Block Discrete Empirical Interpolation Methods

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Abstract
We present two block variants of the discrete empirical interpolation method (DEIM); as a particular application, we will consider a CUR factorization. The block DEIM algorithms are based on the concept of the maximum volume of submatrices and a rank-revealing QR factorization. We also present a version of the block DEIM procedures, which allows for adaptive choice of block size. The results of the experiments indicate that the block DEIM algorithms exhibit comparable accuracy for low-rank matrix approximation compared to the standard DEIM procedure. However, the block DEIM algorithms also demonstrate potential computational advantages, showcasing increased efficiency in terms of computational time.

Keywords: Block DEIM, MaxVol, CUR decomposition, rank-revealing QR factorization, low-rank approximation

1. Introduction

A CUR decomposition approximates a data matrix using a subset of its rows and columns. Such factorization preserves in the reduced matrix, properties such as interpretability, sparsity, and nonnegativity of the original data matrix. In machine learning, one can use a CUR decomposition as an unsupervised feature or sample selection technique. Given an \( m \times n \) matrix \( A \) and a target rank \( k \), a CUR factorization takes the form (In line with [20], we will use the letter \( M \) rather than \( U \) for the middle matrix)

\[
A \approx C M R,
\]

\( m \times n \quad m \times k \quad k \times k \quad k \times n \)

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where $C$ and $R$ (both of full rank) are small subsets of the columns and rows of $A$, respectively. The selected columns and rows tend to capture the important information of $A$. One standard way of constructing the factors $C$ and $R$ of a CUR factorization is to apply the discrete empirical interpolation index selection method (DEIM) to the $k$ dominant right and left singular vectors of $A$, respectively [18]. Given the factors $C$ and $R$, following Sorensen and Embree [18] and others [16, 19], the full-rank middle matrix $M$ can be computed as $(C^TC)^{-1}C^TAR^T(RR^T)^{-1}$.

In this work, we propose three different block DEIM procedures. There are three motivating factors for a block DEIM scheme:

- The DEIM algorithm may be considered a greedy algorithm for finding a submatrix with the maximum absolute determinant in a thin-tall matrix: it locally selects the index corresponding to the largest magnitude element of a vector. A block DEIM method shares the same principle but may be less greedy since the optimization is done over more indices instead of just one.

- The proposed block DEIM procedures will generally have higher flop counts than the standard DEIM algorithm. However, in practice, we expect the block DEIM schemes to have higher flop performance than the classical DEIM algorithm as they are mainly based on level 3 BLAS building blocks, which perform matrix-matrix operations.

- A block DEIM scheme may be a good solution where the DEIM procedure faces a difficult choice when the local maximizer is (nearly) nonunique. Given the basis vectors $v_i$ for $i = 1, \ldots, k$, indeed, in [18, Footnote 3] it is already hinted that a potentially problematic case is if multiple entries in a vector being considered have nearly the same magnitude, e.g., $|\langle v_1 \rangle_\ell | \approx |\langle v_1 \rangle_j |$ for $\ell \neq j$, then the DEIM scheme may sometimes make a relatively arbitrary choice. However, in cases where the nonselected large-magnitude entries in $v_1$ are not influential in the subsequent $v_i$ vectors, their corresponding indices may never be picked, despite their equal importance (see Example 2.1).

Our selection criterion for the block-$b$ case will consist of maximizing the modulus of the determinant (volume) over many possible $b \times b$ submatrices. By default, we set $b$ to 5, but one can choose any value for $b$ as long as it is within the range $2 \leq b < k$. We also discuss the option of taking adaptive values of $b$. 

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The outline of the paper is as follows. Section 2 provides a brief literature review of some existing deterministic CUR approximation algorithms. Section 3 describes how the DEIM scheme can be blocked using either a column-pivoted QR factorization or the concept of the maximum absolute determinant (volume) of submatrices. We discuss the newly proposed block DEIM algorithms and their computational complexities and state a well-known error bound for the approximation. Section 4 reports the results from numerical experiments evaluating the computational efficiency and approximation quality of the various block DEIM procedures. Section 5 summarizes the key points and results of this paper. Some main properties of the methods are summarized in Table 1.

Table 1: Overview of the various variants with their properties. All methods have the singular value decomposition (SVD) as a basis. The quantity $\eta$ appears in error upper bounds and is discussed in Section 3.3.

| Method \ Properties | SVD | Block | Adapt. | Tunable | Greediness | $\eta$ | Speed |
|---------------------|-----|-------|--------|---------|------------|-------|-------|
| Standard DEIM       | +   | –     | –      | –       | High       | Medium| Moderate|
| B-MaxVol (Section 3.1) | +   | +     | –      | +       | Low        | Low   | Fast  |
| B-RRQR (Section 3.2) | +   | +     | –      | +       | Low        | Low   | Fast  |
| B-Adaptive (Section 3.3) | +   | +     | +      | +       | Medium     | Medium| Variable|

2. Review of CUR factorization algorithms

In this section, we summarize some known index selection algorithms for computing a CUR factorization. We denote the spectral norm (2-norm) by $\|\cdot\|$ and the notation $R^+$ denotes the Moore–Penrose pseudoinverse of $R$. We use MATLAB notations to index vectors and matrices, i.e., $A(:, p)$ denotes the $k$ columns of $A$ whose corresponding indices are in vector $p \in \mathbb{N}_k$.

2.1. MaxVol Algorithm

The MaxVol algorithm [11, 12] is a commonly used deterministic method for obtaining a CUR factorization of a matrix. This technique involves selecting a subset of rows and columns from the input matrix to create a smaller, well-conditioned submatrix. The MaxVol scheme is a search method that aims to find the submatrix with the largest volume in a tall-thin matrix. Here, the volume of a matrix is defined as the absolute value of its determinant. The MaxVol method is first introduced by Goreinov et al. [11], who used it to construct a rank-$k$ CUR factorization called the pseudoskeleton approximation. Oseledets and Tyrtyshnikov [17] later developed a cross-approximation
scheme that alternates between selecting rows and columns using the MaxVol algorithm.

Given a tall-thin matrix $U \in \mathbb{R}^{m \times k}$, the MaxVol procedure searches for $k$ row indices such that the resulting $k \times k$ upper submatrix $\hat{U}$ is dominant in $U$ \cite{12}. This means that $|U\hat{U}^{-1}|_{ii} \leq 1$. While the dominant property does not necessarily imply that $\hat{U}$ has the maximum volume, it does guarantee that $\hat{U}$ is locally optimal, meaning that replacing any row in $\hat{U}$ with a row from $U$ that is not already present in $\hat{U}$ will not increase the volume. The procedure for finding a dominant submatrix using the MaxVol algorithm is outlined in Algorithm 1.

**Algorithm 1: MaxVol: Approximation to dominant submatrix \cite{12}**

**Data:** $U \in \mathbb{R}^{m \times k}$ with $m > k$, convergence tolerance $\delta$ (default 0.01)

**Result:** $s \in \mathbb{N}_k$ indices

1. $s \leftarrow k$ first indices of a pivoted rows from LU decomposition of $U$

2. repeat

3. Set $\hat{U} \leftarrow U(s, :)$ and $B \leftarrow U\hat{U}^{-1}$

4. Find the element of maximum absolute value in $B$: $(i, j) \leftarrow \text{argmax} |b_{ij}|$

5. if $|b_{ij}| > 1$, swap rows $i$ and $j$ in $B$: $s(j) = i$

6. until $\forall (i, j): |b_{ij}| < 1 + \delta$

In practice, a useful initialization step for the MaxVol algorithm is to use the pivoted rows from the LU decomposition of the input matrix as the starting point \cite{12}. The parameter $\delta$ is the convergence tolerance to find pivot elements; this parameter serves as a stopping criterion and should be sufficiently small (a good choice can be 0.01) \cite{12}. Note that by swapping the rows as done in Line 5, the volume of the upper submatrix in $B$ is increased, and also in $U$ until convergence. The most expensive part of the iterations is Line 3: this needs a $k \times k$ matrix inversion and $O(mk^2)$ operations for the matrix multiplication. Goreinov et al. \cite{12} describe a speed optimization process that avoids the expensive matrix multiplications and inversions. We refer the reader to \cite{12} for a more detailed explanation of the MaxVol approach.

### 2.2. Discrete Empirical Interpolation Method

The DEIM point selection method is a deterministic greedy index selection algorithm originally presented in the context of model order reduction for nonlinear dynamical systems \cite{2, 7, 18}. \cite{18} show that this procedure is a
viable index selection algorithm for constructing a CUR factorization. To select the indices for a rank-$k$ CUR factorization, first, compute a rank-$k$ SVD of the original matrix. Using as input the top-$k$ right and left singular vectors contained in $V$ and $U$, the DEIM algorithm selects $k$ column and row indices, $p$ and $s$, respectively, as in Algorithm 2. The DEIM procedure selects the indices by processing the singular vectors one at a time. We describe this method using the left singular vectors, and the procedure on the right singular vectors follows similarly.

Starting from the leading right singular vector $u_1$, the first row index $s_1$ corresponds to the entry in $u_1$ with the largest magnitude, i.e., $|u_1(s_1)| = \|u_1\|_{\infty}$ (where $\|\cdot\|_{\infty}$ denotes the infinity norm). The remaining indices $s_j$ for $j = 2, \ldots, k$ are selected so that each index corresponds to the largest magnitude entry in the residual $r_j = u_j - S_{j-1} u_j$, where $S_{j-1}$ is an interpolatory projector computed as $U_{j-1} S_{j-1} (S_{j-1} U_{j-1})^{-1} S_{j-1}^T$. (The linear independence of the columns of $U$ guarantees that $S_{j-1}^T U_{j-1}$ is nonsingular.) As mentioned in our third motivating factor in Section 1, in the case where we have multiple index options, e.g., $|(r_{1j})| = |(r_{2j})|$, the smaller index is picked. For further details about the DEIM scheme, we refer the reader to [7, 18].

Algorithm 2: Discrete empirical interpolation index selection method [7]

| Data: $U \in \mathbb{R}^{m \times k}$ with $k \leq m$ (full rank) |
|-----------------|-----------------|
| Result: Indices $s \in \mathbb{N}_k$ with non-repeating entries |
| $s(1) = \arg\max_{1 \leq i \leq m} |(U(:, 1))_i| |
| for $j = 2, \ldots, k$ do |
| $U(:, j) = U(:, j) - U(:, 1 : j - 1) \cdot (U(s, 1 : j - 1) \setminus U(s, j)) |
| $s(j) = \arg\max_{1 \leq i \leq m} |(U(:, j))_i| |
| end |

2.3. Rank-revealing QR factorization

The classical truncated pivoted QR factorization is another approach for computing a CUR factorization [21]. A pivoted QR factorization of a matrix $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ is of the form

\[ A = QR \]

\[ R = \begin{bmatrix} R_1 & \mathbf{0} \end{bmatrix} \]

\[ Q = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \]

Note that the backslash operator used in the algorithms is a Matlab type notation for solving linear systems and least-squares problems.
\[ A \quad \Pi = \quad Q \quad T, \]
\[ m \times n \quad n \times n \quad m \times n \quad n \times n \]

where \( \Pi \) is a permutation matrix, \( Q \) is a matrix with orthonormal columns, and \( T \) is an upper triangular matrix that satisfies the condition \[ \text{21} \]

\[ |T_{kk}|^2 \geq \sum_{i=k}^{j} |T_{ij}|^2, \quad j = k + 1, \ldots, n, \quad k = 1, \ldots, n. \]

Given \( p \), a vector of indices, we can express \( \Pi \) as \( I(:, p) \). Suppose we partition \( Q \) and \( T \) so that

\[ A(:, :p) = [Q_1 \quad Q_2] \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix} = Q_1 [T_{11} \quad T_{12}] + Q_2 [0 \quad T_{22}], \quad (1) \]

where \( Q_1 \in \mathbb{R}^{m \times k} \), \( Q_2 \in \mathbb{R}^{m \times (n-k)} \), \( T_{11} \in \mathbb{R}^{k \times k} \), \( T_{12} \in \mathbb{R}^{k \times (n-k)} \), \( T_{22} \in \mathbb{R}^{(n-k) \times (n-k)} \), and \( \hat{A}_k := Q_1 [T_{11} \quad T_{12}] \), we have

\[ \|A\Pi - \hat{A}_k\| \leq \|T_{22}\| \]

to be the error bound of a truncated pivoted QR decomposition of \( A \). This implies that \( Q_1 \) is an approximation of the range of \( A \) and as long as \( \|T_{22}\| \) is small, \( A(:, :p) \) can be approximated by \( \hat{A}_k \). For an arbitrary \( k \), the best rank-\( k \) approximation of \( A (A_k) \) from the SVD gives \( \|A - A_k\| = \sigma_{k+1}(A) \). It is always the case that \( \sigma_{k+1}(A) \leq \|T_{22}\| \) \[ \text{21} \].

A factorization is said to be a rank-revealing QR (RRQR) factorization if it satisfies \[ \text{4, 13} \]

\[ \frac{\sigma_k(A)}{f_1(k, n)} \leq \sigma_{\min}(T_{11}) \leq \sigma_k(A), \quad \sigma_{k+1}(A) \leq \sigma_{\max}(T_{22}) \leq f_2(k, n) \sigma_{k+1}(A), \quad (2) \]

where \( \sigma_{\min} \) and \( \sigma_{\max} \) are the minimum and maximum singular values, respectively, and \( f_1(k, n) \) and \( f_2(k, n) \) are functions bounded by a low-degree polynomial in \( k \) and \( n \) \[ \text{4} \]. To compute a pivoted QR factorization, one may use the column-pivoted Gram–Schmidt algorithm \[ \text{10} \]. A QR factorization with column pivoting works well in practice; however, there are examples where it fails to produce a factorization that satisfies \[ \text{2} \] (see, e.g., \[ \text{13} \]). There are several ways to compute an RRQR factorization \[ \text{3, 6, 10, 13} \].

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The computational complexities of these methods are slightly larger than the standard QR decomposition algorithm. The values of $f(k, n)$ and the complexities of different schemes are tabulated in [4].

A rank-revealing QR factorization is based on selecting certain well-conditioned submatrices [6], which is the underlying objective of the maximum volume concept. Notice that from the matrix partition, $Q_1 T_{11}$ equals the first $k$ columns of $A(:,p)$. To construct a CUR decomposition, one may apply a Gram–Schmidt-based pivoted QR algorithm to the matrices $A$ and $A^T$ to obtain the matrices $C$ and $R$, respectively [3, 19]. Alternatively, [21] show how to compute a CUR factorization via a two-sided interpolative decomposition (ID), which in turn can be constructed from a pivoted QR factorization. Using the Q-DEIM approach [8], one can apply a column-pivoted QR procedure on the transpose of the leading $k$ right and left singular vectors to find the indices for constructing the factors $C$ and $R$ in CUR approximation.

We will now use the tools described in this section to design our block variants of the standard DEIM algorithm in the following section. To motivate the discussion, let us first consider a small illustrative example.

**Example 2.1** Consider the matrix of left singular vectors (where, e.g., $\varepsilon = 10^{-15}$)

$$U = \begin{bmatrix} \frac{1}{4}\sqrt{3} + \varepsilon & 0 \\ \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{2} + \varepsilon \\ \frac{1}{4}\sqrt{3} & -\frac{1}{4}\sqrt{2} \end{bmatrix},$$

corresponding to singular values $\sigma_1$, $\sigma_2$.

It may easily be checked that, independent of the $\sigma_i$, standard DEIM will pick the first index, followed by the second. However, it is clear that the second and third indices are a better choice, especially if $\sigma_2$ is close to $\sigma_1$. For instance, if $A = U \cdot \begin{bmatrix} 1 & 0 \\ 0 & 0.99 \end{bmatrix}$, working with a determinant of $2 \times 2$ submatrices gives a better result. Since

$$\left| \det \begin{bmatrix} \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{2} + \varepsilon \\ \frac{1}{4}\sqrt{3} & -\frac{1}{4}\sqrt{2} \end{bmatrix} \right| > \left| \det \begin{bmatrix} \frac{1}{4}\sqrt{3} + \varepsilon & 0 \\ \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{2} + \varepsilon \end{bmatrix} \right|,$$

a block DEIM variant with block size 2 picks the more appropriate indices 2 and 3. Additionally, as noted earlier, the DEIM scheme attempts to minimize the quantity $\| (S^T U)^{-1} \|$, where $S$ is an index selection matrix. From our simple example above, we have that

$$\left\| \left( \begin{bmatrix} \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{2} + \varepsilon \\ \frac{1}{4}\sqrt{3} & -\frac{1}{4}\sqrt{2} \end{bmatrix} \right)^{-1} \right\| < \left\| \left( \begin{bmatrix} \frac{1}{4}\sqrt{3} + \varepsilon & 0 \\ \frac{1}{4}\sqrt{3} & \frac{1}{4}\sqrt{2} + \varepsilon \end{bmatrix} \right)^{-1} \right\|.$$
This implies that the rows selected by the block DEIM schemes we will discuss yield a smaller quantity \( \| (S^T U)^{-1} \| \) compared to the DEIM procedure.

3. Block DEIM

This section introduces three new block variants of the DEIM procedure. We combine the index selection algorithms discussed in Section 2 to design our block DEIM algorithms. The block DEIM algorithms select a \( b \)-size set of indices at each step using a block of singular vectors and then update the subsequent block of vectors using the oblique projection technique in the standard DEIM procedure. The main difference between the block DEIM and the traditional DEIM scheme resides in the \( b \)-size indices selection. In the standard DEIM, we select the indices by processing one singular vector at a time, each iteration step produces an index whilst the block version processes a block of singular vectors at a time, and each step provides an index set of size \( b \). As a result, this may lead to a different selection of indices. For ease of presentation, we assume that the number of singular vectors \( k \) is a multiple of the block size \( b \) and \( 2 \leq b < k \).

3.1. Block DEIM based on maximum volume

As the first block variant, we introduce a block DEIM-MaxVol procedure (B-DEIM-MaxVol). For the standard DEIM method, each next index is picked greedily based on the maximal absolute value of an oblique projected singular vector. For this block variant, in every step, we greedily pick a fixed number (\( b \)) of indices based on an (approximate) maximal volume (absolute value of determinant) of a \( b \times b \) submatrix of the projected singular vectors. To this end, we exploit the MaxVol scheme [12] described in Section 2 to efficiently find a submatrix with the approximately maximal determinant (with a given tolerance \( \delta \)) in a thin-tall matrix. This gives the pseudocode as displayed in Algorithm 3.

In Lines 5 and 6 of Algorithm 3, we use the oblique projection technique as in the standard DEIM scheme to update the subsequent blocks of singular vectors.

We will now describe how Algorithm 3 selects the row indices, the selection of the column indices follows similarly. Algorithm 3 starts from the leading-\( b \) dominant left singular vectors \( U_b \), and the first set of index vector \( s_b \) corresponds to the \( b \) row indices of the dominant submatrix in \( U_b \), which
Algorithm 3: Block DEIM index selection based on MaxVol

**Data:** \( U \in \mathbb{R}^{m \times k}, V \in \mathbb{R}^{n \times k}, k \leq \min(m, n) \), block size \( b \) (with \( b \mid k \)), convergence tolerance \( \delta \) (default 0.01)

**Result:** Indices \( p, s \in \mathbb{N}_+^k \) with non-repeating entries

1. for \( j = 1, \ldots, k/b \) do
   2. \( s((j - 1)b + 1 : jb) = \text{MaxVol}(U(:, (j - 1)b + 1 : jb), \delta) \)
   3. \( p((j - 1)b + 1 : jb) = \text{MaxVol}(V(:, (j - 1)b + 1 : jb), \delta) \)
   4. Let cols = \( jb + 1 : jb + b \)
   5. \( U(:, \text{cols}) = U(:, \text{cols}) - U(:, 1 : jb) \cdot (U(s, 1 : jb) \setminus U(s, \text{cols})) \)
   6. \( V(:, \text{cols}) = V(:, \text{col}) - V(:, 1 : jb) \cdot (V(p, 1 : jb) \setminus V(p, \text{cols})) \)
   7. end

is obtained by applying Algorithm 1 to \( U_b \). Let \( s = [s_b, S_b = I(:, s_b)] \), and define an oblique projection operator as

\[
S_b = U_b(S^T_b U_b)^{-1} S^T_b.
\]

Suppose we have \((j - 1)b\) indices, so that

\[
s_{(j-1)b} = \begin{bmatrix} s_b \\ \vdots \\ s_{(j-1)b} \end{bmatrix}, \quad S_{(j-1)b} = I(:, s_{(j-1)b}), \quad U_{(j-1)b} = [U_b, \ldots, U_{(j-1)b}],
\]

and

\[
S_{(j-1)b} = U_{(j-1)b} (S^T_{(j-1)b} U_{(j-1)b})^{-1} S^T_{(j-1)b}.
\]

Compute the residual \( E_{jb} = U_{jb} - S_{(j-1)b} U_{jb} \) (see Line 5 of the algorithm), and select the next set of \( b \) indices by applying Algorithm 1 to \( E_{jb} \). It is worth noting that, using this oblique projection operator \( S_{(j-1)b} \) on \( U_{jb} \) ensures that the \( s_{(j-1)b} \) entries in \( E_{jb} \) are zero, which guarantees nonrepeating indices. At the end of the iteration, the algorithm returns a column and row index set of size \( k \).

The following are two potential benefits of Algorithm 3 compared to standard DEIM.

- **Approximation-wise**, the greedy selection is not column-by-column, but carried out on a block of columns, possibly leading to a better pick of indices. Since the value of \( b \) is modest (typically 2), this procedure is still very affordable.

- **Computationally**, the block procedure may have some benefits over the vector-variant, for instance in the work for the oblique projection.
The computational cost of this algorithm is dominated by two calls of the MaxVol procedure and the block updates. The initialization step of Algorithm 1 requires a permutation of the input matrix, which can be done via the LU factorization. Given an $n \times b$ matrix, the LU decomposition requires $O(nb^2)$ operations. Furthermore, the dominant cost of each iteration in the MaxVol algorithm is the multiplication of an $n \times b$ matrix and a $b \times b$ matrix, for a cost of $O(nb^2)$ operations. Let $\kappa \in \mathbb{N}_+$ denote the number of iterations performed. The computational complexity of the MaxVol procedure is $O(\kappa nb^2)$. The cost of the two calls of MaxVol is $O(\kappa(m + n)b^2)$ and the block updates cost $O((m + n)kb)$. Given that we have $k/b$ iterations in Algorithm 3, the total cost of the B-DEIM-MaxVol algorithm is $O((m + n)(kbk + k^2))$. A crude bound on the number of iterations in Algorithm 1 is $\kappa \leq \log |\det(\hat{U}_{\text{dom}})| - \log |\det(\hat{U}_{\text{ini}})|)/\log(1 + \delta)$, where $\hat{U}_{\text{ini}}$ is the submatrix at the initialization step and $\hat{U}_{\text{dom}}$ is the dominant submatrix in Algorithm 1, respectively [12].

3.2. Block DEIM based on RRQR

The MaxVol algorithm seeks to find a good approximation of a submatrix with the maximum volume in a given input matrix. It is noted in [8, Remark 2.3] that the pivoting in an RRQR factorization can be interpreted as a greedy volume maximizing scheme. Practical experience shows that the index selection via a column-pivoted QR factorization may be more computationally efficient than the MaxVol method.

Additionally, Khabou et al. [14] propose a block LU factorization with panel rank-revealing pivoting (LU-PRRP) procedure by employing a strong rank-revealing QR (RRQR) panel factorization. The algorithm computes the block LU-PRRP as follows: at each step of the block factorization, a block of columns is factored by performing a strong RRQR factorization [13] on its transpose. Pivoting is done by applying the permutation matrix returned on the entire original matrix followed by an update of the trailing matrix. As noted in [18], the DEIM index selection procedure is equivalent to the index selection of partially pivoted LU decomposition.

With this knowledge, we propose an alternative block DEIM variant (B-DEIM-RRQR), which combines the components of the standard DEIM scheme and an RRQR factorization, implemented in Algorithm 4.

During each step of the index selection process, we utilize a block size, $b$, and a block of singular vectors. Firstly, we perform a QR decomposition with column pivoting on the transpose of the leading-$b$ singular vectors, selecting
Algorithm 4: Block DEIM index selection based on RRQR

Data: \( U \in \mathbb{R}^{m \times k} \), \( V \in \mathbb{R}^{n \times k} \), \( k \leq \min(m,n) \), block size \( b \) (with \( b \mid k \))

Result: Indices \( p, s \in \mathbb{N}_+^k \) with non-repeating entries

1. for \( j = 1, \ldots, k/b \) do
2. Perform a column-pivoted QR on \( U(:,(j-1)b+1:jb)^T \) and \( V(:,(j-1)b+1:jb)^T \), giving the permutations \( \Pi_s \) and \( \Pi_p \)
3. \( s((j-1)b+1:jb) = \Pi_s(1:b) \)
4. \( p((j-1)b+1:jb) = \Pi_p(1:b) \)
5. Let \( \text{cols} = jb+1:jb+b \)
6. \( U(:,\text{cols}) = U(:,\text{cols}) - U(:,1:jb) \cdot (U(s,1:jb) \setminus U(s,\text{cols})) \)
7. \( V(:,\text{cols}) = V(:,\text{col}) - V(:,1:jb) \cdot (V(p,1:jb) \setminus V(p,\text{cols})) \)
8. end

indices corresponding to the first \( b \) pivots as the initial set of indices. We then update the next block of singular vectors based on the updating method used in the B-DEIM-Maxvol algorithm and perform a column-pivoted QR on the transpose of the updated block (repeat these two steps until all \( k \) indices are selected).

The B-DEIM-RRQR may be viewed as a hybrid standard DEIM and QDEIM scheme \[^8\]. The QDEIM selects \( k \) indices by performing one column-pivoted QR while our B-DEIM-RRQR algorithm selects the \( k \) indices by performing \( k/b \) rounds of column-pivoted QR. Note that when the block size \( b = k \), this B-DEIM-RRQR algorithm is just the QDEIM scheme.

The cost of the B-DEIM-RRQR scheme is dominated by two QR factorizations and block updates. Given an \( n \times b \) matrix, a QR factorization requires \( O(nb^2) \) operations hence the cost of the two QR decompositions here is \( O((m+n)b^2) \) and the block updates cost \( O((m+n)kb) \). Since there are \( k/b \) iterations in Algorithm 4, the total cost of the B-DEIM-RRQR scheme is therefore \( O((m+n)(kb+k^2)) \).

### 3.3. Adaptive block DEIM

To combine the strength of standard DEIM with a block version, we also consider adaptive choices for the block size \( b \). In particular, we propose the following variant called AdapBlock-DEIM: Perform block DEIM if, for the singular vector \( \mathbf{v}_j \) being considered the two largest elements are (nearly)
equal (see Example 2.1), i.e.,

\[
\begin{cases}
\text{block DEIM} & \quad \text{if } |(\mathbf{v}_j)_i| \approx |(\mathbf{v}_j)_\ell| \quad \text{for } i \neq \ell, \\
\text{standard DEIM} & \quad \text{otherwise}.
\end{cases}
\]
Algorithm 5: Adaptive block DEIM index selection

Data: $U \in \mathbb{R}^{m \times k}$, $V \in \mathbb{R}^{n \times k}$, $k \leq \min(m, n)$, block size $b$, $\rho$ (default 0.95), tolerance $\delta$ (default 0.01), method ($\text{MaxVol}$ or $\text{QR}$)

Result: Indices $p, s \in \mathbb{N}_{+}^{k}$ with non-repeating entries

1. $j = 1$
2. while $j \leq k$ do
3. if $j > 1$ then
4. $\tilde{u} = U(s(1 : j - 1), 1 : j - 1) \setminus U(s(1 : j - 1), j)$
5. $U(:, j) = U(:, j) - U(:, 1 : j - 1) \cdot \tilde{u}$
6. end if
7. $[u, \text{ind}] = \text{sort}(|U(:, j)|)$ (in descending order)
8. if $(j + b - 1 > k)$ or $(u(2) < \rho \cdot u(1))$ then $s(j) = \text{ind}(1)$; $j = j + 1$
9. else
10..cols = $j + b - 1$
11. if $j > 1$ then
12. $\tilde{U} = U(:, j + 1 : \text{cols}); \quad \hat{U} = U(s(1 : j - 1), j + 1 : \text{cols}))$
13. $\tilde{U} = \tilde{U} - U(:, 1 : j - 1) \cdot (U(s(1 : j - 1), 1 : j - 1) \setminus \tilde{U}$
14. end if
15. if method = $\text{MaxVol}$
16. $s(j : \text{cols}) = \text{MaxVol}(U(:, j : \text{cols}), \delta)$
17. else
18. Perform a column-pivoted QR on $U(:, j : \text{cols})^T$, giving
19. permutation $\Pi_s$
20. $s(j : \text{cols}) = \Pi_s(1 : b)$
21. end if
22. $j = j + b$
23. end if
24. end
25. Repeat the procedure on $V$ to get indices $p$

In Algorithm 5, we show an implementation of the adaptive block DEIM using the block DEIM variants discussed in Section 3. The parameter $\rho$ is the desired lower bound on the ratio $|\langle v_j \rangle_i| / |\langle v_j \rangle_\ell|$ for $i \neq \ell$. We note that although our criterion for switching from a standard DEIM scheme to a block DEIM method is based on how close the two largest entries (magnitude) in the vector being considered are, other criteria can be used.

3.4. Error bounds

The following proposition restates a known theoretical error bound for a CUR approximation, which holds for the block DEIM algorithms proposed in
Lemma 4.1 and 4.2; we provide the necessary details here for the reader’s convenience. Let \( P \in \mathbb{R}^{n \times k} \) and \( S \in \mathbb{R}^{m \times k} \) be matrices with some columns of the identity indexed by the indices selected by employing any of the three block DEIM algorithms.

**Proposition 3.1** \cite{18} Thm. 4.1] Given \( A \in \mathbb{R}^{m \times n} \) and a target rank \( k \), let \( U \in \mathbb{R}^{m \times k} \) and \( V \in \mathbb{R}^{n \times k} \) contain the leading \( k \) left and right singular vectors of \( A \), respectively. Suppose \( C = AP \) and \( R = S^T A \) are of full rank, and \( V^T P \) and \( S^T U \) are nonsingular. Then, with \( M = C^+ A R^+ \), a rank-\( k \) CUR decomposition constructed by either of the block DEIM schemes presented in this chapter satisfies

\[
\| A - CMR \| \leq (\eta_s + \eta_p) \sigma_{k+1} \quad \text{with} \quad \eta_s < \sqrt{\frac{nk}{3}} 2^k, \quad \eta_p < \sqrt{\frac{nk}{3}} 2^k;
\]

where \( \eta_p = \|(V^T P)^{-1}\|, \eta_s = \|(S^T U)^{-1}\| \).

**Proof** Let \( P = P(V^T P)^{-1} V^T \) and \( S = U(S^T U)^{-1} S^T \) be oblique projectors. Note that \( V^T P = V^T \) and \( S U = U \), implying that \( V^T (I - P) = 0 \) and \( (I - S) U = 0 \). Using \( M = C^+ A R^+ \), we have

\[
\| A - CMR \| = \| A - CC^+ A R^+ \| = \| (I - CC^+) A + CC^+ A (I - R^+ R) \| \\
\leq \| (I - CC^+) A \| + \| CC^+ \| \| A (I - R^+ R) \|.
\]

Leveraging the fact that \( CC^+ \) is an orthogonal projector, \( \| CC^+ \| = 1 \) and \cite{18} Lemma 4.1 and 4.2

\[
\| (I - CC^+) A \| \leq \| A (I - P) \| = \| A (I - V V^T) (I - P) \| \\
\leq \| (V^T P)^{-1} \| \| A (I - V V^T) \|,
\]

\[
\| A (I - R^+ R) \| \leq \| (I - S) A \| = \| (I - S) (I - U U^T) A \| \\
\leq \| (S^T U)^{-1} \| \| (I - U U^T) A \|;
\]

we have that

\[
\| A - CMR \| \leq \| (V^T P)^{-1} \| \| A (I - V V^T) \| + \| (S^T U)^{-1} \| \| (I - U U^T) A \|.
\]

Since \( U \) and \( V \) contain the leading \( k \) left and right singular vectors, respectively, \( \| (I - U U^T) A \| = \| A (I - V V^T) \| = \sigma_{k+1} \). Hence

\[
\| A - CMR \| \leq \| (V^T P)^{-1} \| + \| (S^T U)^{-1} \| \cdot \sigma_{k+1}.
\]
Proposition 3.1 suggests that the quality of an index selection method may be assessed using the error constants $\eta_s$ and $\eta_p$. Fig. 1 illustrates the difference in the values of $\eta_s = \| (S^T U)^{-1} \|$ computed by DEIM, B-DEIM-RRQR, and B-DEIM-MaxVol using 50 randomly generated orthonormal matrices of size $10000 \times 100$. In most cases, the block DEIM variants provide smaller values of $\eta_s$; this may be an indication that the indices picked by the block DEIM variants are better for approximating than those selected by the DEIM scheme. We also observe that the values of $\eta_s$ become smaller as we increase the block sizes.

Figure 1: Comparison of the value $\eta_s = \| (S^T U)^{-1} \|$ in DEIM, B-DEIM-RRQR, and B-DEIM-MaxVol with different block sizes using 50 random orthonormal matrices of size $10000 \times 100$. 
4. Numerical Experiments

In this section, we conduct several sets of illustrative experiments to show the effectiveness of the block DEIM variants, i.e., B-DEIM-MaxVol, B-DEIM-RRQR, and AdapBlock-DEIM, proposed in this chapter using synthetic and real data sets. We evaluate the algorithms by applying them to data analysis problems in several application domains: recommendation system analysis, model order reduction, economic modeling, and optimization. We use real-world sparse and dense data matrices with sizes ranging from small to large scale. An overview is presented in Table 2. We compare the performance of our algorithms for constructing a CUR approximation with three state-of-the-art deterministic algorithms: DEIM [18], QDEIM [8], and MaxVol [12]. All these algorithms require the leading $k$ right and left singular vectors to construct a rank-$k$ CUR factorization. We use these two evaluation criteria: the rank-$k$ approximation relative error $\|A - CMR\| / \|A\|$; the computational efficiency, i.e., the runtime scaling for the rank parameter $k$. Here, the runtime measures the time it takes each algorithm to select the desired number of column and row indices. We do not consider the run time for computing the singular vectors since all the methods we consider require the SVD. However, it is important to note that the total cost of selecting the indices may be dominated by the computational cost of the SVD. Our experiments are not meant to be exhaustive; however, they provide clear evidence that the block DEIM schemes proposed in this chapter may provide a comparable low-rank approximation while being computationally more efficient.

In the implementation, we perform the column-pivoted QR factorization and the truncated SVD using the MATLAB built-in functions `qr` and `svds` [1], respectively (and `svd` for small cases). For the MaxVol algorithm, we use a MATLAB implementation by [Kramer and Gorodetsky] [15] made available on GitHub [2]. Unless otherwise stated, in all the experiments we use as default block size $b = 5$ for small/mid-size matrices and $b = 10$ for large-scale matrices, the AdapBlock-DEIM method parameter $\rho = 0.95$, and the MaxVol scheme convergence tolerance $\delta = 0.01$.

**Experiment 4.1** In this first set of experiments, we aim to evaluate how our proposed block-DEIM variants compared with the existing deterministic methods mentioned earlier on a small matrix. Our data set is from the
Table 2: Various examples and dimensions considered.

| Exp. | Domain                  | Matrix   | m     | n     |
|------|------------------------|----------|-------|-------|
| 1    | Recommendation system  | Dense    | 14116 | 100   |
| 2    | Economic modeling      | Sparse   | 29610 | 29610 |
| 3    | Optimization           | Sparse   | 29920 | 29920 |
| 4    | Model order reduction  | Sparse   | 23412 | 23412 |
| 5    | Structural engineering | Sparse   | 22044 | 22044 |
| 6    | Synthetic              | Dense    | 2000  | 4000  |

recommendation system analysis domain, where one is usually interested in making service or purchase recommendations to users. One of the most common techniques for recommendation systems is collaborative filtering, which involves recommending to users items that customers with similar preferences liked in the past. The Jester data set is often used as a benchmark for recommendation system research. This data matrix consists of 73421 users and their ratings for 100 jokes. We only consider users who have ratings for all 100 jokes resulting in a $14116 \times 100$ matrix. We center the matrix by subtracting the mean of each column from all entries in that column.

Based on the observations from Fig. 2, we can conclude that the block DEIM methods generally provide slightly more accurate approximations compared to state-of-the-art methods. It is also important to note that the error of the MaxVol and QDEIM approximations do not always decrease monotonically as the rank $k$ increases. When considering the runtime, both the B-DEIM-MaxVol and B-DEIM-RRQR algorithms demonstrate significantly lower computational times compared to the original DEIM scheme. In these small/mid-scale experiments, the adaptive variants of the block DEIM methods do not seem to improve runtimes compared to the DEIM procedure. There could be several reasons for this observation: the adaptive variants of block DEIM methods involve additional computations and operations compared to the standard DEIM procedure. These additional steps may introduce computational overhead that offsets the potential gains in runtime. In small/mid-scale scenarios, the overhead might outweigh the benefits. On the other hand, it is evident that the B-DEIM-MaxVol algorithm and its adaptive variant are more efficient than the standard MaxVol approach. By utilizing the block DEIM variants, we gain improvements in both accuracy and speed compared to the standard MaxVol method. Additionally, the B-DEIM-RRQR method proves to be equally efficient as the QDEIM procedure while providing a more accurate approximation.
Figure 2: Relative approximation errors (left) and runtimes (right) as a function of $k$ for the block DEIM CUR approximation algorithms compared with some standard CUR approximation algorithms using the Jester data set.

Experiment 4.2 In the subsequent series of experiments, we turn our attention to evaluating the performance of our proposed block-DEIM variants when dealing with large-scale data. With a block size of $b = 10$ selected for this particular set of experiments, our primary goal is to gain insights into how our block-DEIM approaches tackle the challenges presented by large-scale data sets and to assess their effectiveness and efficiency in this context. To conduct these evaluations, we utilize a set of standard test matrices specifically designed for sparse matrix problems. These data matrices are sourced from the publicly available SuiteSparse Matrix Collection. The diverse na-
ture of these matrices allows us to assess the effectiveness of our approaches across various problem domains.

The first test matrix, referred to as \texttt{g7jac100}, is derived from the “Overlapping Generations Model” used to study the social security systems of the G7 nations. It is a sparse matrix with dimensions $29610 \times 29610$ and contains 335972 numerically nonzero entries. Notably, this matrix has a low rank of 21971. The second matrix, named \texttt{net100}, originates from an optimization problem. It has dimensions of $29920 \times 29920$ and contains 2033200 numerically nonzero entries. Similar to the previous matrix, \texttt{net100} also possesses a low rank, specifically 26983. The \texttt{Abacus-shell-ld} matrix, associated with model order reduction, has dimensions $23412 \times 23412$ and represents a rank-2048 structure. It contains 218484 nonzero entries. Lastly, we have \texttt{pkustk01}, a symmetric positive-definite matrix derived from a civil engineering problem. This matrix has dimensions of $22044 \times 22044$, a low rank of 3732, and consists of 979380 nonzero entries.

In the case of large-scale data sets, similar to the small/mid-scale experiments, in Figs. 3, 4, 5, and 6 the block DEIM variants maintain comparable reconstruction errors as the existing methods. This finding aligns with our observations from the small/mid-scale experiments. However, there are notable differences in terms of algorithm efficiency. Unlike the small/mid-scale cases, where the adaptive variants have similar runtimes as the DEIM scheme, in the large-scale experiments, the adaptive variants demonstrate better computational efficiency than the standard DEIM scheme. On the other hand, the B-DEIM-MaxVol and B-DEIM-RRQR schemes showcase better speed efficiency overall. These block DEIM variants prove to be effective in achieving a balance between accuracy and computational efficiency in the context of large-scale data. Consistent with previous findings, the MaxVol algorithm generally remains the least efficient method, with one exception in the case of the \texttt{gijac100} data set. These results highlight the importance of considering the specific characteristics and requirements of the data sets when selecting an appropriate algorithm.
Figure 3: Relative approximation errors (left) and runtimes (right) as a function of $k$ for the block DEIM CUR approximation algorithms compared with some standard CUR approximation algorithms using the $g7jac100$ sparse matrix.
Figure 4: Relative approximation errors (left) and runtimes (right) as a function of $k$ for the block DEIM CUR approximation algorithms compared with some standard CUR approximation algorithms using the net100 sparse matrix.
Figure 5: Relative approximation errors (left) and runtimes (right) as a function of $k$ for the block DEIM CUR approximation algorithms compared with some standard CUR approximation algorithms using the Abacusa-shell-ld sparse matrix.
Figure 6: Relative approximation errors (left) and runtimes (right) as a function of $k$ for the block DEIM CUR approximation algorithms compared with some standard CUR approximation algorithms using the pkustk01 sparse matrix.
**Experiment 4.3** Using two of the block DEIM algorithms proposed: the B-DEIM-MaxVol and B-DEIM-RRQR, we investigate how varying block sizes, i.e., \( b = (2, 5, 10, 20) \) may affect their approximation quality and computational efficiency.

Following the experiments in [21], our test matrix in this experiment is a full-rank data set \( A \in \mathbb{R}^{2000 \times 4000} \) that has the structure of the SVD, i.e., \( A = U \Sigma V^T \). The matrices \( U \) and \( V \) have random orthonormal columns obtained via a QR factorization of a random Gaussian matrix, and the diagonal matrix \( \Sigma \) has entries that are logspace ranging from 1 to \( 10^{-3} \). For each fixed block size, maintaining the properties of \( A \), we generate five different test cases and compute the averages of the evaluation criteria for the range of \( k \) values.

We observe in Fig. 7 that both algorithms become considerably faster for increasing block sizes. On the other hand, the approximation quality of the varying block sizes may not degrade significantly. In this experiment, given the various values of \( k \), the errors are almost similar irrespective of the block size.

**5. Conclusions**

This paper presents various block variants of the discrete empirical interpolation method for computing CUR decompositions. We exploit the advantages of the classical DEIM procedure, a column-pivoted QR decomposition, and the concept of maximum determinant or volume of submatrices to develop these block variants. We have then presented a version of the block DEIM, which allows for an adaptive choice of block size.

We perform the following procedures in the block DEIM based on RRQR; at each iteration step, we compute a QR factorization with column pivoting on the transpose of a block of singular vectors to obtain the indices corresponding to the first \( b \) columns. Then, we update the next block of vectors using the interpolatory projection technique in the DEIM algorithm (repeat these two steps until all indices are selected). A similar procedure is used in the block DEIM based on MaxVol; the difference here is instead of using a column-pivoted QR decomposition, we use the MaxVol method.

Numerical experiments illustrate that the accuracy of a CUR factorization using the newly proposed block DEIM procedures is comparable to the classical DEIM, MaxVol, and QDEIM schemes. The experiments also demonstrate that the block variants, regarding computational speed, may have an advantage over the standard DEIM and MaxVol algorithms. Relative to
the QDEIM algorithm, the B-DEIM-RRQR scheme sometimes yields lesser approximation errors while maintaining comparable runtimes. Using the B-DEIM-RRQR and B-DEIM-MaxVol methods, we have also illustrated how increasing the block size improves the speed of the algorithms but may not necessarily degrade the approximation quality significantly. Table 1 displays a schematic overview of some properties of the various methods. A Matlab code of the proposed algorithms is available via [github.com/perfectyayra](https://github.com/perfectyayra).
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References

[1] J. Baglama and L. Reichel. Augmented implicitly restarted Lanczos bidiagonalization methods. *SIAM J. Sci. Comput.*, 27(1):19–42, 2005.

[2] M. Barrault, Y. Maday, N. C. Nguyen, and A. T. Patera. An ‘empirical interpolation’ method: Application to efficient reduced-basis discretization of partial differential equations. *Comptes Rendus Math.*, 339:667–672, 2004.

[3] M. W. Berry, S. A. Pulatova, and G. W. Stewart. Algorithm 844: Computing sparse reduced-rank approximations to sparse matrices. *ACM Trans. Math. Softw.*, 31(2):252–269, 2005.

[4] C. Boutsidis, P. Drineas, and M. Mahoney. On selecting exactly $k$ columns from a matrix. *Manuscript*, 2008.

[5] T. F. Chan. Rank revealing QR factorizations. *Linear Algebra Appl.*, 88:67–82, 1987.

[6] S. Chandrasekaran and I. C. F. Ipsen. On rank-revealing factorisations. *SIAM J. Matrix Anal. Appl.*, 15(2):592–622, 1994.

[7] S. Chaturantabut and D. C. Sorensen. Nonlinear model reduction via discrete empirical interpolation. *SIAM J. Sci. Comput.*, 32:2737–2764, 2010.

[8] Z. Drmac and S. Gugercin. A new selection operator for the discrete empirical interpolation method—Improved a priori error bound and extensions. *SIAM J. Sci. Comput.*, 38(2):A631–A648, 2016.

[9] K. Goldberg, T. Roeder, D. Gupta, and C. Perkins. Eigentaste: A constant time collaborative filtering algorithm. *Inform. Retrieval*, 4(2):133–151, 2001.
[10] G. Golub and C. F. Van Loan. *Matrix Computations*. Johns Hopkins University Press, Baltimore, 4th edition, 2012.

[11] S. A. Goreinov, E. E. Tyrtyshnikov, and N. L. Zamarashkin. A theory of pseudoskeleton approximations. *Linear Algebra Appl.*, 261(1-3):1–21, 1997.

[12] S. A. Goreinov, I. V. Oseledets, D. V. Savostyanov, E. E. Tyrtyshnikov, and N. L. Zamarashkin. How to find a good submatrix. In *Matrix Methods: Theory, Algorithms And Applications*, pages 247–256. World Scientific, Singapore, 2010.

[13] M. Gu and S. C. Eisenstat. Efficient algorithms for computing a strong rank-revealing QR factorization. *SIAM J. Sci. Comput.*, 17(4):848–869, 1996.

[14] A. Khabou, J. W. Demmel, L. Grigori, and M. Gu. LU factorization with panel rank revealing pivoting and its communication avoiding version. *SIAM J. Matrix Anal. Appl.*, 34(3):1401–1429, 2013.

[15] B. Kramer and A. A. Gorodetsky. System identification method via CUR factorization of Hankel matrix. *SIAM J. Sci. Comput.*, 40(2):A848–A866, 2018.

[16] M. W. Mahoney and P. Drineas. CUR matrix decompositions for improved data analysis. *Proc. Natl. Acad. Sci. USA*, 106:697–702, 2009.

[17] I. Oseledets and E. Tyrtyshnikov. TT-cross approximation for multidimensional arrays. *Linear Algebra Appl.*, 432(1):70–88, 2010.

[18] D. C. Sorensen and M. Embree. A DEIM induced CUR factorization. *SIAM J. Sci. Comput.*, 33(3):A1454–A1482, 2016.

[19] G. W. Stewart. Four algorithms for the efficient computation of truncated pivoted QR approximations to a sparse matrix. *Numer. Math.*, 83:313–323, 1998.

[20] G. Strang. *Linear Algebra and Learning from Data*. SIAM, Philadelphia, 2019.
[21] S. Voronin and P. G. Martinsson. Efficient algorithms for CUR and interpolative matrix decompositions. *Adv. Comput. Math.*, 43:495–516, 2017.