of the blurring matrix arising in 3-D image restoration with zero boundary conditions can be reduced to finding the best rank-1 approximation of the scaled PSF array, which is a well known problem in tensor decomposition literature [4, 5, 11]. We also give the weights and demonstrate their effects on the PSF array. The numerical results show that the “scaled” version is better than the “unscaled” one. After submitting this manuscript to SIMAX, we learned that the idea of using the weighted PSF array to compute the best Kronecker product approximation was already suggested (without proofs) in a talk given by Misha Kilmer at the 2006 SIAM annual meeting.¹

This paper is organized as follows. Section 2 contains some concepts and notation that will be needed in other sections. A brief account of the modeling of image deblurring with zero boundary is given in section 3. In section 4 we explain the best Kronecker product approximation for 2-D image deblurring. The extension of the best Kronecker product approximation to three dimensions is discussed and formulated in section 5. Section 6 contains some experimental results.

¹See http://www.tufts.edu/~mkilmer01/list_of_medicalimaging.html under the heading “Structured Matrices and Tensors...”

2. Notation and preliminaries. We consider a tensor as a generalization of vectors and matrices of high dimensions. In this framework vectors and matrices can be considered as tensors of order one and two, respectively. Tensors will be denoted by calligraphic letters, e.g, $\mathcal{A}, \mathcal{B}$, matrices by capital roman letters, and vectors by small roman letters. Let $\mathcal{A}$ denote a tensor in $\mathbb{R}^{I_1 \times I_2 \times I_3}$. Different “dimensions” of tensors are referred to as *modes*. We will use both standard subscripts and “MATLAB-like” notation: a particular tensor element will be denoted in two equivalent ways:

$$\mathcal{A}(i, j, k) = a_{ijk}.$$

The Frobenius norm of $\mathcal{A}$ is defined

$$(2.1) \quad \|\mathcal{A}\| = \left(\sum_{i,j,k} a_{ijk}^2 \right)^{1/2}.$$

A fiber is a subtensor, where all indices but one are fixed. For example, mode-2 fibers of $\mathcal{A}$ have the following form:

$$\mathcal{A}(i, :, j) \in \mathbb{R}^{I_2}.$$

Next, we define *mode- p multiplication of a tensor by a matrix* as follows. For concreteness we first let $p = 1$. The mode-1 product of a tensor $\mathcal{A} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ by a matrix $W \in \mathbb{R}^{K \times I_1}$ is defined as

$$(2.2) \quad \mathbb{R}^{K \times I_2 \times I_3} \ni \mathcal{B} = (W)_1 \cdot \mathcal{A}, \quad b_{ki_2 i_3} = \sum_{i_1=1}^{I_1} w_{ki_1} a_{i_1 i_2 i_3}.$$

This means that all column vectors (mode-1 fibers) in the order-3 tensor are multiplied by the matrix W . Similarly, mode-2 multiplication by a matrix X means that all row vectors (mode-2 fibers) are multiplied by the matrix X . Mode-3 multiplication is defined similarly. In the case when tensor $\times$ matrix multiplication is performed in all modes in the same formula, we omit the subscripts and write

$$(2.3) \quad (X, Y, Z) \cdot \mathcal{A},$$

where the mode of each multiplication is understood from the order in which the matrices appear. We next introduce a couple of variants of the reshaping of matrices that will be used in the following sections. Let

$$(2.4) \quad A = [\mathbf{a}_1, \dots, \mathbf{a}_p] \in \mathbb{R}^{p \times p}$$

be a matrix with columns $\mathbf{a}_1, \dots, \mathbf{a}_p$. The $\text{vec}(\cdot)$ operator transforms the matrix A into the following vector:

$$\text{vec}(A) = \begin{pmatrix} \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_p \end{pmatrix} \in \mathbb{R}^{p^2}.$$

It is clear that $\|\text{vec}(A)\| = \|A\|$. Similarly, for the block matrix

$$(2.5) \quad A = \begin{pmatrix} A_{11} & \dots & A_{1m} \\ \vdots & & \vdots \\ A_{m1} & \dots & A_{mm} \end{pmatrix},$$

where for every i, j the matrix $A_{i,j} \in \mathbb{R}^{p \times p}$ has the form (2.4), we define

$$\tilde{A} = (\text{vec}(A_{11}) \quad \dots \quad \text{vec}(A_{m1}) \quad \dots \quad \text{vec}(A_{1m}) \quad \dots \quad \text{vec}(A_{mm}))^\top \in \mathbb{R}^{m^2 \times p^2}.$$

Obviously, $\|A\| = \|\tilde{A}\|$. If $A = (A_{ij})_{1 \leq i,j \leq n}$ is a three level block matrix in which A_{ij} are block matrices of the form (2.5), we define the operator Γ to act on A as

$$\Gamma(A)(:, :, (j-1)n+i) = \tilde{A}_{ij}, \quad i, j = 1, \dots, n.$$

The structure of $\Gamma(A) \in \mathbb{R}^{m^2 \times p^2 \times n^2}$ can be seen in Figure 1. It is easy to see that

$$(2.6) \quad \|A\| = \|\Gamma(A)\|.$$

FIG. 1. Tensor $\Gamma(A)$ of order three.

2.1. Toeplitz matrices. A matrix $A = (a_{ij})_{i,j=1,\dots,n}$ is Toeplitz if the same elements appear in its diagonals. These matrices have special structure and properties. For example, matrix-vector multiplication for these matrices can be carried out in $O(n \log n)$ [3]. In this paper we have banded Toeplitz matrices

$$(2.7) \quad A = \begin{pmatrix} a_l & \dots & a_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ a_n & & & & a_1 \\ & \ddots & & \ddots & \\ 0 & & a_n & \dots & a_l \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

Here we use

$$A = \text{toep}(\mathbf{a}, l), \quad \mathbf{a} = [a_1, \dots, a_n]^\top \in \mathbb{R}^n,$$

to denote the Toeplitz matrix A given in (2.7), which can be constructed just by the vector $\mathbf{a}$. Here, l refers to the l th elements of the vector $\mathbf{a}$ that appears on the main diagonal of A . By introducing the shift matrix Z as

$$(2.8) \quad Z = \begin{pmatrix} 0 & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & 0 \end{pmatrix} \in \mathbb{R}^{n \times n},$$

the matrix (2.7) can be written as

$$A = [Z^{l-1}\mathbf{a}, \dots, Z\mathbf{a}, \mathbf{a}, Z^\top \mathbf{a}, \dots, Z^{(n-l)\top} \mathbf{a}].$$

Here for every j ,

$$Z^j \mathbf{a} = [a_{j+1}, \dots, a_n, 0, \dots, 0]^\top$$

and

$$Z^{j\top} \mathbf{a} = [0, \dots, 0, a_1, \dots, a_{n-j}]^\top.$$

2.2. Kronecker product. Let $A \in \mathbb{R}^{n \times n}$ and $B \in \mathbb{R}^{m \times m}$ be two matrices. The Kronecker product $A \otimes B$ of these matrices is defined

$$(2.9) \quad A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{n1}B & \cdots & a_{nn}B \end{pmatrix}.$$

3. The blurring operator in image restoration with zero boundary conditions. In this section we study the structure of the blurring operator in the image restoration problem with zero boundary conditions. We first consider the one dimensional case. Here the discrete version of the blurring process (1.1) can be written as the following convolution equation:

$$(3.1) \quad y_i = \sum_{j=-\infty}^{\infty} h_{i-j} x_j, \quad i = 1, \dots, n,$$

where x, y denote true and blurred images (signals), respectively.

The vector $[h_k]_{k=-\infty, \dots, \infty}$, which will be named the PSF array, denotes the discrete version of point spread function. This shows that every element y_i of the blurred image can be obtained from convolution of the PSF array with the true scene. Here h_0 , the weight of x_i in construction of y_i , is called the center of the PSF array. In all applications except a finite number of elements around the center are zero. So if $h_i, i = 1-l, \dots, n-l$ are the nonzero elements of the PSF, by (3.1) the process of finding the blurred signal $\mathbf{y} = [y_1, \dots, y_n]^\top$ can be modeled as

$$(3.2) \quad \begin{pmatrix} h_{n-l} & \cdots & h_0 & \cdots & h_{1-l} & & \\ & \ddots & & \ddots & & \ddots & \\ & & \ddots & & \ddots & \ddots & \\ & & & \ddots & & \ddots & \\ & & & & h_{n-l} & \cdots & h_0 & \cdots & h_{1-l} \end{pmatrix} \begin{pmatrix} x_{l-n+1} \\ \vdots \\ x_0 \\ x_1 \\ \vdots \\ x_n \\ x_{n+1} \\ \vdots \\ x_{n+l-1} \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}.$$

The subvectors $\mathbf{x}_l = [x_{l-n+1}, \dots, x_0]^\top$ and $\mathbf{x}_r = [x_{n+1}, \dots, x_{n+l-1}]^\top$ are named boundaries of the vector $\mathbf{x} = [x_1, \dots, x_n]^\top$. In the zero boundary case $\mathbf{x}_l$ and $\mathbf{x}_r$ are zero.

So (3.2) becomes

$$(3.3) \quad \begin{pmatrix} h_0 & \cdots & h_{1-l} & & 0 \\ \vdots & \ddots & & \ddots & \\ h_{n-l} & & & h_{1-l} & \\ & \ddots & & & \ddots \\ 0 & & h_{n-l} & \cdots & h_0 \end{pmatrix} \begin{pmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ \vdots \\ y_n \end{pmatrix}.$$

For simplicity of notation, let $\mathbf{p} = [p_1, \dots, p_n]$, where $p_i = h_{i-l}, i = 1, \dots, n$, denote the nonzero part of the PSF array. By this notation (index shifting) the blurring model can be rewritten as

$$(3.4) \quad A\mathbf{x} = \mathbf{y}, \quad A = \begin{pmatrix} p_l & \cdots & p_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ p_n & & & p_1 & \\ & \ddots & & & \ddots \\ 0 & & p_n & \cdots & p_l \end{pmatrix}.$$

The blurring matrix $A = \text{toep}(\mathbf{p}, l)$ is a banded Toeplitz matrix, and p_l is the center of the PSF array $\mathbf{p}$.

This modeling can be extended to higher dimensions. For example, in the 2-D image restoration problem with zero boundaries, if $X, Y \in \mathbb{R}^{m \times n}$ are true and blurred images, respectively, and $P = [\mathbf{p}_1, \dots, \mathbf{p}_n] \in \mathbb{R}^{m \times n}$ is the PSF array with center $p_{l,q}$ (the weight of $X(i, j)$ in the construction of $Y(i, j)$), the blurring process can be modeled as

$$(3.5) \quad K\mathbf{x} = \mathbf{y},$$

where $\mathbf{x} = \text{vec}(X)$, $\mathbf{y} = \text{vec}(Y)$, and

$$(3.6) \quad K = \begin{pmatrix} T_q & \cdots & T_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ T_n & & & T_1 & \\ & \ddots & & & \ddots \\ 0 & & T_n & \cdots & T_q \end{pmatrix}$$

is block Toeplitz with Toeplitz blocks (BTTB) constructed by P . For every i , T_i is the Toeplitz matrix

$$T_i = \text{toep}(\mathbf{p}_i, l),$$

where $\mathbf{p}_i$ is the i th column of the PSF array [8].

Also for the 3-D problem, where $\mathcal{X}, \mathcal{Y} \in \mathbb{R}^{m \times n \times p}$ and $\mathcal{P} \in \mathbb{R}^{m \times n \times p}$, denote the true image, blurred image, and PSF array with center $\mathcal{P}_{l,q,r}$, respectively; the blurring operator can be obtained as

$$(3.7) \quad A = \begin{pmatrix} K_r & \cdots & K_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ K_p & & & K_1 & \\ & \ddots & & & \ddots \\ 0 & & K_p & \cdots & K_r \end{pmatrix}.$$

Here each K_i is a banded BTTB matrix as expressed in (3.6), constructed by $\mathcal{P}(:, :, i)$. So A is a multilevel block Toeplitz matrix with BTTB blocks and the blurring process with zero boundaries can be formulated as

$$A\mathbf{x} = \mathbf{y},$$

where

$$(3.8) \quad \mathbf{y} = [\text{vec}(\mathcal{Y}(:, :, 1))^T, \dots, \text{vec}(\mathcal{Y}(:, :, n))^T]^T,$$

$$(3.9) \quad \mathbf{x} = [\text{vec}(\mathcal{X}(:, :, 1))^T, \dots, \text{vec}(\mathcal{X}(:, :, n))^T]^T.$$

Thus we have demonstrated that a 2-D or 3-D image restoration problem can be modeled as a large scale linear system, with a multilevel Toeplitz coefficient matrix. To solve such a linear system it is necessary to use an iterative method, with a suitable preconditioner to improve the rate of convergence [6, 7, 18]. To construct a preconditioner various approximations of the blurring operator have been used, e.g., circulant approximation [7], incomplete Lanczos decomposition [18], and Kronecker product approximation [9, 13, 17, 12, 19]. In [9] Kamm and Nagy showed that for 2-D image restoration with zero boundary conditions the problem of determining the best Kronecker product approximation is equivalent to finding the best rank-1 approximation of the scaled PSF array with a size much smaller than that of the blurring matrix. Recently, this problem has been studied also for other boundary conditions [13, 17, 10]. In the rest of this paper, we extend the best Kronecker approximation result of [9] to the 3-D image restoration problem. However, to set the stage we first consider the 2-D case.

4. The Kronecker product approximation in the 2-D image restoration problem. We first consider the special case in which the blurring of the columns and rows are independent, i.e., the point spread array is separable and can be written as $P = \mathbf{b}\mathbf{c}^T$, where $\mathbf{b}$ and $\mathbf{c}$ are the vertical and horizontal PSF arrays with centers l and q , respectively. Consequently, the blurring matrix in (3.5) is the Kronecker product of two matrices $C = \text{toep}(\mathbf{c}, q)$ and $B = \text{toep}(\mathbf{b}, l)$ [9, 8],

$$(4.1) \quad K = C \otimes B.$$

By this structure, (3.5) can be rewritten

$$Y = BXC^T.$$

For nonsingular matrices B and C , the solution X is

$$X = B^{-1}YC^{-T},$$

which shows that solving the equation with Kronecker product structure matrices is much easier than in the general case. For a nonseparable PSF array, the blurring matrix can be approximated by a Kronecker product of two matrices, which can be used as a preconditioner. The approximation problem can be written as the following minimization problem:

$$(4.2) \quad \min_{\mathbf{b}, \mathbf{c}} \|K - C \otimes B\|,$$

where $B = \text{toep}(\mathbf{b}, l)$, $C = \text{toep}(\mathbf{c}, q)$, and K is a BTTB matrix defined in (3.6). Recall that by the Van Loan and Pitsianis approach [19], we have

$$(4.3) \quad \min \|K - C \otimes B\| = \min \|\widetilde{K} - \widetilde{C \otimes B}\| = \min \|\widetilde{K} - \text{vec}(C)\text{vec}(B)^T\|,$$

which shows that (4.2) is equivalent to finding the best rank-1 approximation of the matrix $\tilde{K}$. In [9] it is shown that, since K is banded BTTB blurring matrix corresponding to the PSF array P defined in (3.6), (4.3), in turn, is equivalent to

$$(4.4) \quad \min_{B,C} \|K - C \otimes B\| = \min_{\mathbf{b}, \mathbf{c}} \|R_l(P - \mathbf{b}\mathbf{c}^\top)R_q^\top\|,$$

where for $t = l, q$,

$$(4.5) \quad R_t = \text{diag}(\sqrt{n-t+1}, \sqrt{n-t+2}, \dots, \sqrt{n}, \sqrt{n-1}, \dots, \sqrt{t}).$$

This means that the problem of computing the best Kronecker product approximation of a large blurring matrix is reduced to computing the best rank-1 approximation of the scaled PSF array, which is much smaller in size. With the singular value decomposition $R_l P R_q = U \Sigma V^\top$, the solution is

$$\begin{aligned} \mathbf{b} &= R_l^{-1} \sqrt{\sigma_1} \mathbf{u}_1, & \mathbf{c} &= R_q^{-1} \sqrt{\sigma_1} \mathbf{v}_1, \\ B &= \text{toep}(\mathbf{b}, l), & C &= \text{toep}(\mathbf{c}, q), \end{aligned}$$

where $\mathbf{u}_1$ and $\mathbf{v}_1$ are the singular vectors corresponding to the largest singular value σ_1 .

These results have been proved in [9]. In the generalization to 3-D problems, we will need some details of proof for the 2-D case. But if we use the approach of [9], we will face some difficulties. Hence we present an alternative proof which allows us to generalize more easily the result to 3-D problems.

LEMMA 4.1. *Let K and $C \otimes B$ be the banded BTTB blurring matrices corresponding to the PSF arrays $P \in \mathbb{R}^{m \times n}$ and $\tilde{P} = \mathbf{b}\mathbf{c}^\top \in \mathbb{R}^{m \times n}$, respectively, with the centers located at position (l, q) . Then*

$$\|K - C \otimes B\| = \|R_l(P - \mathbf{b}\mathbf{c}^\top)R_q^\top\|,$$

where $R_t, t = l, q$, are defined in (4.5).

Proof. Let $P = [\mathbf{p}_1, \dots, \mathbf{p}_n] \in \mathbb{R}^{m \times n}$ be the PSF array with the center located at the (l, q) position. Then the blurring model is

$$K \text{vec}(X) = \text{vec}(Y),$$

where

$$K = \begin{pmatrix} T_q & \cdots & T_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ T_n & & & & T_1 \\ & \ddots & & \ddots & \\ 0 & & T_n & \cdots & T_q \end{pmatrix},$$

and for every k , $T_k = \text{toep}(\mathbf{p}_k, l)$. Let $K = [K_1, \dots, K_n]$, where K_j is the j th block column of K . In this case K_j has the following structure:

$$K_j = \begin{pmatrix} T_{q-j+1} \\ \vdots \\ T_n \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad 1 \leq j \leq q,$$

and

$$K_j = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ T_1 \\ \vdots \\ T_{n-j+q} \end{pmatrix}, \quad q+1 \leq j \leq n.$$

For $1 \leq j \leq q$,

$$(4.6) \quad \tilde{K}_j = \begin{pmatrix} \text{vec}(T_{q-j+1})^\top \\ \vdots \\ \text{vec}(T_n)^\top \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} \text{vec}(\text{toep}(\mathbf{p}_{q-j+1}, l))^\top \\ \vdots \\ \text{vec}(\text{toep}(\mathbf{p}_n, l))^\top \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

But, for every vector $\mathbf{a}$,

$$\text{toep}(\mathbf{a}, l) = [Z^{l-1}\mathbf{a}, \dots, Z\mathbf{a}, Z^0\mathbf{a}, Z^\top\mathbf{a}, \dots, Z^{(n-l)^\top}\mathbf{a}],$$

and so it is easy to see that

$$\text{vec}(\text{toep}(\mathbf{a}, l))^\top = \mathbf{a}^\top [Z^{(l-1)^\top}, \dots, Z^\top, Z^0, Z, \dots, Z^{n-l}].$$

Therefore, (4.6) can be written

$$\tilde{K}_j = \begin{pmatrix} \mathbf{p}_{q-j+1}^\top \\ \vdots \\ \mathbf{p}_n^\top \\ 0 \\ \vdots \\ 0 \end{pmatrix} [Z^{(l-1)^\top}, \dots, Z^\top, Z^0, Z, \dots, Z^{n-l}], \quad 1 \leq j \leq q.$$

On the other hand we have

$$Z^{q-j} P^\top = \begin{pmatrix} \mathbf{p}_{q-j+1}^\top \\ \vdots \\ \mathbf{p}_n^\top \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad 1 \leq j \leq q,$$

so for $1 \leq j \leq q$,

$$\tilde{K}_j = Z^{q-j} P^\top [Z^{(l-1)^\top}, \dots, Z^\top, Z^0, Z, \dots, Z^{n-l}].$$

Similarly, for $q+1 \leq j \leq n$,

$$\tilde{K}_j = Z^{(j-q)^\top} P^\top [Z^{(l-1)^\top}, \dots, Z^\top, Z^0, Z, \dots, Z^{n-l}].$$

Therefore, $\tilde{K}$ can be written

$$(4.7) \quad \tilde{K} = \begin{pmatrix} \tilde{K}_1 \\ \vdots \\ \tilde{K}_q \\ \vdots \\ \tilde{K}_n \end{pmatrix} = \begin{pmatrix} Z^{q-1} \\ \vdots \\ Z^0 \\ \vdots \\ Z^{(n-q)\top} \end{pmatrix} P^\top \begin{pmatrix} Z^{(l-1)\top} & \dots & Z^0 & \dots & Z^{n-l} \end{pmatrix}.$$

With the definition $E_t = [Z^{(t-1)\top}, \dots, Z^0, \dots, Z^{(n-t)\top}]^\top$, (4.7) becomes

$$(4.8) \quad \tilde{K} = E_q P^\top E_l^\top.$$

Using the same technique we get

$$(4.9) \quad \widetilde{C \otimes B} = E_q(\mathbf{c}\mathbf{b}^\top)E_l.$$

Hence,

$$(4.10) \quad \begin{aligned} \|K - C \otimes B\| &= \|\tilde{K} - \widetilde{C \otimes B}\| = \|E_q(P^\top - \mathbf{c}\mathbf{b}^\top)E_l^\top\| \\ &= \|E_l(P - \mathbf{b}\mathbf{c}^\top)E_q^\top\|. \end{aligned}$$

Since $Z^j = \sum_{i=1}^j e_i e_{i+j}^\top$, it is easy to see that E_t has orthogonal columns:

$$\begin{aligned} E_t^\top E_t &= \sum_{j=0}^{t-1} Z^j{}^\top Z^j + \sum_{j=0}^{n-t} Z^j Z^j{}^\top = \sum_{j=0}^{t-1} \sum_{i=j+1}^n e_i e_i^\top + \sum_{j=1}^{n-t} \sum_{i=1}^{n-j} e_i e_i^\top \\ &= \text{diag}(1, 2, \dots, t-1, t, t, \dots, t) \\ &\quad + \text{diag}(n-t, n-t, \dots, n-t, n-t, n-t-1, \dots, 0) \\ &= \text{diag}(n-t+1, n-t+2, \dots, n-1, n, n-1, \dots, t-1, t). \end{aligned}$$

By definition $R_t = \text{diag}(\sqrt{n-t+1}, \sqrt{n-t+2}, \dots, \sqrt{n}, \sqrt{n-1}, \dots, \sqrt{t})$. Thus $Q_t = E_t R_t^{-1}$ is an orthogonal matrix, $E_t = Q_t R_t$, and (4.10) becomes

$$\|K - C \otimes B\| = \|R_l(P - \mathbf{b}\mathbf{c}^\top)R_q\|.$$

This proves the lemma. $\square$

Lemma 4.1 can be generalized as follows.

LEMMA 4.2. *Let K and $\sum_{i=1}^r C_i \otimes B_i$ be the BTTB matrices corresponding to the PSF arrays $P \in \mathbb{R}^{m \times n}$ and $\bar{P} = \sum_{i=1}^r \mathbf{b}_i \mathbf{c}_i^\top \in \mathbb{R}^{m \times n}$, respectively, with centers located at the (l, q) position. Then*

$$\left\| K - \sum_{i=1}^r C_i \otimes B_i \right\| = \left\| R_l \left(P - \sum_{i=1}^r \mathbf{b}_i \mathbf{c}_i^\top \right) R_q^\top \right\|.$$

Proof. The proof is similar to Lemma 4.1. $\square$

5. The Kronecker product approximation in the 3-D problem. In 3-D image restoration with zero boundaries we have a linear system in which the coefficient matrix is block Toeplitz with BTTB blocks. We now formulate the best Kronecker product approximation problem for the 3-D problem and give its solution. To see the advantage of a separable PSF array in three dimensions, consider the separable PSF array $\mathcal{P} = \mathbf{b} \circ \mathbf{c} \circ \mathbf{d}$ ($\circ$ denotes the outer product, i.e., $\mathcal{P}_{i,j,k} = b_i c_j d_k$) with $\mathcal{P}_{l,q,r} = b_l c_q d_r$ as its center. It is easy to see that the blurring process can be modeled as

$$(D \otimes C \otimes B)x = y,$$

where the vectors y, x are defined in (3.8) and (3.9), respectively. Also

$$D = \text{toep}(\mathbf{d}, r), \quad C = \text{toep}(\mathbf{c}, q), \quad B = \text{toep}(\mathbf{b}, l).$$

In this case, using tensor notation, we have

$$\mathcal{Y} = (B, C, D) \cdot \mathcal{X},$$

and for nonsingular B, C, D matrices, the solution is

$$\mathcal{X} = (B^{-1}, C^{-1}, D^{-1}) \cdot \mathcal{Y}.$$

Now as in the 2-D case we want to find the best Kronecker product approximation of a multilevel Toeplitz matrix with BTTB blocks to be used as a preconditioner. Here we show that finding the best Kronecker approximation of this multilevel matrix is equivalent to finding the best rank-1 approximation of the scaled PSF array, for which the size of the problem is much smaller than for the original problem. In [12] the authors used a rank-1 approximation of the PSF array to construct a preconditioner for 3-D image deblurring but their Kronecker approximation is not optimal. In the following theorem we give the optimal Kronecker product approximation of the blurring matrix in the 3-D image deblurring problem with zero boundary conditions.

THEOREM 5.1. *Let A and $D \otimes C \otimes B$ be the block Toeplitz matrices with BTTB blocks corresponding to the PSF arrays $\mathcal{P} \in \mathbb{R}^{m \times n \times p}$ and $\overline{\mathcal{P}} = \mathbf{b} \circ \mathbf{c} \circ \mathbf{d} \in \mathbb{R}^{m \times n \times p}$, respectively, such that their centers are located at the (l, q, r) position. Then*

$$(5.1) \quad \|A - D \otimes C \otimes B\| = \|(R_l, R_q, R_r) \cdot (\mathcal{P} - \mathbf{b} \circ \mathbf{c} \circ \mathbf{d})\|,$$

where R_t , $t = l, q, r$, are defined in (4.5).

Proof. Let

$$A = \begin{pmatrix} K_r & \cdots & K_1 & & 0 \\ \vdots & \ddots & & \ddots & \\ K_n & & & & K_1 \\ & \ddots & & \ddots & \\ 0 & & K_n & \cdots & K_r \end{pmatrix}$$

be the blurring matrix corresponding to the PSF array $\mathcal{P}$. A is block Toeplitz with BTTB blocks, where for every i , K_i is a BTTB matrix of the form (3.6). Let A_k be the k th block column of A ; then by the definition of the operator Γ ,

$$\Gamma(A)(:, :, (k-1)n+1 : kn) = \Gamma(A_k), \quad \Gamma(A_k) \in \mathbb{R}^{m^2 \times n^2 \times p}.$$

We now explore the structure of $\Gamma(A_k)$. For $1 \leq k \leq r$,

$$A_k = \begin{pmatrix} K_{r-k+1} \\ \vdots \\ K_n \\ 0 \\ \vdots \\ 0 \end{pmatrix}.$$

It is easy to see that $\Gamma(A_k)$ has the following form:

$$(5.2) \quad \Gamma(A_k)(:, :, i) = \begin{cases} \tilde{K}_{r-k+i}, & 1 \leq i \leq n-r+k, \\ 0, & n-r+k < i \leq n, \end{cases} \quad i = 1, \dots, n.$$

Similarly, for $r+1 \leq k \leq n$,

$$(5.3) \quad \Gamma(A_k)(:, :, i) = \begin{cases} 0, & 1 \leq i \leq k-r, \\ \tilde{K}_{i-k+r}, & k-r+1 \leq i \leq n, \end{cases} \quad i = 1, \dots, n.$$

The details are illustrated in Figure 2. By using the relation (4.8) in the proof of Lemma 4.1, we have

$$(5.4) \quad \tilde{K}_j = E_q P(:, :, j)^\top E_l^\top, \quad j = 1, \dots, p.$$

FIG. 2. $\Gamma(A_k)$, for $k \leq r$ and $k > r$, from left to right, respectively.

By (5.4) and using the structure of the $\Gamma(A_k)$ in (5.2) and (5.3), we can write

$$(5.5) \quad \Gamma(A_k) = (E_q, E_l)_{1:2} \cdot \mathcal{T}^k,$$

where, for $1 \leq k \leq r$,

$$\mathcal{T}^k(:, :, i) = \begin{cases} \mathcal{P}(:, :, r-k+i)^\top, & 1 \leq i \leq n-r+k, \\ 0, & \text{else,} \end{cases} \quad i = 1, \dots, n,$$

and for $r+1 \leq k \leq n$,

$$\mathcal{T}^k(:, :, i) = \begin{cases} 0, & 1 \leq i \leq k-r, \\ \mathcal{P}(:, :, i-k+r)^\top, & k-r+1 \leq i \leq n, \end{cases} \quad i = 1, \dots, n.$$

The structure of $\mathcal{T}^k$ can be seen in Figure 3.

FIG. 3. $\mathcal{T}^k$, for $k \leq r$ and $k > r$, from left to right, respectively.

Defining $\mathcal{P}^\top$ as

$$\mathcal{P}^\top(:, :, j) = \mathcal{P}(:, :, j)^\top, \quad j = 1, \dots, p,$$

for $1 \leq k \leq r$, $\mathcal{T}^k$ can be written as

$$\mathcal{T}^k = (Z^{r-k})_3 \cdot \mathcal{P}^\top,$$

and by (5.5) we have,

$$\Gamma(A_k) = (E_q, E_l, Z^{r-k}) \cdot \mathcal{P}^\top.$$

In the same way, for $r+1 \leq k \leq n$, $\Gamma(A_k)$ has the following structure:

$$\Gamma(A_k) = (E_q, E_l, Z^{(k-r)^\top}) \cdot \mathcal{P}^\top.$$

Therefore, from this result, the structure of A_k , and the relation between $\Gamma(A)$ and $\Gamma(A_k)$, we can write

$$\Gamma(A) = \left(E_q, E_l, \begin{pmatrix} Z^{r-k} \\ \vdots \\ Z^0 \\ \vdots \\ Z^{(n-r)^\top} \end{pmatrix} \right) \cdot \mathcal{P}^\top = (E_q, E_l, E_r)_{1:3} \cdot \mathcal{P}^\top.$$

Analogously we have

$$\Gamma(D \otimes C \otimes B) = (E_q, E_l, E_r) \cdot (\mathbf{c} \circ \mathbf{b} \circ \mathbf{d}).$$

Therefore, by the definition of $\Gamma(\cdot)$ and (2.6),

$$\begin{aligned} \|A - D \otimes C \otimes B\| &= \|\Gamma(A - D \otimes C \otimes B)\| = \|\Gamma(A) - \Gamma(D \otimes C \otimes B)\| \\ &= \|(E_q, E_l, E_r) \cdot (\mathcal{P}^\top - \mathbf{c} \circ \mathbf{b} \circ \mathbf{d})\| \\ &= \|(E_l, E_q, E_r) \cdot (\mathcal{P} - \mathbf{b} \circ \mathbf{c} \circ \mathbf{d})\| \\ &= \|(R_l, R_q, R_r) \cdot (\mathcal{P} - \mathbf{b} \circ \mathbf{c} \circ \mathbf{d})\|. \end{aligned}$$

The last equation comes from the invariance of the Frobenius norm under multiplication by an orthogonal matrix in an arbitrary mode. This proves the theorem. $\square$

The previous theorem shows that the problem

$$(5.6) \quad \min_{D,C,B} \|A - D \otimes C \otimes B\|$$

is equivalent to

$$(5.7) \quad \min_{\widehat{\mathbf{b}}, \widehat{\mathbf{c}}, \widehat{\mathbf{d}}} \|\widehat{\mathcal{P}} - \widehat{\mathbf{b}} \circ \widehat{\mathbf{c}} \circ \widehat{\mathbf{d}}\|,$$

where $\widehat{\mathcal{P}} = (R_l, R_q, R_r)_{1:3} \cdot \mathcal{P}$. Given the solution $\widehat{\mathbf{b}}, \widehat{\mathbf{c}}$ and $\widehat{\mathbf{d}}$ of (5.7), the solution of (5.6) is

$$B = \text{toep}(\mathbf{b}, l), \quad C = \text{toep}(\mathbf{c}, q), \quad D = \text{toep}(\mathbf{d}, r),$$

where

$$(5.8) \quad \mathbf{b} = R_l^{-1} \widehat{\mathbf{b}}, \quad \mathbf{c} = R_q^{-1} \widehat{\mathbf{c}}, \quad \mathbf{d} = R_r^{-1} \widehat{\mathbf{d}}.$$

Although, unlike the 2-D case, there is no known closed-form solution of the approximation problem (5.7), it can be shown that this minimization problem is well defined [4, Corollary 4.5], and there are several methods for computing the best rank-1 approximation of a tensor [5, 11]. The results of Theorem 5.1 can be generalized as follows.

PROPOSITION 5.2. *Let A and $\sum_{i=1}^k D_i \otimes C_i \otimes B_i$ be the block Toeplitz matrices with BTTB blocks corresponding to the PSF arrays $\mathcal{P} \in \mathbb{R}^{m \times n \times p}$ and $\overline{\mathcal{P}} = \sum_{i=1}^k \mathbf{b}_i \circ \mathbf{c}_i \circ \mathbf{d}_i \in \mathbb{R}^{m \times n \times p}$, respectively, such that their centers are located at the (l, q, r) position. Then*

$$\left\| A - \sum_{i=1}^k D_i \otimes C_i \otimes B_i \right\| = \left\| (R_l, R_q, R_r) \cdot \left(\mathcal{P} - \sum_{i=1}^k \mathbf{b}_i \circ \mathbf{c}_i \circ \mathbf{d}_i \right) \right\|.$$

Proof. The proof is similar to that of Theorem 5.1. $\square$

So, with $\widehat{\mathcal{P}} = (R_l, R_q, R_r) \cdot \mathcal{P}$, we have

$$(5.9) \quad \min \left\| A - \sum_{i=1}^k D_i \otimes C_i \otimes B_i \right\| = \min \left\| \widehat{\mathcal{P}} - \sum_{i=1}^k \widehat{\mathbf{b}}_i \circ \widehat{\mathbf{c}}_i \circ \widehat{\mathbf{d}}_i \right\|.$$

Then

$$\mathbf{b}_i = R_l^{-1} \widehat{\mathbf{b}}_i, \quad \mathbf{c}_i = R_q^{-1} \widehat{\mathbf{c}}_i, \quad \mathbf{d}_i = R_r^{-1} \widehat{\mathbf{d}}_i,$$

where $\widehat{\mathbf{b}}_i$, $\widehat{\mathbf{c}}_i$, and $\widehat{\mathbf{d}}_i$ are the solutions to the right-hand side problem in (5.9). That problem is the rank- k CANDECOMP/PARAFAC decomposition of the tensor $\widehat{\mathcal{P}}$ [11].

6. Numerical results. In this section, we present some numerical experiments that illustrate the effectiveness of our preconditioner. Here we consider a 3-D MRI test problem presented in [12]. The true image is a tensor $\mathcal{X} \in \mathbb{R}^{128 \times 128 \times 27}$. Six 128×128 slices are given in Figure 4. The known true image is artificially blurred with a known space invariant PSF, and 1% white noise is added to the blurred image. We simulate blurring effects caused by partial volume averaging in spiral CT [21], which can be approximated well by a 3-D Gaussian PSF,

$$p(x, y, z) = (p_1(x, y, z) + p_2(x, y, z) + p_3(x, y, z))/3,$$

FIG. 4. Slices from the MRI test problem.

FIG. 5. The relative errors $\hat{r}_k$ (left) and r_k (right) for $k = 1, \dots, 20$.

where

$$p_i(x, y, z) = \frac{1}{\sqrt{2\pi^3}\sigma_i^3} e^{-(x^2+y^2+z^2)/2\sigma_i^2}.$$

Here we choose $\sigma_1 = 1$, $\sigma_2 = 1.5$, and $\sigma_3 = 2$. The discrete PSF is $\mathcal{P} \in \mathbb{R}^{128 \times 128 \times 27}$, with center $\mathcal{P}(65, 65, 14)$.

To investigate the approximation power of our approach, we first compute the best rank- k approximation (the CANDECOMP/PARAFAC decomposition) of the scaled PSF tensor $\hat{\mathcal{P}}$ for $k = 1, \dots, 20$ in (5.9),

$$\hat{\mathcal{P}} \approx \sum_{i=1}^k \hat{\mathbf{b}}_i \circ \hat{\mathbf{c}}_i \circ \hat{\mathbf{d}}_i.$$

FIG. 6. Relative errors versus iterations for CGLS with different preconditioners.

Then, we compute the relative errors $\hat{r}_k$,

$$\hat{r}_k = \frac{\left\| A - \sum_{i=1}^k D_i \otimes C_i \otimes B_i \right\|}{\|A\|}, \quad k = 1, \dots, 20,$$

where

$$D_i = \text{toep}(R_{14}^{-1} \hat{\mathbf{d}}_i, 14), \quad C_i = \text{toep}(R_{65}^{-1} \hat{\mathbf{c}}_i, 65), \quad B_i = \text{toep}(R_{65}^{-1} \hat{\mathbf{b}}_i, 65).$$

The relative errors are plotted in the left of Figure 5.

The authors in [12] used rank-k approximations of the PSF tensor $\mathcal{P}$ rather than scaled PSF array $\hat{\mathcal{P}}$ to construct Kronecker product approximations. The right side of Figure 5 shows the corresponding relative errors r_k . Clearly, for this example our approach gives a much better approximation of the blurring operator.

As was suggested in [12], a regularized version of the proposed approximation can be used as a preconditioner in solving the restoration problem with iterative methods. This regularized preconditioner, for example, can be obtained by truncated singular value decomposition (TSVD) approximation. For any matrix $M \in R^{N \times N}$, with SVD $M = U \Sigma V^T$, then for a threshold τ , its TSVD approximation is $\bar{M} = U \bar{\Sigma} V^T$, where the diagonal elements of $\bar{\Sigma}$ are given by

$$(6.1) \quad \bar{\sigma}_i = \begin{cases} \sigma_i, & \sigma_i > \tau, \\ 0 & \text{otherwise.} \end{cases}$$

Let M be a Kronecker product approximation, i.e, $M = D \otimes C \otimes B$, where the SVDs of D, C , and B are given by

$$D = U_d \Sigma_d V_d^T, \quad C = U_c \Sigma_c V_c^T, \quad B = U_b \Sigma_b V_b^T.$$

Then the SVD of M is $M = U \Sigma V^T$, where

$$U = U_d \otimes U_c \otimes U_b, \quad V = V_d \otimes V_c \otimes V_b, \quad \Sigma = \Sigma_d \otimes \Sigma_c \otimes \Sigma_b.$$

FIG. 7. Relative errors versus iterations for MRNSD with different preconditioners.

We first solve the restoration problem without any preconditioner using the conjugate gradient for the least square problems (CGLS) method [1]. Second, we use the original PSF array to construct a Kronecker product preconditioner, referred to as “No-Weighted Kron,” and solve the restoration problem by the Preconditioned CGLS method. Finally we use our proposed method to construct a preconditioner (“Weighted Kron”). In both cases we use $\tau = 0.05$. Figure 6 shows the relative errors as a function of the number of iterations. We also solve the problem using the modified residual norm steepest descent (MRNSD) method [14]. Figure 7 shows the relative errors of the MRNSD method in conjunction with different preconditioning methods.

Figure 8 shows the restored images of slice 5 after 30 iterations by different methods. The same results for slice 15 can be seen in Figure 9.

These figures show the effect of the proposed preconditioner in improving the rate of convergence in iterative methods in restoration of the true image.

7. Conclusion. In this paper, we have proposed a new method to find the best Kronecker product approximation of multilevel structured matrices that occur in 3-D image deblurring problems with zero boundary conditions. The experimental results show the quality of this approximation. The results of this paper can be extended to other boundary conditions, e.g., antireflexive (M. Kilmer, personal communication).

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FIG. 8. *Noisy Blurred Slice 5. Restored Slice 5 by MRNSD without preconditioner and with No-Weighted Kron and Weighted Kron preconditioners, at iteration 30.*

FIG. 9. *Noisy Blurred Slice 5. Restored Slice 5 by MRNSD without preconditioner and with No-Weighted Kron and Weighted Kron preconditioners, at iteration 30.*

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