

## APPROXIMATION WITH KRONECKER PRODUCTS

C.F. VAN LOAN and N. PITSIANIS

*Department of Computer Science*

*Cornell University*

*Ithaca, New York 14853, U.S.A.*

*cv@cs.cornell.edu*

**ABSTRACT.** Let  $A$  be an  $m$ -by- $n$  matrix with  $m = m_1 m_2$  and  $n = n_1 n_2$ . We consider the problem of finding  $B \in \mathbb{R}^{m_1 \times n_1}$  and  $C \in \mathbb{R}^{m_2 \times n_2}$  so that  $\|A - B \otimes C\|_F$  is minimized. This problem can be solved by computing the largest singular value and associated singular vectors of a permuted version of  $A$ . If  $A$  is symmetric, definite, non-negative, or banded, then the minimizing  $B$  and  $C$  are similarly structured. The idea of using Kronecker product preconditioners is briefly discussed.

**KEYWORDS.** Kronecker product, preconditioners, block matrices.

### 1 Background

Suppose  $A \in \mathbb{R}^{m \times n}$  with  $m = m_1 m_2$  and  $n = n_1 n_2$ . This paper is about the minimization of

$$\phi_A(B, C) = \|A - B \otimes C\|_F^2$$

where  $B \in \mathbb{R}^{m_1 \times n_1}$ ,  $C \in \mathbb{R}^{m_2 \times n_2}$ , and " $\otimes$ " denotes the Kronecker product.

Our interest in this problem stems from preliminary experience with Kronecker product preconditioners in the conjugate gradient setting. Suppose  $A \in \mathbb{R}^{n \times n}$  with  $n = n_1 n_2$  and that  $M$  is the preconditioner. For this solution process to be successful, the preconditioner should "capture" the essence of  $A$  as much as possible subject to the constraint that a linear system  $Mz = r$  is "easy" to solve. In our context, we capture  $A$  through the minimization  $\phi_A(B, C)$  with  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$ . Systems of the form  $Mz \equiv (B \otimes C)z = r$  are easy to solve because only  $O(n^{3/2})$  flops are required if  $n_1 \approx n_2 \approx \sqrt{n}$ . To appreciate this point, observe that  $(B \otimes C)z = r$  is equivalent to

$$CZB^T = R \tag{1}$$

where  $Z$  and  $R$  are  $n_2$ -by- $n_1$  matrices whose columns are segments of the vectors  $z$  and  $r$  respectively:

$$\begin{aligned} Z(:, k) &= z((k-1)n_2 + 1:kn_2) \\ R(:, k) &= r((k-1)n_2 + 1:kn_2) \end{aligned} \quad k = 1:n_1.$$

(At this point the reader may wish to review the algebra of Kronecker products. See [21] or [29].) If  $B$  and  $C$  are nonsingular and we apply Gaussian elimination with partial pivoting to produce the factorizations  $P_1B = L_1U_1$  and  $P_2C = L_2U_2$ , then  $2(n_1^3 + n_2^3)/3$  flops are required. The ensuing multiple triangular system solves involve an additional  $2(n_1^2n_2 + n_1n_2^2)$  flops. If  $n = n_1^2 = n_2^2$ , then a total of  $16n^{3/2}/3$  flops are needed.

An instructive way to look at the above solution process is to recognize that

$$(P_1 \otimes P_2)(B \otimes C) = (L_1 \otimes L_2)(U_1 \otimes U_2)$$

is an  $LU$  (with partial pivoting) factorization of  $B \otimes C$ . This illustrates the adage that a given factorization of  $B \otimes C$  can usually be obtained by taking the Kronecker product of the corresponding  $B$  and  $C$  factorizations:

$$\text{Cholesky: } \begin{aligned} B &= L_1L_1^T \\ C &= L_2L_2^T \end{aligned} \Rightarrow (B \otimes C) = (L_1 \otimes L_2)(L_1 \otimes L_2)^T$$

$$\text{QR: } \begin{aligned} B &= Q_1R_1 \\ C &= Q_2R_2 \end{aligned} \Rightarrow (B \otimes C) = (Q_1 \otimes Q_2)(R_1 \otimes R_2)^T$$

$$\text{SVD: } \begin{aligned} B &= U_1\Sigma_1V_1^T \\ C &= U_2\Sigma_2V_2^T \end{aligned} \Rightarrow (B \otimes C) = (U_1 \otimes U_2)(\Sigma_1 \otimes \Sigma_2)(V_1 \otimes V_2)^T$$

$$\text{Schur: } \begin{aligned} B &= U_1D_1U_1^H \\ C &= U_2D_2U_2^H \end{aligned} \Rightarrow (B \otimes C) = (U_1 \otimes U_2)(D_1 \otimes D_2)(U_1 \otimes U_2)^H$$

Here we are exploiting the fact that

$$\text{Kronecker products of } \left\{ \begin{array}{l} \text{orthogonal} \\ \text{triangular} \\ \text{diagonal} \end{array} \right\} \text{ matrices are } \left\{ \begin{array}{l} \text{orthogonal} \\ \text{triangular} \\ \text{diagonal} \end{array} \right\}.$$

For a practical illustration of Kronecker product factorizations, see [10] where the idea is applied with QR in a photogrammetry application.

Some factorizations are not "preserved" when Kronecker products are taken:

- A real Schur decomposition of  $B \otimes C$  is not obtained by taking the Kronecker product of the real Schur decompositions of  $B$  and  $C$  because the 2-by-2 bumps in the factors can create "block bumps" in the product. The computational ramifications of this fact are discussed in [3, 13].

- If  $QR$  with column pivoting is used to produce the factorizations  $B\Pi_1 = Q_1R_1$  and  $C\Pi_2 = Q_2R_2$ , then  $(B \otimes C)(\Pi_1 \otimes \Pi_2) = (Q_1 \otimes Q_2)(R_1 \otimes R_2)$  is *not* the factorization rendered by the same algorithm applied to  $B \otimes C$ .

Despite these anomalies, it is clear that the solution of Kronecker product systems is a nice problem with much structure to exploit. Not only are  $O(n^{3/2})$  solution procedures available, but the form of (1) suggests opportunities for using the level-3 BLAS and parallel processing.

The act of finding good preconditioners through an appropriately constrained minimization of  $\|A - M\|_F$  is not new. For example, [5] derives a useful class of preconditioners for the case when  $A$  is Toeplitz by solving

$$\min_{M \text{ circulant}} \|A - M\|_F$$

Generalizations of this for matrices with Toeplitz blocks are discussed in [6].

Our presentation is organized as follows. First, we characterize the optimum Kronecker factors  $B$  and  $C$  in terms of the singular value decomposition of a permuted version of  $A$ . Algorithms for determining  $B$  and  $C$  are discussed in §3 and §4. The important cases when  $A$  is banded, non-negative, symmetric, and definite are handled in §5 along with some additional specially structured examples. In §6 we briefly examine the use of Kronecker product preconditioners.

We conclude this section with a few pointers to related work. The Kronecker product has a long history in mathematics and an excellent review is offered in [18]. Computational aspects of the operation are detailed in [25, 9].

Kronecker products arise in a number of applied areas. See [1, 28, 4, 17, 26] for Kronecker product discussions of generalized spectra, higher order statistics, systems theory, image processing, and photogrammetry.

In recent years there have been a number of developments that point to an increased role of the Kronecker product in the area of high performance matrix computations. In [22] is developed a parallel programming methodology that revolves around the Kronecker product. See also [23]. In [27, 29] is shown how the organization of fast transforms is clarified through the "language" of Kronecker products.

## 2 The rank-1 approximation

Consider the uniform blocking of an  $m_1 m_2$ -by- $n_1 n_2$  matrix  $A$ .

$$A = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1,n_1} \\ A_{21} & A_{22} & \cdots & A_{2,n_1} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m_1,1} & A_{m_1,2} & \cdots & A_{m_1,n_1} \end{bmatrix}, \quad A_{ij} \in \mathbb{R}^{m_2 \times n_2}. \quad (2)$$

Using Matlab colon notation, the  $(i, j)$  block is given by

$$A_{ij} = A((i-1)m_2 + 1:im_2, (j-1)n_2 + 1:jn_2),$$

the submatrix defined by rows  $(i-1)m_2 + 1$  to  $im_2$  and columns  $(j-1)n_2 + 1$  to  $jn_2$ . It is not hard to show using the definition of the Kronecker product that

$$\phi_A(B, C) = \sum_{i=1}^{m_1} \sum_{j=1}^{n_1} \|A_{ij} - b_{ij}C\|_F^2. \quad (3)$$

By keeping the  $B$  matrix "intact," we also have

$$\phi_A(B, C) = \sum_{i=1}^{m_2} \sum_{j=1}^{n_2} \|\hat{A}_{ij} - c_{ij}B\|_F^2, \quad (4)$$

where

$$\hat{A}_{ij} = A(i:m_2:m, j:n_2:n)$$

is the  $m_1$ -by- $n_1$  submatrix defined by rows  $i, i + m_2, i + 2m_2, \dots, i + (m_1 - 1)m_2$  and columns  $j, j + n_2, j + 2n_2, \dots, j + (n_1 - 1)n_2$ . Thinking of matrices at the block level is the key to high performance matrix computations. See [15].

To proceed further with the analysis of  $\phi_A(B, C)$ , we require the *vec* operation, which is a way of turning matrices into vectors by "stacking" the columns:

$$X \in \mathbb{R}^{p \times q} \Rightarrow \text{vec}(X) = \begin{bmatrix} X(1:p, 1) \\ X(1:p, 2) \\ \vdots \\ X(1:p, q) \end{bmatrix} \in \mathbb{R}^{pq}.$$

It turns out that the *vec* operator can be used to express the minimization of  $\|A - B \otimes C\|_F^2$  as a rank-1 approximation problem. The idea is to rearrange  $A$  into another matrix  $\tilde{A}$  so that the sum of squares that arise in  $\|A - B \otimes C\|_F^2$  is exactly the same as the sum of squares that arise in  $\|\tilde{A} - \text{vec}(B)\text{vec}(C)^T\|_F^2$ . For example, in a 4-by-4 problem with 2-by-2 blocks,

$$\|A - B \otimes C\|_F = \left\| \begin{bmatrix} a_{11} & a_{21} & a_{12} & a_{22} \\ a_{31} & a_{41} & a_{32} & a_{42} \\ a_{13} & a_{23} & a_{14} & a_{24} \\ a_{33} & a_{43} & a_{34} & a_{44} \end{bmatrix} - \begin{bmatrix} b_{11} \\ b_{21} \\ b_{12} \\ b_{22} \end{bmatrix} [c_{11} \ c_{21} \ c_{12} \ c_{22}] \right\|_F.$$

Refer to the above permuted version of  $A$  as  $\tilde{A}$ . Note that  $\tilde{A}$  is *not* of the form  $PAQ$  where  $P$  and  $Q$  are permutation matrices. Indeed, in our example

- the four rows of  $\tilde{A}$  are  $\text{vec}$ 's of the 2-by-2 blocks of  $A$ :

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \Rightarrow \tilde{A} = \begin{bmatrix} \text{vec}(A_{11})^T \\ \text{vec}(A_{21})^T \\ \text{vec}(A_{12})^T \\ \text{vec}(A_{22})^T \end{bmatrix}.$$

- the  $\text{vec}$ 's of the 2-by-2 blocks of  $\tilde{A}^T$  are columns of  $A$ :

$$\tilde{A} = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix} \Rightarrow A = [\text{vec}(\tilde{A}_{11}^T) \mid \text{vec}(\tilde{A}_{12}^T) \mid \text{vec}(\tilde{A}_{21}^T) \mid \text{vec}(\tilde{A}_{22}^T)].$$

In general, if  $m = m_1 m_2$ ,  $n = n_1 n_2$ ,  $A \in \mathbb{R}^{m \times n}$ , and we have the blocking (2), then we define the *rearrangement* of  $A$  (relative to the blocking parameters  $m_1$ ,  $m_2$ ,  $n_1$ , and  $n_2$ ) by

$$\mathcal{R}(A) = \begin{bmatrix} A_1 \\ \vdots \\ A_{n_1} \end{bmatrix}, \quad A_j = \begin{bmatrix} \text{vec}(A_{1,j})^T \\ \vdots \\ \text{vec}(A_{m_1,j})^T \end{bmatrix}, \quad j = 1:n_1. \quad (5)$$

Note that  $\mathcal{R}(A)$  has  $m_1 n_1$  rows and  $m_2 n_2$  columns. Thus,  $\mathcal{R}(A)$  need not be the same size as  $A$ . For example, if  $m = m_1 m_2 = 2 \cdot 2$  and  $n = n_1 n_2 = 3 \cdot 2$ , then  $A$  is 4-by-6 but

$$\mathcal{R}(A) = \begin{bmatrix} a_{11} & a_{21} & a_{12} & a_{22} \\ a_{31} & a_{41} & a_{32} & a_{42} \\ a_{13} & a_{23} & a_{14} & a_{24} \\ a_{33} & a_{43} & a_{34} & a_{44} \\ a_{15} & a_{25} & a_{16} & a_{26} \\ a_{35} & a_{45} & a_{36} & a_{46} \end{bmatrix}.$$

We are now set to establish a key result that connects the problem of minimizing  $\phi_A(B, C)$  with the problem of approximating  $\tilde{A}$  with a rank-1 matrix.

**Theorem 1** Assume that  $A \in \mathbb{R}^{m \times n}$  with  $m = m_1 m_2$  and  $n = n_1 n_2$ . If  $B \in \mathbb{R}^{m_1 \times n_1}$  and  $C \in \mathbb{R}^{m_2 \times n_2}$ , then

$$\|A - B \otimes C\|_F = \|\mathcal{R}(A) - \text{vec}(B)\text{vec}(C)^T\|_F.$$

**Proof.** By applying the  $\text{vec}$  operator in (3) we get:

$$\begin{aligned} \|A - B \otimes C\|_F^2 &= \sum_{j=1}^{n_1} \sum_{i=1}^{m_1} \|\text{vec}(A_{ij}) - b_{ij}\text{vec}(C)\|_2^2 \\ &= \sum_{j=1}^{n_1} \sum_{i=1}^{m_1} \|\text{vec}(A_{ij})^T - b_{ij}\text{vec}(C)^T\|_2^2 \\ &= \sum_{j=1}^{n_1} \|A_j - B(:,j)\text{vec}(C)^T\|_F^2 \\ &= \|\mathcal{R}(A) - \text{vec}(B)\text{vec}(C)^T\|_F^2. \quad \square \end{aligned}$$

The approximation of a given matrix by a rank-1 matrix has a well-known solution in terms of the singular value decomposition.

**Corollary 2** Assume that  $A \in \mathbb{R}^{m \times n}$  with  $m = m_1 m_2$  and  $n = n_1 n_2$ . If  $\tilde{A} = \mathcal{R}(A)$  has singular value decomposition

$$U^T \tilde{A} V = \Sigma = \text{diag}(\sigma_i)$$

where  $\sigma_1$  is the largest singular value, and  $U(:, 1)$  and  $V(:, 1)$  are the corresponding singular vectors, then the matrices  $B \in \mathbb{R}^{m_1 \times n_1}$  and  $C \in \mathbb{R}^{m_2 \times n_2}$  defined by  $\text{vec}(B) = \sigma_1 U(:, 1)$  and  $\text{vec}(C) = V(:, 1)$  minimize  $\|A - B \otimes C\|_F$ .

**Proof.** See [15, p. 73].  $\square$

The definition (5) of  $\mathcal{R}(A)$  is in terms of the blocks  $A_{ij}$  in (2). An alternative characterization can be obtained in terms of the columns of  $A$ . In particular, we show that

$$\mathcal{R}(A) = \begin{bmatrix} \tilde{A}_{11} & \cdots & \tilde{A}_{1,n_2} \\ \vdots & \ddots & \vdots \\ \tilde{A}_{n_1,1} & \cdots & \tilde{A}_{n_1,n_2} \end{bmatrix}. \quad (6)$$

where  $\tilde{A}_{ij} \in \mathbb{R}^{m_1 \times m_2}$  is defined by

$$\text{vec}(\tilde{A}_{ij}^T) = A(:, (i-1)n_2 + j) \quad 1 \leq i \leq n_1, 1 \leq j \leq n_2.$$

In view of (5) we need only confirm that

$$A_i = \begin{bmatrix} \text{vec}(A_{1,i})^T \\ \vdots \\ \text{vec}(A_{m_1,i})^T \end{bmatrix} = [\tilde{A}_{i,1} \mid \tilde{A}_{i,2} \mid \cdots \mid \tilde{A}_{i,n_2}]. \quad (7)$$

For  $s = 1:m_2$ ,  $p = 1:n_2$ , and  $q = 1:m_2$  we have

$$[A_i]_{s,(p-1)m_2+q} = [\text{vec}(A_{s,i})^T]_{(p-1)m_2+q} = A((s-1)m_2 + q, (i-1)n_2 + p).$$

But (7) immediately follows because we also have

$$[\tilde{A}_{i,1} \mid \tilde{A}_{i,2} \mid \cdots \mid \tilde{A}_{i,n_2}]_{s,(p-1)m_2+q} = [\tilde{A}_{i,p}]_{sq} = A((s-1)m_2 + q, (i-1)n_2 + p).$$

### 3 SVD framework

The Golub-Reinsch SVD algorithm can be used for computing the largest singular value and corresponding singular vectors of  $\mathcal{R}(A)$ . However, in view of the potentially large dimension of  $\tilde{A} = \mathcal{R}(A)$  in some applications, it may be more appropriate to use the SVD Lanczos process described in [12]. Here is how to proceed with the computation of  $B \in \mathbb{R}^{m_1 \times n_1}$  and  $C \in \mathbb{R}^{m_2 \times n_2}$ :

#### Framework 1.

```

C = initial guess.
v1 ← vec(C)/||C||F
p0 ← v1; β0 ← 1; j ← 0; u0 ← 0
while βj ≠ 0 (or some other less stringent criteria.)
  vj+1 ← pj/βj
  j ← j + 1
  rj ←  $\tilde{A}v_j - \beta_{j-1}u_{j-1}$ 
  αj ← ||rj||2
  uj ← rj/αj
  pj ←  $\tilde{A}^T u_j - \alpha_j v_j$ ;
  βj ← ||pj||2
end {while}

```

Compute the largest singular value  $\sigma_1$  and associated left and right singular vectors  $u_B$  and  $v_B$  of the bidiagonal matrix with diagonal  $\alpha_1, \dots, \alpha_j$  and upper diagonal  $\beta_1, \dots, \beta_{j-1}$ .

Define  $B$  by  $\text{vec}(B) = \sigma_1[u_1, \dots, u_j]u_B$  and  $C$  by  $\text{vec}(C) = [v_1, \dots, v_j]v_B$

There are many subtleties associated with the Lanczos process and we refer the reader to [8] or [15, p. 98ff] for details.

Our only implementation discussion concerns the matrix-vector products  $\tilde{A}x$  and  $\tilde{A}^T x$  that are required by the iteration. The explicit formation of  $\mathcal{R}(A) = \tilde{A}$  is *not* necessary. For example, working with the characterization (5), here is a dot product formulation for  $y \leftarrow \tilde{A}x$ :

```

for j = 1:n1
  for i = 1:m1
    y((j-1)m1 + i) ← vec(Aij)Tx
  end
end
end

```

A saxpy-based procedure for  $y \leftarrow \tilde{A}^T x$  proceeds as follows:

```

y(1:m2n2) ← 0
for j = 1:n1
  for i = 1:m1
    y ← y + x((j-1)m1 + i)vec(Aij)
  end
end
end

```

By working with (6) we have the following alternative block formulation for  $y \leftarrow \tilde{A}x$ :

```

y(1:m1n1) ← 0
for i = 1:n1
  rows = (i-1)m1 + 1:i m1
  for j = 1:n2
    Define Z ∈ ℝm1 × m2 by vec(ZT) = A(:, (i-1)n2 + j)
    y(rows) ← y(rows) + Zx((j-1)m2 + 1:j m2)
  end
end

```

end  
end

Likewise, we can formulate a procedure for  $y \leftarrow \tilde{A}^T x$  that is based upon (6):

```

y(1:m2n2) ← 0
for i = 1:n2
  rows = (i - 1)m2 + 1:i m2
  for j = 1:n1
    Define Z ∈ ℝm2 × m1 by vec(ZT) = A(:, (j - 1)n2 + i)
    y(rows) ← y(rows) + ZT x((j - 1)m1 + 1:j m1)
  end
end
end

```

Each of these products requires  $2m_1 n_1 m_2 n_2 = 2mn$  flops assuming that  $\tilde{A}$  is treated as a dense matrix.

#### 4 The separable least squares framework

Note that if we fix  $C$ , then the problem of minimizing  $\phi_A(B, C) = \|A - B \otimes C\|_F$  is a linear least squares problem with unknowns  $b_{ij}$ . Likewise, if  $B$  is fixed, then the minimization of  $\phi_A$  is a linear least squares problem in the  $c_{ij}$ . The following theorem specifies the solution to these linear least squares problems and requires the concept of matrix trace:

$$X \in \mathbb{R}^{q \times q} \Rightarrow \text{tr}(X) = \sum_{i=1}^q x_{ii}.$$

**Theorem 3** Suppose  $m = m_1 m_2$ ,  $n = n_1 n_2$ , and  $A \in \mathbb{R}^{m \times n}$ . If  $C \in \mathbb{R}^{m_2 \times n_2}$  is fixed, then the matrix  $B \in \mathbb{R}^{m_1 \times n_1}$  defined by

$$b_{ij} = \frac{\text{tr}(A_{ij}^T C)}{\text{tr}(C^T C)} \quad 1 \leq i \leq m_1, 1 \leq j \leq n_1 \quad (8)$$

minimizes  $\|A - B \otimes C\|_F$  where  $A_{ij} = A((i-1)m_2 + 1:i m_2, (j-1)n_2 + 1:j n_2)$ . Likewise, if  $B \in \mathbb{R}^{m_1 \times n_1}$  is fixed, then the matrix  $C \in \mathbb{R}^{m_2 \times n_2}$  defined by

$$c_{ij} = \frac{\text{tr}(\hat{A}_{ij}^T B)}{\text{tr}(B^T B)} \quad 1 \leq i \leq m_2, 1 \leq j \leq n_2 \quad (9)$$

minimizes  $\|A - B \otimes C\|_F$  where  $\hat{A}_{ij} = A(i:m_2:m, j:n_2:n)$ .

**Proof.** Since

$$\begin{aligned} \|A_{ij} - b_{ij} C\|_F^2 &= \text{tr}((A_{ij} - b_{ij} C)^T (A_{ij} - b_{ij} C)) \\ &= \|A_{ij}\|_F^2 - 2b_{ij} \text{tr}(C^T A_{ij}) + b_{ij}^2 \|C\|_F^2 \end{aligned}$$

it follows from (2.2) that

$$\frac{\partial \phi_A(B, C)}{\partial b_{ij}} = -2 \text{tr}(C^T A_{ij}) + 2b_{ij} \|C\|_F^2.$$

Setting these partials to zero defines the required matrix  $B$ . The proof of (9) is similar.  $\square$



The above result suggests that we can compute  $B$  and  $C$  by taking the *separable least squares* described in [2]. The idea is to minimize  $\phi_A(B, C)$  by alternately improving the  $B$  and  $C$  matrices through a sequence of linear least squares optimizations:

### Framework 2.

$C = C_0$  (given starting matrix)

**Repeat:**

$$\gamma \leftarrow \text{tr}(C^T C)$$

for  $i = 1:m_1$

for  $j = 1:n_1$

$$b_{ij} \leftarrow \text{tr}(C^T A_{ij})/\gamma$$

$$\beta \leftarrow \text{tr}(B^T B)$$

for  $i = 1:m_2$

for  $j = 1:n_2$

$$c_{ij} \leftarrow \text{tr}(B^T \hat{A}_{ij})/\beta$$

This process requires  $4m_1n_1m_2n_2 = 4mn$  flops per iteration, the same as Framework 1. Other methods for nonlinear least squares problems with variables that separate are discussed in [14, 24].

Framework 2 amounts to a power method for the largest singular value of  $\tilde{A} = \mathcal{R}(A)$ . To see this we switch to "tilde-space" and observe that if

$$\phi(b, c) = \|\tilde{A} - bc^T\|_F^2 \quad b \in \mathbb{R}^{m_1n_1}, c \in \mathbb{R}^{m_2n_2},$$

then the gradient is given by

$$\nabla\phi(b, c) = -2 \begin{bmatrix} \tilde{A}c - (c^T c)b \\ \tilde{A}^T b - (b^T b)c \end{bmatrix}.$$

If  $b$  is fixed, then the minimizing  $c$  is obtained by setting  $c = \tilde{A}^T b / b^T b$  for then the  $c$ -partials are all zero. Likewise, if  $c$  is fixed, then the minimizing  $b$  is given by  $b = \tilde{A}c / c^T c$ . After  $k$  passes through the iteration

$c = c_0$  (given starting vector)

**Repeat:**

$$b \leftarrow \tilde{A}c / c^T c$$

$$c \leftarrow \tilde{A}^T b / b^T b$$

the vector  $c$  is in the direction of  $(\tilde{A}^T \tilde{A})^k c_0$  and the vector  $b$  is in the direction of  $(\tilde{A} \tilde{A}^T)^{k-1} \tilde{A} c_0$ .

The practical implementation of this framework involves all the subtleties that are associated with the power method. See [30] for a discussion.

## 5 Structured problems

As we alluded to in §1, the Kronecker product of two structured matrices is usually structured in the same way:

If  $B$  and  $C$  are  $\left\{ \begin{array}{l} \text{banded} \\ \text{non-negative} \\ \text{symmetric} \\ \text{positive definite} \\ \text{stochastic} \\ \text{orthogonal} \end{array} \right\}$ , then  $B \otimes C$  is  $\left\{ \begin{array}{l} \text{banded} \\ \text{non-negative} \\ \text{symmetric} \\ \text{positive definite} \\ \text{stochastic} \\ \text{orthogonal} \end{array} \right\}$ .

We are interested in the structure of the solution to the Kronecker approximation problem given that  $A$  is structured. In the following subsections we use Corollary 2 and Theorem 3 to establish a number results about structured problems.

### 5.1 BANDEDNESS

We first show how bandedness in  $A$  "shows up" in  $B$  and  $C$ .

**Theorem 4** Suppose  $n = n_1 n_2$ ,  $A \in \mathbb{R}^{n \times n}$  has bandwidth  $pn_2$ , and that each block in

$$A = \begin{bmatrix} A_{11} & \cdots & A_{1,n_1} \\ \vdots & \ddots & \vdots \\ A_{n_1,1} & \cdots & A_{n_1,n_1} \end{bmatrix} \quad A_{ij} \in \mathbb{R}^{n_2 \times n_2}$$

has bandwidth  $q$  or less. If  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$  minimize  $\|A - B \otimes C\|_F$ , then  $B$  has bandwidth  $p$  and  $C$  has bandwidth  $q$ .

**Proof.** Since  $A$  has bandwidth  $pn_2$ , it follows that  $A_{ij} = 0$  if  $|i - j| > p$ . From (3) we have  $b_{ij} = 0$  whenever  $|i - j| > p$ . Since each  $A_{ij}$  has bandwidth  $q$ , it follows that the minimization of  $\|A_{ij} - b_{ij}C\|_F$  requires setting  $c_{rs}$  to zero whenever  $|r - s| > q$ . Thus, a minimizing  $C$  must have bandwidth  $q$ .  $\square$

### 5.2 NON-NEGATIVITY

We first show that if  $A$  and  $C$  are non-negative, then the  $B$  that minimizes  $\phi_A(B, C)$  is also non-negative.

**Theorem 5** If  $m = m_1 m_2$ ,  $n = n_1 n_2$ ,  $A \in \mathbb{R}^{m \times n}$ , and  $C \in \mathbb{R}^{m_2 \times n_2}$  are non-negative, then there exists a non-negative  $B \in \mathbb{R}^{m_1 \times n_1}$  that minimizes  $\|A - B \otimes C\|_F$ .

**Proof.** Using the non-negativity of  $C$  and Theorem 3,

$$b_{ij} = \frac{\text{tr}(A_{ij}^T C)}{\text{tr}(C^T C)} \geq 0$$

for  $i = 1:m_1$  and  $j = 1:n_1$ .  $\square$

In the same way, we can show that if  $A$  and  $B$  are non-negative, then the  $C$  that minimizes  $\|A - B \otimes C\|_F$  is also non-negative. Thus, if we start with a non-negative  $C$  in Framework 2, then all subsequent  $B$  and  $C$  matrices are non-negative. The following theorem shows that this restriction poses no difficulty because the optimum  $B$  and  $C$  are also non-negative.

**Theorem 6** If  $m = m_1 m_2$ ,  $n = n_1 n_2$ , and  $A \in \mathbb{R}^{m \times n}$  is non-negative, then there exist non-negative matrices  $B \in \mathbb{R}^{m_1 \times n_1}$  and  $C \in \mathbb{R}^{m_2 \times n_2}$  such that  $\|A - B \otimes C\|_F$  is minimized.

**Proof.** Note that  $\tilde{A} = \mathcal{R}(A)$  has non-negative entries and let  $\sigma_1$  be its largest singular value. Peron-Frobenius theory tells us that there exist non-negative  $u \in \mathbb{R}^{m_1 n_1}$  and  $v \in \mathbb{R}^{m_2 n_2}$  so that  $\tilde{A}^T \tilde{A} v = \sigma_1^2 v$  and  $\tilde{A} \tilde{A}^T u = \sigma_1^2 u$ . (See [20, p.503].) But  $u$  and  $v$  are the right and left singular vectors of  $\tilde{A}$  and so the matrices  $B$  and  $C$  as specified in Corollary 2 are non-negative.  $\square$

### 5.3 SYMMETRY

Turning next to the issue of symmetry, we show that if  $A$  and  $C$  are symmetric, then a symmetric  $B$  can be found to minimize  $\phi_A(B, C)$ .

**Theorem 7** If  $n = n_1 n_2$ ,  $A \in \mathbb{R}^{n \times n}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$  are symmetric, then there exists a symmetric  $B \in \mathbb{R}^{n_1 \times n_1}$  that minimizes  $\|A - B \otimes C\|_F$ .

**Proof.** Since  $A$  is symmetric,  $A_{ji} = A_{ij}^T$ . Using elementary properties of the trace we have

$$b_{ij} = \frac{\text{tr}(A_{ij}^T C)}{\text{tr}(C^T C)} = \frac{\text{tr}(A_{ji} C)}{\text{tr}(C^T C)} = \frac{\text{tr}(C A_{ji})}{\text{tr}(C^T C)} = \frac{\text{tr}(A_{ji}^T C)}{\text{tr}(C^T C)} = b_{ji}$$

for all  $1 \leq i, j \leq n_1$ . It follows that  $B$  is symmetric.  $\square$

It is equally straightforward to establish that a symmetric  $C$  can be found to minimize  $\|A - B \otimes C\|_F$  if  $A$  and  $B$  are symmetric.

Analogous results are applicable if the "frozen factor" is skew-symmetric:

**Theorem 8** If  $n = n_1 n_2$ ,  $A \in \mathbb{R}^{n \times n}$  is symmetric and  $C \in \mathbb{R}^{n_2 \times n_2}$  is skew-symmetric, then there exists a skew-symmetric  $B \in \mathbb{R}^{n_1 \times n_1}$  that minimizes  $\|A - B \otimes C\|_F$ .

**Proof.**

$$b_{ij} = \frac{\text{tr}(A_{ij}^T C)}{\text{tr}(C^T C)} = -\frac{\text{tr}(A_{ji}^T C)}{\text{tr}(C^T C)} = -b_{ji}. \quad \square$$

The optimum Kronecker approximation of a symmetric matrix may have skew-symmetric factors as consideration of the following example shows:

$$A = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

For this particular  $A$ , it is not possible to find symmetric  $B$  and  $C$  for which we have  $A = B \otimes C$ . The following theorem summarizes the situation.

**Theorem 9** Suppose  $n = n_1 n_2$  and  $A \in \mathbb{R}^{n \times n}$  is symmetric. If  $\|A - B \otimes C\|_F$  cannot be minimized by symmetric matrices  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$ , then it can be minimized by skew-symmetric matrices  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$ .

**Proof.** For any positive integer  $q$ , define the following orthogonal subspaces of  $\mathbb{R}^{q^2}$ :

$$S_+^{(q)} = \{x \in \mathbb{R}^{q^2} : x = \text{vec}(X) \text{ for some symmetric } X \in \mathbb{R}^{q \times q}\}$$

$$S_-^{(q)} = \{x \in \mathbb{R}^{q^2} : x = \text{vec}(X) \text{ for some skew-symmetric } X \in \mathbb{R}^{q \times q}\}$$

Note that  $\mathbb{R}^{q^2} = S_+^{(q)} \oplus S_-^{(q)}$ .

Now suppose that  $y = \mathcal{R}(A)x$  and that  $X \in \mathbb{R}^{n_2 \times n_2}$  and  $Y \in \mathbb{R}^{n_1 \times n_1}$  are defined by  $x = \text{vec}(X)$  and  $y = \text{vec}(Y)$ , respectively. From (2)) we know that

$$[Y]_{ij} = \text{vec}(A_{ij})^T x = \text{tr}(A_{ij}^T X) \quad 1 \leq i, j \leq n_1.$$

If  $x \in S_+^{(n_2)}$ , then since  $A$  is symmetric we have

$$[Y]_{ij} - [Y]_{ji} = \text{tr}((A_{ij}^T - A_{ji}^T)X) = \text{tr}((A_{ij}^T - A_{ij})X) = \text{vec}(A_{ij}^T - A_{ij})^T x = 0$$

since  $\text{vec}(A_{ij}^T - A_{ij}) \in S_-^{(n_2)}$ . Thus,

$$x \in S_+^{(n_2)} \Rightarrow \mathcal{R}(A)x \in S_+^{(n_1)}$$

Likewise,

$$x \in S_-^{(n_2)} \Rightarrow \mathcal{R}(A)x \in S_-^{(n_1)}$$

and so  $(S_+^{(n_2)}, S_+^{(n_1)})$  and  $(S_-^{(n_2)}, S_-^{(n_1)})$  are singular subspace pairs for  $\mathcal{R}(A)$ . It follows that the largest singular value and corresponding singular vectors must be associated with one of these pairs.  $\square$

Theorem 9 can also be established by observing that if  $A$  is symmetric, then

$$P_{n_1} \mathcal{R}(A) P_{n_2}^T = \mathcal{R}(A)$$

where  $P_q$  designates the *vec permutation matrix* on  $\mathbb{R}^{q^2}$ :

$$P_q \text{vec}(X) = \text{vec}(X^T) \quad X \in \mathbb{R}^{q \times q}.$$

This permutation connects the *vec* of a matrix and the *vec* of its transpose. See [19] for further details.

#### 5.4 POSITIVE DEFINITENESS

We first show that if the initial guess matrix in Framework 2 is positive definite, then all subsequent  $B$  and  $C$  iterates are positive definite.

**Theorem 10** *If  $n = n_1^2$ ,  $A \in \mathbb{R}^{n \times n}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$  are symmetric positive definite, then there exists a symmetric positive definite  $B \in \mathbb{R}^{n_1 \times n_1}$  that minimizes  $\phi_A(B, C)$ . Likewise, if  $B \in \mathbb{R}^{n_1 \times n_1}$  is symmetric positive definite, then there exists a symmetric positive definite  $C \in \mathbb{R}^{n_2 \times n_2}$  that minimizes  $\phi_A(B, C)$ .*

**Proof.** If each entry  $b_{ij}$  in  $B \in \mathbb{R}^{n_1 \times n_1}$  satisfies  $b_{ij} = \text{tr}(C^T A_{ij}) / \text{tr}(C^T C)$ , and if  $y \in \mathbb{R}^{n_1}$ , then using the linearity of the trace we have

$$y^T B y = \sum_{i=1}^{n_1} \sum_{j=1}^{n_1} b_{ij} y_i y_j = \sum_{i=1}^{n_1} \sum_{j=1}^{n_1} y_i y_j \text{tr}(C^T A_{ij}) / \text{tr}(C^T C) = \text{tr}(C^T \hat{A}) \quad (10)$$

where

$$\hat{A} = \sum_{i=1}^{n_1} \sum_{j=1}^{n_1} y_i y_j A_{ij}.$$

The matrix  $\hat{A}$  is positive definite because for any  $z \in \mathbb{R}^{n_1}$  we have

$$0 < (z \otimes y)^T A (z \otimes y) = \begin{bmatrix} z_1 y^T & \cdots & z_{n_1} y^T \end{bmatrix} [A_{ij}] \begin{bmatrix} z_1 y \\ \vdots \\ z_{n_1} y \end{bmatrix} = z^T \hat{A} z.$$

Since  $C$  is positive definite, it has a Cholesky factorization  $C = LL^T$ . From (10) and the fact that the trace is invariant under similarity transformations, gives

$$y^T B y = \text{tr}(C^T \hat{A}) = \text{tr}(LL^T \hat{A}) = \text{tr}(L^{-1}(LL^T \hat{A})L) = \text{tr}(L^T \hat{A} L) > 0.$$

The proof that  $C$  is positive definite when  $B$  is given is similar.  $\square$

The next result shows that if  $A$  is symmetric and positive definite, then the same can be said about the optimum  $B$  and  $C$ .

**Theorem 11** *If  $n = n_1 n_2$  and  $A \in \mathbb{R}^{n \times n}$  is symmetric positive definite, then there exists symmetric positive definite  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$  that minimize  $\phi_A(B, C)$ .*

**Proof.** From Theorem 9 we may select the optimum  $B$  and  $C$  to be either both skew-symmetric or both symmetric. We first show that the latter must be the case.

If  $B$  is skew-symmetric, then there exists a real orthogonal  $U_B$  such that

$$U_B^T B U_B = B_1 \quad (11)$$

where  $B_1$  is a direct sum of 1-by-1 and 2-by-2 skew-symmetric blocks. The 1-by-1's are (of course) zero and the 2-by-2's have the form

$$M = \begin{bmatrix} 0 & m \\ -m & 0 \end{bmatrix}$$

and correspond to the complex conjugate eigenpairs of  $B$ . The decomposition (11) is just the real Schur decomposition. Note that the unitary matrix

$$Z = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}$$

diagonalizes  $M$ :

$$Z^H M Z = \begin{bmatrix} im & 0 \\ 0 & -im \end{bmatrix}.$$

Let  $V_B$  be the unitary matrix that has copies of  $Z$  on the diagonal which correspond to the 2-by-2 blocks in  $B_1$ , and which is the identity elsewhere. It follows that

$$V_B^H U_B^T B U_B V_B = D_B$$

is diagonal. Let us refer to this decomposition as the *structured Schur decomposition* of  $B$ . Assume that  $C$  is also skew-symmetric and let

$$V_C^H U_C^T C U_C V_C = D_C$$

be its structured Schur decomposition. For a matrix  $H$ , let  $|H|$  be the matrix obtained by taking the absolute values of each entry. Since

$$Z \left| \begin{bmatrix} im & 0 \\ 0 & -im \end{bmatrix} \right| Z^H = |m| I_2$$

it is easy to check that the matrices

$$B_+ = U_B V_B |D_B| V_B^H U_B^T$$

$$C_+ = U_C V_C |D_C| V_C^H U_C^T$$

are real and symmetric.

Let  $Q = Q_B \otimes Q_C$  where  $Q_B = U_B V_B$  and  $Q_C = U_C V_C$ . Define the *off* operation on matrices as follows:

$$\text{off}(M) = \sum_{i \neq j} m_{ij}^2.$$

Setting  $D_A$  to be the diagonal part of  $Q^H A Q$ , we see that

$$\begin{aligned} \|A - B_+ \otimes C_+\|_F^2 &= \|Q^H A Q - |D_B| \otimes |D_C|\|_F^2 \\ &= \text{off}(Q^H A Q) + \|D_A - |D_B| \otimes |D_C|\|_F^2 \end{aligned}$$

while

$$\begin{aligned} \|A - B \otimes C\|_F^2 &= \|Q^H A Q - D_B \otimes D_C\|_F^2 \\ &= \text{off}(Q^H A Q) + \|D_A - D_B \otimes D_C\|_F^2. \end{aligned}$$

Since  $Q^H A Q$  is positive definite,  $D_A$  has positive diagonal entries. Moreover,  $D_B \otimes D_C$  is a real diagonal matrix with some negative diagonal entries. It follows that

$$\|D_A - |D_B| \otimes |D_C|\|_F^2 < \|D_A - D_B \otimes D_C\|_F^2.$$

and so

$$\|A - B_+ \otimes C_+\|_F < \|A - B \otimes C\|_F.$$

This shows that a skew-symmetric pair cannot minimize  $\phi_A(B, C)$ .

Knowing now that the optimizing  $B$  and  $C$  are symmetric, it remains for us to show that they are both positive definite. Suppose

$$Q_1^T B Q_1 = D_1 = \text{diag}(\lambda_1, \dots, \lambda_{n_1})$$

$$Q_2^T C Q_2 = D_2 = \text{diag}(\mu_1, \dots, \mu_{n_2})$$

are Schur decompositions. Set  $Q = Q_1 \otimes Q_2$  and let  $D = \text{diag}(d_1, \dots, d_n)$  be the diagonal part of  $F = Q^T A Q$ . Thus,

$$\begin{aligned} \|A - B \otimes C\|_F^2 &= \|Q^T(A - B \otimes C)Q\|_F^2 \\ &= \|F - D_1 \otimes D_2\|_F^2 = \|D - D_1 \otimes D_2\|_F^2 + \text{off}(F). \end{aligned}$$

Note that

$$\|D - D_1 \otimes D_2\|_F^2 = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} (d_{(i-1)n_2+j} - \lambda_i \mu_j)^2.$$

Since  $D$  has positive diagonal entries and

$$(d_{(i-1)n_2+j} - \lambda_i \mu_j)^2 - (d_{(i-1)n_2+j} - |\lambda_i \mu_j|)^2 = |\lambda_i|^2 |\mu_j|^2 - \lambda_i^2 \mu_j^2 > 0,$$

it follows that the  $\lambda_i$  and  $\mu_j$  should all have the same sign. Otherwise,  $B$  and  $C$  will not render the minimum sum of squares. Since  $\phi_A(-B, -C) = \phi_A(B, C)$ , we may assume without loss of generality that this sign is positive. This implies that symmetric positive definite  $B$  and  $C$  may be chosen to be minimize  $\phi_A(B, C)$ .  $\square$

## 5.5 SUMS OF KRONECKER PRODUCTS

Next, we consider the situation when the matrix  $A$  to be approximated is a sum of Kronecker products:

$$A = \sum_{i=1}^p (G_i \otimes F_i).$$

Assume that each  $G_i$  is  $m_1$ -by- $n_1$  and each  $F_i$  is  $m_2$ -by- $n_2$ . It follows that if  $f_i = \text{vec}(F_i)$  and  $g_i = \text{vec}(G_i)$ , then

$$\bar{A} = \mathcal{R}(A) = \sum_{i=1}^p \mathcal{R}(G_i \otimes F_i) = \sum_{i=1}^p g_i f_i^T$$

is a rank- $p$  matrix. This has two important ramifications. First, it means that matrix-vector products of the form  $\bar{A}x$  and  $\bar{A}^T x$  cost  $O((m+n)p)$  flops where  $m = m_1 m_2$  and  $n = n_1 n_2$ . Second, it means that the optimum  $B$  and  $C$  are linear combinations of the  $G_i$  and  $F_i$ :

$$B = \alpha_1 G_1 + \dots + \alpha_p G_p$$

$$C = \beta_1 F_1 + \dots + \beta_p F_p$$

The problem of approximating matrices of the form  $(I \otimes F) + (G \otimes I)$  is discussed further in §6.

## 5.6 APPROXIMATION WITH LINEAR HOMOGENEOUS CONSTRAINTS

Consider the problem of approximating  $A$  with a Kronecker product  $B \otimes C$  that has a prescribed structure. If the constraints on  $B$  and  $C$  are linear and homogeneous, then we are looking at a problem with the following form:

$$\begin{aligned} \min \quad & \|A - B \otimes C\|_F. \\ S_1^T \text{vec}(B) &= 0 \\ S_2^T \text{vec}(C) &= 0 \end{aligned} \quad (12)$$

Here,  $A \in \mathbb{R}^{m \times n}$ ,  $m = m_1 m_2$ ,  $n = n_1 n_2$ ,  $B \in \mathbb{R}^{m_1 \times n_1}$ ,  $C \in \mathbb{R}^{m_2 \times n_2}$ ,  $S_1 \in \mathbb{R}^{m_1 n_1 \times p_1}$ ,  $S_2 \in \mathbb{R}^{m_2 n_2 \times p_2}$ , and we assume that  $S_1$  and  $S_2$  have full column rank. By choosing these constraint matrices properly, we can force  $B$  and  $C$  to take on any prescribed sparsity pattern. Circulant, Toeplitz, Hankel, and Hamiltonian structures can also be imposed.

To solve the constrained problem we follow the techniques espoused in [11] where various modified eigenvalue problems are discussed. Let  $b = \text{vec}(B)$ ,  $c = \text{vec}(C)$ , and assume that we have the QR factorizations

$$S_1 = Q_1 \begin{bmatrix} R_1 \\ 0 \end{bmatrix} \quad S_2 = Q_2 \begin{bmatrix} R_2 \\ 0 \end{bmatrix} \quad (13)$$

where  $R_1$  and  $R_2$  are square. If

$$Q_1^T \mathcal{R}(A) Q_2 = \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix}, \quad Q_1^T b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}, \quad Q_2^T c = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}$$

are partitioned conformably with (13), then (12) transforms to the problem of minimizing

$$\left\| \begin{bmatrix} \tilde{A}_{11} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{22} \end{bmatrix} - \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix}^T \right\|_F$$

subject to the constraints

$$\begin{bmatrix} R_1^T & | & 0 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = 0, \quad \begin{bmatrix} R_2^T & | & 0 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = 0.$$

It follows that  $b_1$  and  $c_1$  are both zero and that the optimum  $b_2$  and  $c_2$  can be obtained by solving the unconstrained problem

$$\min \| \tilde{A}_{22} - b_2 c_2^T \|_F.$$

Collecting results, we see that  $B$  and  $C$  are prescribed by

$$\text{vec}(B) = Q_1 \begin{bmatrix} 0 \\ b_2 \end{bmatrix}, \quad \text{vec}(C) = Q_2 \begin{bmatrix} 0 \\ c_2 \end{bmatrix}.$$

## 5.7 STOCHASTIC AND ORTHOGONAL PROBLEMS

The non-negative matrix  $A \in \mathbb{R}^{n \times n}$  is *stochastic* if  $e_n^T A = e_n^T$  where  $e_n$  is the  $n$ -vector of ones. If  $n = n_1 n_2$  and  $B \in \mathbb{R}^{n_1 \times n_1}$  and  $C \in \mathbb{R}^{n_2 \times n_2}$  minimize  $\phi_A(B, C)$ , then it does *not*



follow that  $B$  and  $C$  are stochastic. For example, if

$$A = \begin{bmatrix} .1 & .5 & .2 & .6 \\ .4 & .1 & .1 & .2 \\ .2 & .0 & .3 & .1 \\ .3 & .4 & .4 & .1 \end{bmatrix},$$

then, after normalizing  $B$  and  $C$  so that  $b_{11} + b_{21} = 1$  we have

$$B = \begin{bmatrix} .6228 & .5939 \\ .3772 & .4298 \end{bmatrix} \quad C = \begin{bmatrix} .3610 & .6657 \\ .5560 & .3512 \end{bmatrix}.$$

Note that  $B$  and  $C$  are not quite stochastic. Thus, to get the best stochastic Kronecker product approximation we must apply a constrained nonlinear least squares solver to the problem

$$\begin{aligned} \min & \quad \|A - B \otimes C\|_F \\ e_{n_1}^T B &= e_{n_1}^T, B \geq 0 \\ e_{n_2}^T C &= e_{n_2}^T, C \geq 0 \end{aligned}$$

Another structured problem that is not solvable by our SVD framework is the case when  $A$  is orthogonal and we insist that the optimizing  $B$  and  $C$  be orthogonal. It does *not* follow that orthogonal  $B$  and  $C$  minimize  $\phi_A(B, C)$ . Thus, we are led to another constrained nonlinear least squares problem:

$$\begin{aligned} \min & \quad \|A - B \otimes C\|_F \\ B^T B &= I_{n_1} \\ C^T C &= I_{n_2} \end{aligned}$$

A reasonable initial guess  $(B_0, C_0)$  in this setting is to set  $B_0$  and  $C_0$  to be the closest orthogonal matrices to the  $B$  and  $C$  that minimize  $\phi_A(B, C)$ .

## 6 Kronecker product preconditioners

To acquire some intuition about the use of Kronecker products as pre-conditioners, consider the  $Ax = b$  problem where

$$A = a_1(I_{n_1} \otimes I_{n_2}) + a_2(I_{n_1} \otimes J_{n_2}) + a_3(J_{n_1} \otimes I_{n_2}) + a_4(J_{n_1} \otimes J_{n_2}), \quad (14)$$

$n = n_1 n_2$ , and  $J_m$  is the  $m$ -by- $m$  symmetric tridiagonal matrix

$$J_m = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$

Matrices with this structure arise in many applications. For example, the usual discretization of Poisson's equation on a rectangle with the Dirichlet stencil

$$\begin{array}{|c|c|c|} \hline a_3 & a_2 & a_3 \\ \hline a_2 & a_1 & a_2 \\ \hline a_3 & a_2 & a_3 \\ \hline \end{array} = \begin{array}{|c|c|c|} \hline 0 & -1 & 0 \\ \hline -1 & 4 & -1 \\ \hline 0 & -1 & 0 \\ \hline \end{array}$$

leads to

$$A = (2I_{n_1} - J_{n_1}) \otimes I_{n_2} + I_{n_1} \otimes (2I_{n_2} - J_{n_2}). \quad (15)$$

In computer vision, the Laplace stencil defined by

$$\begin{array}{|c|c|c|} \hline a_3 & a_2 & a_3 \\ \hline a_2 & a_1 & a_2 \\ \hline a_3 & a_2 & a_3 \\ \hline \end{array} = \begin{array}{|c|c|c|} \hline -1 & -4 & -1 \\ \hline -4 & 20 & -4 \\ \hline -1 & -4 & -1 \\ \hline \end{array}$$

is frequently used and this leads to

$$A = (2I_{n_1} - J_{n_1}) \otimes (5I_{n_2} - \frac{1}{2}J_{n_2}) + (5I_{n_1} - \frac{1}{2}J_{n_1}) \otimes (2I_{n_2} - J_{n_2}).$$

In either case, if we define the constants

$$\alpha_1 = 2, \quad \alpha_2 = 2 \left( a_2 - \sqrt{a_2^2 - a_1 a_3} \right) / a_1,$$

$$\beta_1 = a_1/4, \quad \beta_2 = a_1 a_3 \left( (a_2 - \sqrt{a_2^2 - a_1 a_3}) / 4 \right),$$

then it can be shown that

$$A = (\alpha_1 I_{n_1} + \alpha_2 J_{n_1}) \otimes (\beta_1 I_{n_2} + \beta_2 J_{n_2}) + (\beta_1 I_{n_1} + \beta_2 J_{n_1}) \otimes (\alpha_1 I_{n_2} + \alpha_2 J_{n_2}).$$

Thus,  $A$  is the sum of two Kronecker products and the remarks made in §5.5 apply. Since the rank of  $\tilde{A}$  is two, the singular vectors that define the optimal  $B$  and  $C$  can be computed in  $O(n)$  flops. These matrices are tridiagonal, symmetric, and positive definite in view of the discussions in §5.

Let us focus on the case when  $A$  is given by (15). For simplicity, define the 1-2-1 tridiagonal matrix

$$T_m = 2I_m - J_m$$

and note that

$$A = T_{n_1} \otimes I_{n_2} + I_{n_1} \otimes T_{n_2}.$$

From §5.5 we know that the optimizing  $B$  and  $C$  have the form

$$B = b_1 I_{n_1} + b_2 T_{n_1}$$

$$C = c_1 I_{n_2} + c_2 T_{n_2}.$$

The matrix  $T_m$  has known eigenvalues:

$$Q_m^T T_m Q_m = D_m = \text{diag}(\lambda_1^{(m)}, \dots, \lambda_m^{(m)}), \quad \lambda_j^{(m)} = 4 \sin^2 \left( \frac{j\pi}{2(m+1)} \right).$$

Using this result, it can be shown that the Kronecker approximation problem involves choosing  $b_1, b_2, c_1,$  and  $c_2$  so that

$$\begin{aligned} \|A - B \otimes C\|_F^2 &= \|(T_{n_1} \otimes I_{n_2} + I_{n_1} \otimes T_{n_2}) - (b_1 I_{n_1} + b_2 T_{n_1}) \otimes (c_1 I_{n_2} + c_2 T_{n_2})\|_F^2 \\ &= \|(D_{n_1} \otimes I_{n_2} + I_{n_1} \otimes D_{n_2}) - (b_1 I_{n_1} + b_2 D_{n_1}) \otimes (c_1 I_{n_2} + c_2 D_{n_2})\|_F^2 \\ &= \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} [(\lambda_i^{(n_1)} + \lambda_j^{(n_2)}) - (b_1 + b_2 \lambda_i^{(n_1)})(c_1 + c_2 \lambda_j^{(n_2)})]^2 \end{aligned}$$

is minimized. The eigenvalue distribution of  $M^{-1}A$ , which is crucial to the success of  $M = B \otimes C$  as a preconditioner, can also be examined in closed form once  $b_1, b_2, c_1,$  and  $c_2$  are known:

$$\lambda_{ij}(M^{-1}A) = \frac{\lambda_i^{(n_1)} + \lambda_j^{(n_2)}}{(b_1 + b_2 \lambda_i^{(n_1)})(c_1 + c_2 \lambda_j^{(n_2)})}. \quad (16)$$

We ran some experiments in the square case  $n_1 = n_2 = \sqrt{n}$ . It can be shown that about  $10n$  flops are required to solve a system of the form  $Mz = r$  assuming that the  $LDL^T$  factorizations of  $B$  and  $C$  are available. By way of comparison, about  $9n$  flops are involved when an incomplete Cholesky (IC) preconditioner is used. In the following table we compare these two preconditioners:

$\sqrt{n}$	IC Iterations	Kronecker Iterations
16	14	19
32	23	33
64	39	56
128	51	74
256	66	93

Table 1. Comparison of Preconditioners on Model Problem

Random right hand sides were used with termination criteria  $r^T A r \leq 10^{-6}$  where  $r = b - Ax$  is the residual of the approximate solution. We have no "proof" why reasonable convergence occurs before  $\sqrt{n}$  steps. A plot of the spectrum of  $M^{-1}A$  using (16) reveals that many eigenvalues of  $M^{-1}A$  are clustered about 1. However, the clustering is not definitive enough to suggest that  $O(\sqrt{n})$  convergence is provable.

The Kronecker preconditioner applied to the above model problem compares favorably with many of the other block preconditioners that are reported in [7]. In a distributed memory environment, we suspect that the Kronecker approach may be very attractive because the preconditioner equation  $CZB^T = R$  is structured perfectly for parallel computation—but that is the subject of ongoing research.

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