ALTERNATING ENERGY MINIMIZATION METHODS FOR
MULTI-TERM MATRIX EQUATIONS

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Abstract. We develop computational methods for approximating the solution of a linear multi-term matrix equation in low rank. We follow an alternating minimization framework, where the solution is represented as a product of two matrices, and approximations to each matrix are sought by solving certain minimization problems repeatedly. The solution methods we present are based on a rank-adaptive variant of alternating energy minimization methods that builds an approximation iteratively by successively computing a rank-one solution component at each step. We also develop efficient procedures to improve the accuracy of the low-rank approximate solutions computed using these successive rank-one update techniques. We explore the use of the methods with linear multi-term matrix equations that arise from stochastic Galerkin finite element discretizations of parameterized linear elliptic PDEs, and demonstrate their effectiveness with numerical studies.

Key words. low-rank approximation, alternating energy minimization, stochastic Galerkin methods, matrix equations

AMS subject classifications. 35R60, 60H35, 65F10, 65N30

1. Introduction. We are interested in computing a low-rank approximate solution of a Kronecker-product structured linear system

\[ Au = b, \]

(1.1)

where \( A = \sum_{i=0}^{m} G_i \otimes K_i \) is symmetric positive definite, \( \otimes \) is the Kronecker product, \( \{K_i\}_{i=0}^{m} \in \mathbb{R}^{n_1 \times n_1}, \{G_i\}_{i=0}^{m} \in \mathbb{R}^{n_2 \times n_2}, \{f_i\}_{i=0}^{r} \in \mathbb{R}^{n_1}, \) and \( \{g_i\}_{i=0}^{r} \in \mathbb{R}^{n_2} \). Systems with such structure arise in the discretization of linear elliptic PDEs in high dimensions [2, 18, 19, 20] and stochastic Galerkin finite element discretization of parameterized linear elliptic PDEs [11, 22, 25, 38]. The solution vector \( u \in \mathbb{R}^{n_1 n_2} \) consists of \( n_2 \) subvectors of dimension \( n_1 \), i.e., \( u = [u_1^T, \ldots, u_{n_2}^T]^T \), where \( \{u_i\}_{i=1}^{n_2} \in \mathbb{R}^{n_1} \). It also has an alternative representation in matrix format, \( U = [u_1, \ldots, u_{n_2}] \in \mathbb{R}^{n_1 \times n_2} \), for which the system equivalent to (1.1) is the linear multi-term matrix equation [31]

\[ \sum_{i=0}^{m} K_i U G_i^T = B, \]

(1.2)

where \( B = \sum_{i=0}^{r} f_i g_i^T \in \mathbb{R}^{n_1 \times n_2} \) and it is assumed that \( m, r \ll n_1, n_2 \). The system matrices \( K_i \) and \( G_i \) obtained from discretization methods are typically sparse and, thus, for moderately large system matrices, Krylov subspace methods [29, 30] and multigrid methods [3, 9, 21] have been natural choices to solve such systems.

The dimensions of the system matrices grow rapidly, however, if a solution is sought on a refined grid or (in the case of stochastic Galerkin methods) if the so-called parametric space is high-dimensional. For large \( n_1 \) and \( n_2 \), direct applications...
of standard iterative methods may be computationally prohibitive and storing or explicitly forming the matrix $U$ may be prohibitive in terms of memory. Instead of computing an exact solution of (1.2), we are interested in inexpensive computation of an approximate solution of low rank. To achieve this goal, we begin by introducing a factored representation of $U \in \mathbb{R}^{n_1 \times n_2}$:

$$U = VW^T,$$

where, if $U$ is of full rank $m := \min(n_1, n_2)$, $V \in \mathbb{R}^{n_1 \times m}$ and $W \in \mathbb{R}^{n_2 \times m}$. Our aim is to find a low-rank approximation to this factored matrix of the form

(1.3) $U_p = V_p W_p^T \in \mathbb{R}^{n_1 \times n_2},$

where $V_p = [v_1, \ldots, v_p] \in \mathbb{R}^{n_1 \times p}$ and $W_p = [w_1, \ldots, w_p] \in \mathbb{R}^{n_2 \times p}$ and $p \ll m$, and we want to derive solution algorithms for computing $U_p$ that operate only on the factors $V_p$ and $W_p$ without explicitly forming $U_p$.

One such solution algorithm has been developed for matrix completion/sensing [14, 16], which, at the $p$th iteration, computes $V_p$ and $W_p$ by alternately solving certain minimization problems. Although the algorithm computes highly accurate approximations, it can become very expensive as $p$ increases. Another approach is to use successive rank-one approximations and successively compute pairs of vectors $\{(v_i, w_i)\}_{i=1}^p$ to build the factors $V_p$ and $W_p$ of (1.3) until a stopping criterion is satisfied. The $p$th iteration starts with $V_{p-1}$ and $W_{p-1}$ and constructs $v_p$ and $w_p$ as the solutions of certain minimization problems. This approach for solving parameterized PDEs is one component of a methodology known as Proper Generalized Decomposition (PGD) [26, 27, 37]. As observed in those works, using only successive rank-one approximations is less expensive but may not be practical because it typically results in approximate solutions with an unnecessarily large value of $p$ for satisfying a certain error tolerance.

Our goal in this study is to develop solution algorithms that preserve only the good properties of the above two types of solution strategies, i.e., algorithms that compute an accurate solution in a computationally efficient way. In developing such algorithms, we take our cue from PGD methods, in which, to improve accuracy, the successive rank-one constructions are supplemented with an updating procedure that is performed intermittently during the iteration. Inspired by this approach, we propose a solution algorithm that adaptively computes approximate solutions in an inexpensive way via the successive rank-one approximation method. This is then supplemented by an enhancement procedure, which effectively improves the accuracy of the resulting approximate solutions. We propose two novel enhancement procedures developed by modifying some ideas used for matrix completion problems [16].

Some other rank-adaptive approaches for approximating solutions of parameterized or high-dimensional PDEs in low-rank format are as follows. A method in [4] uses alternating energy minimization techniques in combination with tensor-train decompositions [28]. One can incrementally compute rank-one solution pairs by solving a residual minimization problem, an approach known as alternating least-squares (ALS) methods, which has been used to compute low-rank approximate solutions of parameterized PDEs in [5, 6], and to solve matrix recovery problems, matrix sensing and completion problems, [13, 14, 16, 32]. In [31], an adaptive iterative procedure to solve the matrix equation (1.2) is given, which incrementally computes a set of orthonormal basis vectors for use in representing the spatial part of the solution, $V_p$. See [36] for an overview of other computational approaches for solving linear matrix equations.
An outline of the paper is as follows. In Section 2, we introduce and derive alternating energy minimization (AEM) methods using the well-known general projection framework and discuss a collection of methods developed for constructing low-rank approximate solutions of the form (1.3). In Section 3, we discuss enhancement procedures and derive two new approaches for performing such updates. In Section 4, we measure the effectiveness and the efficiency of the variants of the methods with numerical experiments. Finally, in Section 5, we draw some conclusions.

2. Alternating energy minimization (AEM) methods. In this section, we derive AEM methods for solving the matrix equation (1.2) from the optimal projection framework, and review two variants of such methods. We first introduce some notation. Capital and small letters are used to denote matrices and vectors, respectively. As a special case, a zero-column matrix is indicated by using a subscript 0, e.g., \( X_0 \in \mathbb{R}^{n_1 \times 0} \). An inner product between two matrices \( X, Y \in \mathbb{R}^{n_1 \times n_2} \) is defined as \( \langle X, Y \rangle \equiv \text{tr}(X^T Y) = \text{tr}(XY^T) = \sum_{i,j} X_{ij} Y_{ij} \), where \( \text{tr} \) is the trace operator, and \( \text{tr}(X) = \sum_{i=1}^n x_{ii} \) if \( X \in \mathbb{R}^{n \times n} \). The norm induced by \( \langle \cdot, \cdot \rangle \) is the Frobenius norm \( \|X\|_F = \sqrt{\langle X, X \rangle} \). For shorthand notation, we introduce a linear operator \( A(X) = \sum_{i=0}^m K_i X G_i^T \) for \( X \in \mathbb{R}^{n_1 \times n_2} \). Using this, we can define the weighted inner product \( \langle X, Y \rangle_A = \langle A(X), Y \rangle = \langle X, A(Y) \rangle \) and the induced \( A \)-norm \( \|\cdot\|_A \). Finally, \( \text{vec} \) denotes a vectorization operator, \( \text{vec}(X) = x \), where \( X = [x_1, \ldots, x_{n_2}] \in \mathbb{R}^{n_1 \times n_2} \) and \( x = [x_1^T, \ldots, x_{n_2}^T]^T \in \mathbb{R}^{n_1 n_2} \), where \( x_i \in \mathbb{R}^{n_1} \), for \( i = 1, \ldots, n_2 \).

2.1. General projection framework. For the computation of \( V_p \) and \( W_p \) in (1.3), we rely on the classical theory of orthogonal (Galerkin) projection methods [33, Proposition 5.2]. Let \( K \subset \mathbb{R}^{n_1 \times n_2} \) be a search space in which an approximate solution \( U_p \in \mathbb{R}^{n_1 \times n_2} \) is sought, and let \( L \) be a constraint space onto which the residual \( B - A(U_p) \) is projected. Following [33, Proposition 5.2], if the system matrix \( A \) is symmetric positive definite and \( L = K \), then a matrix \( U_p^* \) is the result of an orthogonal projection onto \( L \) if and only if it minimizes the \( A \)-norm of the error over \( K \), i.e.,

\[
U_p^* = \arg \min_{U_p \in K} J_A(U_p),
\]

where the objective function is

\[
J_A(U_p) = \frac{1}{2} \|U - U_p\|_A^2.
\]

Because we seek a factored representation of \( U_p \), we slightly modify (2.1) to give

\[
J_A(V_p, W_p) = \frac{1}{2} \|U - V_p W_p^T\|_A^2,
\]

and obtain a new minimization problem

\[
\min_{V_p \in \mathbb{R}^{n_1 \times p}, W_p \in \mathbb{R}^{n_2 \times p}} J_A(V_p, W_p).
\]

Since \( J_A \) is quadratic, gradients with respect to \( V_p \) and \( W_p \) can be easily obtained as

\[
\nabla_{V_p} J_A = (A(V_p W_p^T) - B) W_p = \sum_{i=0}^m (K_i V_p W_p^T G_i^T) W_p - B W_p,
\]

\[
\nabla_{W_p} J_A = (A(V_p W_p^T) - B)^T V_p = \sum_{i=0}^m (K_i V_p W_p^T G_i^T)^T V_p - B^T V_p.
\]
Employing the first-order optimality condition on (2.4)–(2.5) (i.e., setting (2.4) and (the transpose of) (2.5) to be zero) results in the set of equations

$$\sum_{i=0}^{m} (K_i V_p W_p^T G_i^T) W_p = BW_p \in \mathbb{R}^{n_1 \times p},$$

$$\sum_{i=0}^{m} V_p^T (K_i V_p W_p^T G_i^T) = V_p^T B \in \mathbb{R}^{p \times n_2}.$$  

These equations can be interpreted as projections of the residual $B - \mathcal{A}(V_p W_p^T)$ onto the spaces spanned by the columns of $W_p$ and $V_p$, respectively.

Given (2.6)–(2.7), a widely used strategy for solving the minimization problem (2.3) is to compute each component of the solution pair $(V_p, W_p)$ alternately [4, 5, 6, 13, 14, 16]. That is, one can fix $W_p$ and solve the system of equations of order $n_1 p$ in (2.6) for $V_p$, and then one can fix $V_p$ and solve the system of equations of order $n_2 p$ in (2.7) for $W_p$. However, in this approach, suitable choices of $p$ for satisfying a fixed error tolerance are typically not known a priori. Thus, adaptive schemes that incrementally compute solution pairs $(v_i, w_i)$ have been introduced [16, 26, 27, 37]. All of these schemes are based on alternately solving two systems of equations for two types of variables in an effort to minimize a certain error measure. In this study, we employ alternating methods for minimizing the energy norm of the error (2.3) and, thus, we refer to approaches of this type as alternating energy minimization (AEM) methods. In the following sections, we present two adaptive variants of AEM methods: a Stage-$p$ AEM method and a successive rank-one AEM method.

### 2.2. Stage-$p$ AEM method.

An alternating minimization method that entails solving a sequence of least-squares problems whose dimensions increase with $p$ was developed in [16] for solving matrix-recovery problems [13, 14, 16]. We adapt this approach to the energy minimization problem (2.3) and refer to it as the Stage-$p$ AEM method. It is an iterative method that runs until an approximate solution satisfies a stopping criterion (e.g., the relative residual $\|B - \mathcal{A}(V_p W_p^T)\|_F \leq \epsilon \|B\|_F$ with a user-specified stopping tolerance $\epsilon$). At the $p$th iteration, called a “stage” in [16], this method seeks $p$-column factors $V_p$ and $W_p$ determining an approximate solution by initializing $W_p^{(0)}$ and solving the following systems of equations in sequence:

$$\sum_{i=0}^{m} (K_i) V_p^{(k)} (W_p^{(k-1)} G_i W_p^{(k-1)})^T = BW_p^{(k-1)},$$

$$\sum_{i=0}^{m} (V_p^{(k)} K_i V_p^{(k)}) W_p^{(k)} G_i^T = V_p^{(k)} B,$$

for $k = 1, \ldots, k_{\text{max}}$, where the superscript indicates the number of alternations between the two systems of equations (2.8)–(2.9). Note that the method can also begin by initializing $V_p^{(0)}$ and alternating between (2.9) and (2.8). Algorithm 2.1 summarizes the entire procedure. For the initialization of $W_p^{(0)}$ (line 3), one step of the singular value projection method [15] is performed with the exact settings from [16, Algorithm 3]. The CheckConvergence procedure (line 9) is detailed in Section 3.

Systems of equations for “vectorized” versions of the matrix factors $V_p$ and $W_p$
Algorithm 2.1 Stage-p AEM method

**INPUT:** $p_{\text{max}}$: the maximum number of solution pairs,
$k_{\text{max}}$: the maximum number of alternations in each stage,
$\epsilon$: a parameter for checking convergence,

1: function STAGEpAEM($p_{\text{max}}, k_{\text{max}}, \epsilon$)
2:    for $p = 1, \ldots, p_{\text{max}}$ do
3:        $[V_p^{(0)}, W_p^{(0)}] = \text{first } p \text{ singular vectors of } V_{p-1}W_{p-1}^T - \frac{3}{4}(A(V_{p-1}W_{p-1}^T) - B)$
4:        for $k = 1, \ldots, k_{\text{max}}$ do
5:            $V_p^{(k)} \leftarrow \text{solve } (2.8)$
6:            $W_p^{(k)} \leftarrow \text{solve } (2.9)$
7:        end for
8:        $V_p, W_p \leftarrow \text{CheckConvergence}(V_p, W_p, \epsilon)$
9:    end for
10: end function

can be derived\(^1\) from (2.8) and (2.9) as follows

\[
\sum_{i=0}^{m} [(W_p^{(k-1)T}G_iW_p^{(k-1)}) \otimes K_i] \text{vec}(V_p^{(k)}) = \text{vec}(BW_p^{(k-1)}),
\]

\[
\sum_{i=0}^{m} [(V_p^{(k)T}K_iV_p^{(k)}) \otimes G_i] \text{vec}(W_p^{(k)}) = \text{vec}(B^TV_p^{(k)}).
\]

Thus, solving (2.8) and (2.9) is equivalent to solving coupled linear systems with coefficient matrices of dimensions $n_1p \times n_1p$ and $n_2p \times n_2p$, respectively, which are smaller than that of the original system (1.2) when $p$ is small. However, the reduced matrix factors (of size $p \times p$) are dense, even if the original ones are sparse, and so as $p$ increases, the computational costs for solving (2.8)–(2.9) increase and the Stage-p AEM method may be impractical for large-scale problems.

### 2.3. Successive rank-one AEM method

We now describe a successive rank-one (S-rank-1) approximation method which, at each iteration, adds a rank-one correction to the current iterate. This is a basic component of PGD methods [26, 27, 37] for solving parameterized PDEs. The method only requires solutions of linear systems with coefficient matrices of size $n_1 \times n_1$ and $n_2 \times n_2$ rather than coupled systems like those in the Stage-p AEM method that grow in size with the step counter $p$.

Assume that $p - 1$ pairs of solutions are computed, giving $V_{p-1}$ and $W_{p-1}$. The next step is to compute a new solution pair $(v_p, w_p)$ by choosing the objective function

\[
J_A(v_p, w_p) = \frac{1}{2}\|U - V_{p-1}W_{p-1}^T - v_p w_p^T\|_A^2,
\]

and solving the following minimization problem

\[
\min_{v_p \in \mathbb{R}^{n_1}, w_p \in \mathbb{R}^{n_2}} J_A(v_p, w_p).
\]

---

\(^1\)The left-hand sides of (2.10)–(2.11) are derived using vec$(KUG^T) = (G \otimes K)\text{vec}(U)$. Note that (2.11) is derived by first transposing (2.9) and then vectorizing the resulting equation. In the sequel, vectorized versions of equations for the factor $W_p$ are derived by first taking the transpose.
The gradients of $J_A$ with respect to $v_p$ and $w_p$ are

\begin{align}
\nabla_{v_p} J_A &= \left( A(v_p w_p^T) + A(V_{p-1} W_{p-1}^T) - B \right) w_p, \\
\nabla_{w_p} J_A &= \left( A(v_p w_p^T) + A(V_{p-1} W_{p-1}^T) - B \right)^T v_p.
\end{align}

Employing the first-order optimality conditions (setting (2.12) and (2.13) to zero) results in systems of equations for which, in a succession of steps $k = 1, \ldots, k_{\text{max}}$, $v_p$ is updated using fixed $w_p$ and then $w_p$ is updated using fixed $v_p$:

\begin{align}
\sum_{i=0}^{m} (K_i)_{v_p} (w_p^{(k-1)T} G_i w_p^{(k-1)})^T &= B w_p^{(k-1)} - A(V_{p-1} W_{p-1}^T) w_p^{(k-1)}, \\
\sum_{i=0}^{m} (v_p^{(k)}^T K_i v_p^{(k)}) w_p^{(k)} (G_i^T) &= v_p^{(k)T} B - v_p^{(k)T} A(V_{p-1} W_{p-1}^T).
\end{align}

Algorithm 2.2 summarizes this procedure, which randomly initializes $w_p^{(0)}$ and then alternately solves (2.14)–(2.15). Like the Stage-$p$ AEM method, the algorithm can start with either $w_p^{(0)}$ or $v_p^{(0)}$.

**2.4. Algebraic interpretation of the methods.** Algorithms 2.1 and 2.2 both entail an “outer iteration” with counter $p$ and an “inner iteration” with counter $k$, and both are designed to minimize the objective function (2.2). It is instructive to see the difference between the two methods in vectorized format. To this end, let

$$A_w(u_i, w_j) = \sum_{i=0}^{m} K_i (w_j G_i w_i) \in \mathbb{R}^{n_1 \times n_1}, \quad A_v(v_i, v_j) = \sum_{i=0}^{m} G_i (v_j^T K_i^T v_i) \in \mathbb{R}^{n_2 \times n_2},$$

and let us assume $p = 2$ for simplifying the presentation.

Both methods seek solution pairs $(V_2, W_2)$ satisfying the systems of equations (2.6)–(2.7), which can be written in a vectorized form:

\begin{align}
\begin{bmatrix}
A_w(u_1, v_1) & A_w(u_1, v_2) \\
A_w(u_2, v_1) & A_w(u_2, v_2)
\end{bmatrix}
\begin{bmatrix}
v_1 \\
v_2
\end{bmatrix}
&= 
\begin{bmatrix}
B w_1 \\
B w_2
\end{bmatrix}, \\
\begin{bmatrix}
A_v(v_1, v_1) & A_v(v_1, v_2) \\
A_v(v_2, v_1) & A_v(v_2, v_2)
\end{bmatrix}
\begin{bmatrix}
w_1 \\
w_2
\end{bmatrix}
&= 
\begin{bmatrix}
B^T v_1 \\
B^T v_2
\end{bmatrix}.
\end{align}
In the second outer iteration, the Stage-$p$ AEM method alternately solves fully coupled linear systems (2.8)–(2.9) specified by $W_2^{(k-1)}$ and $V_2^{(k)}$, which can be written in vectorized form as in (2.16)–(2.17):

$$
\begin{bmatrix}
A_w(w_1^{(k-1)}, w_1^{(k-1)}) & A_w(w_2^{(k-1)}, w_2^{(k-1)}) \\
A_w(w_2^{(k-1)}, w_1^{(k-1)}) & A_w(w_2^{(k-1)}, w_2^{(k-1)})
\end{bmatrix}
\begin{bmatrix}
v_1^{(k)} \\
v_2^{(k)}
\end{bmatrix} =
\begin{bmatrix}
Bw_1^{(k-1)} \\
Bw_2^{(k-1)}
\end{bmatrix},
$$

(2.18)

In contrast, the S-rank-1 method seeks approximate solutions of (2.16)–(2.17) by solving systems of equations associated with only the diagonal blocks. In the first iteration, the method alternates between the following equations to find $v_1$ and $w_1$:

$$
\begin{bmatrix}
A_w(w_1^{(k-1)}, w_1^{(k-1)}) \\
A_v(v_1^{(k)}, v_1^{(k)})
\end{bmatrix}
\begin{bmatrix}
v_1^{(k)} \\
w_1^{(k)}
\end{bmatrix} =
\begin{bmatrix}
Bw_1^{(k-1)} \\
B^Tv_1^{(k)}
\end{bmatrix}.
$$

In the second iteration, the method alternately solves the systems of equations in the second rows of the following equations:

$$
\begin{bmatrix}
A_w(w_1^{(k-1)}, w_1^{(k-1)}) & A_w(w_2^{(k-1)}, w_2^{(k-1)}) \\
A_v(v_1^{(k)}, v_1^{(k)}) & A_v(v_2^{(k)}, v_2^{(k)})
\end{bmatrix}
\begin{bmatrix}
v_1^{(k)} \\
w_1^{(k)}
\end{bmatrix} =
\begin{bmatrix}
Bw_1^{(k-1)} \\
B^Tv_1^{(k)}
\end{bmatrix}.
$$

Because $v_1$ and $w_1$ are fixed, the $(2,1)$-block matrices are multiplied with $v_1$ and $w_1$ and the resulting vectors are moved to the right-hand sides. Then solving the equations associated with the $(2,2)$-block matrices gives $v_2^{(k)}$ and $w_2^{(k)}$. As illustrated in this example, the S-rank-1 AEM method approximately solves (2.16)–(2.17) by taking the matrices in the lower-triangular blocks to the right-hand sides and solving only the systems associated with the diagonal blocks, as opposed to solving fully coupled systems as in the Stage-$p$ AEM method.

The system matrices that arise in Algorithm 2.1 have reduced factors that are dense but small (of size $p \times p$) and their counterpart factors are large but sparse. In Algorithm 2.2, the system matrices are sparse and of order $n_1$ and $n_2$ (as the reduced factors are of size $1 \times 1$). Thus in both cases, we may use Krylov subspace methods to solve the systems. Then, with the iteration counter $p$, the cost of the Stage-$p$ AEM method grows quadratically (since the reduced factors are dense), whereas that of the S-rank-1 AEM method grows linearly with $p$. Thus, using the Stage-$p$ AEM method can be impractical for large-scale applications. On the other hand, as the S-rank-1 AEM method employs only the lower-triangular part of the system matrices, convergence tends to be slow and the level of accuracy that can be achieved in a small number of steps is limited. To overcome these shortcomings, in the next section, we will consider several ways to modify and enhance them to improve accuracy.

Remark 2.1. The Stage-$p$ AEM and S-rank-1 AEM methods can be seen as two extreme versions of AEM methods. The former solves fully coupled systems and the latter sequentially solves systems associated with the diagonal blocks. Although it has not been explored in this study, in an intermediate approach, more than one consecutive pair of solution vectors $(\{v_p, \ldots, v_{p+\ell}\}, \{w_p, \ldots, w_{p+\ell}\})$, with $\ell \in \mathbb{N}$, can be computed in a coupled manner at each outer iteration.
3. Enhancements. We now describe variants of the S-rank-1 AEM method that perform extra computations to improve accuracy. The general strategy is to compute an enhancement of the approximate solution at every \( n_{\text{update}} \) outer iterations of the S-rank-1 AEM method, as specified in Algorithms 3.1–3.3.

Algorithm 3.1 Enhanced AEM method

\[ \text{INPUT: } p_{\text{max}}, k_{\text{max}}, n_{\text{update}}, \text{ and } \epsilon \]
1: \text{function ENHANCEDAEM}(p_{\text{max}}, k_{\text{max}}, n_{\text{update}}, \epsilon)  
2: \text{for } p = 1, \ldots, p_{\text{max}} \text{ do}  
3: \quad v_p, w_p \leftarrow \text{RANKONECORRECTION}(V_{p-1}, W_{p-1}, k_{\text{max}})  
4: \quad \text{Add to solution matrices, } V_p \leftarrow [V_{p-1}, v_p], W_p \leftarrow [W_{p-1}, w_p]  
5: \quad \text{if } p \mod n_{\text{update}} == 0 \text{ then}  
6: \quad \quad V_p, W_p \leftarrow \text{ENHANCEMENT}(V_p, W_p)  
7: \quad \text{end if}  
8: \quad V_p, W_p \leftarrow \text{CHECKCONVERGENCE}(V_p, W_p, \epsilon)  
9: \text{end for}  
10: \text{end function}

Algorithm 3.2 Rank one correction

\[ \text{INPUT: } V_{p-1}, W_{p-1}, \text{ and } k_{\text{max}} \]
1: \text{function RANKONECORRECTION}(V_{p-1}, W_{p-1}, k_{\text{max}})  
2: \quad \text{Set a random initial guess for } w_p^{(0)}.  
3: \quad \text{for } k = 1, \ldots, k_{\text{max}} \text{ do}  
4: \quad \quad v_p^{(k)} \leftarrow \text{solve (2.14)}  
5: \quad \quad w_p^{(k)} \leftarrow \text{solve (2.15)}  
6: \quad \text{end for}  
7: \quad v_p \leftarrow v_p^{(k)} \text{ and } w_p \leftarrow w_p^{(k)}  
8: \text{end function}

Algorithm 3.3 Checking for convergence

\[ \text{INPUT: } V_p, W_p, \text{ and } \epsilon \]
1: \text{function CHECKCONVERGENCE}(V_p, W_p, \epsilon)  
2: \quad \text{if } \|V_p W_p^T - V_{p-1} W_{p-1}^T\|_F \leq \epsilon \|V_p W_p^T\|_F \text{ then}  
3: \quad V_p, W_p \leftarrow \text{ENHANCEMENT}(V_p, W_p)  
4: \quad \text{if } \|V_p W_p^T - V_{p-1} W_{p-1}^T\|_F \leq \epsilon \|V_p W_p^T\|_F \text{ then} \text{ Stop}  
5: \quad \text{end if}  
6: \text{end if}  
7: \text{end function}

We present three enhancement procedures, one taken from the literature and two new ones. These are (i) a procedure adopted from an updating technique developed in [37, Section 2.5], which defines one variant of PGD methods; (ii) a refined version of this approach, which only solves systems associated with the diagonal blocks of the system matrices but incorporates information (upper-triangular blocks) in a manner similar to Gauss-Seidel iterations; and (iii) an adaptive enhancement of the Stage-\( p \) AEM method that decreases costs with negligible impact on accuracy. In discussing
these ideas, we distinguish updated solutions using the notation, \( \overline{v}_i, \overline{w}_i \) (for vectors), and \( \overline{V}_p = [\overline{v}_1, \ldots, \overline{v}_p], \overline{W}_p = [\overline{w}_1, \ldots, \overline{w}_p] \) (for matrices).

Before we detail each method, we first elaborate on the CheckConvergence procedure in Algorithm 3.3. This checks the relative difference between the current iterate and the previous iterate \( \|V_p W_p^T - V_{p-1} W_{p-1}^T\|_F \leq \varepsilon \|V_p W_p^T\|_F \) in the Frobenius norm.\(^2\) If this condition is met, we apply the Enhancement procedure and check the convergence with the same criterion. The purpose of this extra enhancement is to help prevent Algorithm 3.1 from terminating prematurely (i.e., the stopping condition can be met when Algorithm 3.1 stagnates.).

### 3.1. PGD-updated AEM

Suppose the factors \( V_p \) and \( W_p \) obtained from RankOneCorrection do not satisfy the first-order optimality conditions (2.6)–(2.7). An enhancement like that of the PGD update \([26, 27, 37]\) modifies one of these factors (e.g., the one corresponding to the smaller dimension \( n_1 \) or \( n_2 \)) by solving the associated minimization problem for \( V_p \) (given \( W_p \), when \( n_1 < n_2 \)) or for \( W_p \) (given \( V_p \) when \( n_1 > n_2 \)) so that one of the first-order conditions holds. We outline the procedure for approximating \( W_p \); the procedure for \( V_p \) is analogous. The basic procedure is to solve the optimization problem \( \min_{W_p \in \mathbb{R}^{n_2 \times p}} J_A(V_p, W_p) \) every \( n_{\text{update}} \) steps. In place of \( V_p \), an orthonormal matrix \( \tilde{V}_p \) is used, so that the construction entails solving
\[
\overline{W}_p = \arg \min_{W_p \in \mathbb{R}^{n_2 \times p}} J_A(\tilde{V}_p, W_p),
\]
where \( J_A \) is the quadratic objective function defined in (2.2). The gradient of the objective function \( J_A \) with respect to \( W_p \) can be computed as
\[
\nabla_{W_p} J_A = \left( A(\tilde{V}_p W_p^T) - B \right)^T \tilde{V}_p = \sum_{i=0}^{m} (K_i \tilde{V}_p W_p^T G_i^T)^T \tilde{V}_p - B^T \tilde{V}_p.
\]
Thus, solving the minimization problem (3.1) by employing the first-order optimality condition is equivalent to solving a system of equations similar in structure to (2.7),
\[
\sum_{i=0}^{m} (\tilde{V}_p^T K_i \tilde{V}_p) \overline{W}_p^T (G_i^T) = \tilde{V}_p^T B \in \mathbb{R}^{p \times n_2}.
\]

Compared to the original system (1.2), the dimension of this matrix is reduced via a “single-sided” reduction; in (3.2), the reduction is on the side of the first dimension, i.e., \( n_1 \) is reduced to \( p \). The vectorized form of this system, for \( p = 2 \), is
\[
\begin{bmatrix}
A_v(\tilde{v}_1, \tilde{v}_1) & A_v(\tilde{v}_1, \tilde{v}_2) \\
A_v(\tilde{v}_2, \tilde{v}_1) & A_v(\tilde{v}_2, \tilde{v}_2)
\end{bmatrix}
\begin{bmatrix}
\overline{w}_1 \\
\overline{w}_2
\end{bmatrix}
= \begin{bmatrix}
B^T \tilde{v}_1 \\
B^T \tilde{v}_2
\end{bmatrix},
\]
which has structure like that of the second system in (2.18) of the Stage-\( p \) AEM method. We summarize this single-sided enhancement method in Algorithm 3.4.

**Remark 3.1.** Another approach for computing a set of orthonormal basis vectors and computing a low-rank solution by solving a reduced system of type (3.2) is given in [31]. The MultiRB method of [31] incrementally computes a set of orthonormal basis vectors for the spatial part of the solution (i.e., \( \tilde{V}_p \in \mathbb{R}^{n_1 \times p} \)) using rational Krylov subspace methods and solves a reduced system for \( \overline{W}_p \) and, consequently, \( U_p = \tilde{V}_p \overline{W}_p^T \).

\(^2\)To compute \( \|V_p W_p^T\|_F^2 \), we form \( X = (V_p^T V_p) \odot (W_p^T W_p) \in \mathbb{R}^{p \times p} \), where \( \odot \) is the Hadamard product, and then sum-up all the elements of \( X \). The product \( V_p W_p^T \) is never explicitly formed.
Algorithm 3.4 PGD-update enhancement

| Input: \( V_p \) and \( W_p \) |
|---|
| 1: function PGDupdate \((V_p, W_p)\) |
| 2: if \( n_1 < n_2 \) then |
| 3: \( W_p \leftarrow \) orthonormalize \( W_p \). |
| 4: \( \tilde{V}_p \leftarrow \) solve \( \sum_{i=0}^{m} (K_i \tilde{V}_p (\tilde{W}_p^T G_i \tilde{W}_p))^T = B \tilde{W}_p \) |
| 5: \( V_p \leftarrow \tilde{V}_p \) |
| 6: else |
| 7: \( \tilde{V}_p \leftarrow \) orthonormalize \( V_p \). |
| 8: \( \tilde{W}_p \leftarrow \) solve \( \sum_{i=0}^{m} (\tilde{V}_p^T K_i \tilde{V}_p) \tilde{W}_p^T (G_i^T) = \tilde{V}_p^T B \) |
| 9: \( W_p \leftarrow \tilde{W}_p \) |
| 10: end if |
| 11: end function |

Algorithm 3.5 PGD/GS enhancement

| Input: \( V_p \) and \( W_p \) |
|---|
| 1: function PGD/GS \((V_p, W_p)\) |
| 2: for \( l = 1, \ldots, p \) do |
| 3: \( \tilde{v}_l \leftarrow \) solution of equation (3.3) |
| 4: \( \tilde{w}_l \leftarrow \) solution of equation (3.4) |
| 5: end for |
| 6: \( V_p \leftarrow \tilde{V}_p, W_p \leftarrow \tilde{W}_p \) |
| 7: end function |

3.2. PGD/Gauss–Seidel-updated AEM. The second strategy for enhancement, like the “unenhanced” S-rank-1 AEM method (and in contrast to PGD-updated AEM), only requires solutions of linear systems with coefficient matrices of dimensions \( n_1 \times n_1 \) and \( n_2 \times n_2 \), independent of \( p \). As observed in Section 2.4, the S-rank-1 AEM method loosely corresponds to solving lower block-triangular systems of equations. We modify these computations by using more information (from the upper triangular part), as soon as it becomes available. This leads to a method that resembles the (block) Gauss–Seidel method for linear systems [12]. Suppose \( \{(v_i, w_i)\}_{i=1}^{p} \) are obtained from \( p \) iterations of Algorithm 3.1. When the condition on line 5 of Algorithm 3.1 is met, these quantities will be updated in sequence to produce \( \{(\tilde{v}_l, \tilde{w}_l)\}_{l=1}^{p} \) using the most recently computed quantities. In particular, suppose the updated pairs \( \{(\tilde{v}_i, \tilde{w}_i)\}_{i=1}^{p} \) have been computed. Then the \( l \)th pair \((v_l, w_l)\) is updated as follows. First, given \( w_l \), the update \( \tilde{v}_l \) is computed by solving

\[
A_w(w_l, w_l)\tilde{v}_l = Bw_l - \sum_{i=1}^{l-1} A_w(w_l, \tilde{w}_i)\tilde{v}_i - \sum_{i=l+1}^{p} A_w(w_l, w_i)v_i.
\]

Then given \( \tilde{v}_l, \tilde{w}_l \) is computed by solving

\[
A_s(\tilde{v}_l, \tilde{w}_l)\tilde{w}_l = B^T \tilde{v}_l - \sum_{i=1}^{l-1} A_s(\tilde{v}_l, \tilde{v}_i)\tilde{w}_i - \sum_{i=l+1}^{p} A_s(\tilde{v}_l, v_i)w_i.
\]

With \( p = 2 \) as an example, in vector format, the first step of this enhancement is
to update \((v_1, w_1)\) to \((\overline{v}_1, \overline{w}_1)\) by solving the following equations:

\[
\begin{bmatrix}
A_w(w_1, w_1) & A_w(w_1, w_2) \\
A_v(\overline{v}_1, \overline{v}_1) & A_v(\overline{v}_1, \overline{v}_2)
\end{bmatrix}
\begin{bmatrix}
\overline{v}_1 \\
\overline{v}_2
\end{bmatrix} =
\begin{bmatrix}
Bw_1 \\
B\overline{v}_1
\end{bmatrix},
\]

and the second step is to update \((v_2, w_2)\) to \((\overline{v}_2, \overline{w}_2)\) by solving the second row of the following equations:

\[
\begin{bmatrix}
A_w(w_1, w_1) & A_w(w_1, w_2) \\
A_w(w_2, w_1) & A_w(w_2, w_2) \\
A_v(\overline{v}_1, \overline{v}_1) & A_v(\overline{v}_1, \overline{v}_2) \\
A_v(\overline{v}_2, \overline{v}_1) & A_v(\overline{v}_2, \overline{v}_2)
\end{bmatrix}
\begin{bmatrix}
\overline{v}_1 \\
\overline{v}_2
\end{bmatrix} =
\begin{bmatrix}
Bw_1 \\
B\overline{v}_1 \\
Bw_2 \\
B\overline{v}_2
\end{bmatrix}.
\]

This strategy, which we call the PGD/GS enhancement, is summarized in Algorithm 3.5. It is an alternative to Algorithm 3.4 and is also applied every \(n_{\text{update}}\) outer iterations. For a comparison of Algorithms 3.4 and 3.5, note that Algorithm 3.4 (PGD-update) works with a larger system but it can exploit the matricized representation (3.2). Once the system matrices \(G_i = \tilde{W}_p^TG_i\tilde{W}_p\) or \(K_i = \tilde{V}_p^TK_i\tilde{V}_p\) are formed, if it is not too large, the system in (3.2) (of order \(n_{2p}\) in this example) can be solved using a single application of an iterative method such as the preconditioned conjugate gradient (PCG) method. In contrast, Algorithm 3.5 (PGD/GS) requires sequential updates of individual components in equations (3.3)-(3.4), but with smaller blocks, of order \(n_1\) and \(n_2\). As we will show in Section 4, the PGD/GS-updated AEM method exhibits better performance in some error measures.

We have found that in practice, the enhancement procedure can be improved by updating only a chosen subset of solution pairs rather than all the solution pairs \(\{(v_i, w_i)\}_{i=1}^p\). We discuss a criterion to choose such a subset next.

### 3.3. Reduced stage-\(p\) AEM method

The third enhancement procedure excerpt of and modifies certain computations in the Stage-\(p\) AEM method (Lines 5 and 6 in Algorithm 2.1) in a computationally efficient way. The procedure adaptively chooses solution pairs to be updated and solves reduced systems to update only those pairs. Let us assume for now that a subset of the solution pairs to be updated has been chosen. Denote the set of indices of those solution pairs by \(\ell(p) \subseteq \{1, \ldots, p - 1\} \setminus \ell(p)\). Then the update is performed by solving the following equations for \(\overline{V}_{\ell(p)}\) and \(\overline{W}_{\ell(p)}\):

\[
\sum_{i=0}^{m}(K_i)\overline{V}_{\ell(p)}(\tilde{W}_{\ell(p)}^TG_i\tilde{W}_{\ell(p)})^T = B\tilde{W}_{\ell(p)} - \sum_{i=0}^{m}(K_i)V_{\ell'(p)}(\tilde{W}_{\ell(p)}^TG_iW_{\ell'(p)})^T,
\]

where \(\tilde{W}_{\ell(p)}\) is obtained by orthonormalizing the columns of \(W_{\ell(p)}\), and

\[
\sum_{i=0}^{m}(\tilde{V}_{\ell(p)}^TK_i\tilde{V}_{\ell(p)})\overline{W}_{\ell(p)}(G_i^T) = \tilde{V}_{\ell(p)}^TB - \sum_{i=0}^{m}(\tilde{V}_{\ell(p)}^TK_iV_{\ell'(p)})W_{\ell'(p)}(G_i^T),
\]

where \(\tilde{V}_{\ell(p)}\) is obtained by orthonormalizing the columns of \(V_{\ell(p)}\). Then, \(V_{\ell(p)}\) and \(W_{\ell(p)}\) are updated to \(\overline{V}_{\ell(p)}\) and \(\overline{W}_{\ell(p)}\), while \(V_{\ell'(p)}\) and \(W_{\ell'(p)}\) remain the same.
Let \( (Ω, F, P) \) be a probability space and let \( D = [0, 1] \times [0, 1] \) be the spatial domain. Next, let \( ξ_i : Ω → Γ_i ⊂ R, \) for \( i = 1, \ldots, m, \) be independent and identically distributed random variables and define \( ξ = [ξ_1, \ldots, ξ_m]. \) Then, \( ξ : Ω → Γ \) where \( Γ = \prod_{i=1}^{m} Γ_i \) denotes the image. Given a second-order random field \( a : D × Γ → R, \) we consider the following boundary value problem with constant forcing term \( f(x) = 1. \) Find \( u : D × Γ → R \) such that

\[
\begin{align*}
-\nabla \cdot (a(x, ξ) \nabla u(x, ξ)) &= f(x) & \text{in } D × Γ, \\
u(x, ξ) &= 0 & \text{on } ∂D × Γ.
\end{align*}
\]

### 4. Numerical experiments

In this section, we present the results of numerical experiments with the algorithms described in Sections 2 and 3. For benchmark problems, we consider stochastic diffusion problems, where the stochasticity is assumed to be characterized by a prescribed set of real-valued random variables. We apply suitable stochastic Galerkin finite element discretizations to these problems, which results in linear multi-term matrix equations of the form (1.2) whose system matrices are symmetric positive-definite. All numerical experiments are performed on an INTEL 3.1 GHz i7 CPU, with 16 GB RAM, using MATLAB R2019b.

#### 4.1. Stochastic Diffusion Problems

Let \( (Ω, F, P) \) be a probability space and let \( D = [0, 1] \times [0, 1] \) be the spatial domain. Next, let \( ξ_i : Ω → Γ_i ⊂ R, \) for \( i = 1, \ldots, m, \) be independent and identically distributed random variables and define \( ξ = [ξ_1, \ldots, ξ_m]. \) Then, \( ξ : Ω → Γ \) where \( Γ = \prod_{i=1}^{m} Γ_i \) denotes the image. Given a second-order random field \( a : D × Γ → R, \) we consider the following boundary value problem with constant forcing term \( f(x) = 1. \) Find \( u : D × Γ → R \) such that

\[
\begin{align*}
-\nabla \cdot (a(x, ξ) \nabla u(x, ξ)) &= f(x) & \text{in } D × Γ, \\
u(x, ξ) &= 0 & \text{on } ∂D × Γ.
\end{align*}
\]

### Algorithm 3.6 Reduced stage-\( p \) enhancement

**Input:** \( V_p, W_p, \) and \( τ \)

1. **function** Rstagep\((V_p, W_p, τ)\)
2.   Normalize the columns: \( \tilde{v}_i = \frac{v_i}{∥v_i∥_2}, \tilde{w}_i = \frac{w_i}{∥w_i∥_2} \) for \( i = 1, \ldots, p \)
3.   Compute \( β_V = \tilde{V}^T_{p-1} \tilde{v}_p, β_W = \tilde{W}^T_{p-1} \tilde{w}_p \)
4.   Select \( ℓ(p) = \{i ∈ \{1, \ldots, p-1\} | ||β_V||_i > τ \text{ or } ||β_W||_i > τ\} \)
5.   \( \hat{W}ℓ(p) ← \text{orthonormalize } Wℓ(p)\)
6.   \( \hat{V}ℓ(p) ← \text{solve (3.5)}\)
7.   \( \hat{V}ℓ(p) ← \text{orthonormalize } Vℓ(p)\)
8.   \( Wℓ(p) ← \text{solve (3.6)}\)
9.   \( Vℓ(p) = \hat{V}ℓ(p), Wℓ(p) = \hat{W}ℓ(p)\)
10. **end function**
In particular, we will assume that the input random field $a(x, \xi)$ has the affine form

$$
(4.2) \quad a(x, \xi) = a_0(x) + \sum_{i=1}^{m} a_i(x)\xi_i,
$$

which has the same structure as a truncated Karhunen-Loève (KL) expansion [24], and we will choose the $\xi_i$ to be independent uniform random variables. Recall that if we denote the joint probability density function of $\xi$ by $\rho(\xi)$ then the expected value of a random function $v(\xi)$ on $\Gamma$ is $\langle v \rangle_{\rho} = \int_{\Gamma} v(\xi) \rho(\xi) d\xi$.

For the discretization, we consider the stochastic Galerkin method [1, 11, 25, 38], which seeks an approximation to the solution of the following weak formulation of (4.1): Find $u(x, \xi) \in V = H^1_0(D) \otimes L^2_{\rho}(\Gamma)$ such that

$$
(4.3) \quad \left\langle \int_{D} a(x, \xi) \nabla u(x, \xi) \cdot \nabla v(x, \xi) dx \right\rangle_{\rho} = \left\langle \int_{D} f(x)v(x, \xi)dx \right\rangle_{\rho}, \quad \forall v \in V.
$$

In particular, we seek a finite-dimensional approximation of the solution of the form

$$
\tilde{u}(x, \xi) = \sum_{s=1}^{n_s} \sum_{i=1}^{n_{x,s}} u_{\rho,s}(x) \psi_s(\xi),
$$

where $\{\phi_i\}_{i=1}^{n_{x,s}}$ is a set of standard finite element basis functions, which arises from using continuous piecewise bilinear approximation on a uniform mesh of square elements (Q1 elements\(^3\)) and $n_x$ is related to the refinement level of the spatial mesh. In addition, $\{\psi_s\}_{s=1}^{n_s}$ is chosen to be a finite subset of the set of orthonormal polynomials that provides a basis for $L^2_{\rho}(\Gamma)$ (also known as a generalized polynomial chaos (gPC) [39]). As the random variables are uniformly distributed, we use $m$-variate normalized Legendre polynomials $\{\psi_s(x)\}_{s=1}^{n_s}$, which are constructed as products of univariate Legendre polynomials, $\psi_s(\xi) = \prod_{i=1}^{m} \pi_{d_i(s)}(\xi_i)$. Here, $d(s) = (d_1(s), \ldots, d_m(s))$ is a multi-index and $\pi_{d_i(s)}$ is the $d_i(s)$-order univariate Legendre polynomial in $\xi_i$. A set of multi-indices $\{d(s)\}_{s=1}^{n_s}$ is specified as a set $\Lambda_{m,d_{\text{tot}}} = \{d(s) \in \mathbb{N}_0^m : \|d(s)\|_1 \leq d_{\text{tot}}\}$, where $\mathbb{N}_0$ is the set of non-negative integers, $\|d(s)\|_1 = \sum_{j=1}^{m} d_j(s)$, and $d_{\text{tot}}$ defines the maximal degree of $\{\psi_s(\xi)\}_{s=1}^{n_s}$. With this setting, the number of gPC basis functions is $n_s = \dim(\Lambda_{m,d_{\text{tot}}}) = (m + d_{\text{tot}})! / m!d_{\text{tot}}!$.

Employing a Galerkin projection to (4.3) onto the chosen finite-dimensional space (i.e., using the same test basis functions as the trial basis functions) and ordering the coefficients of the solution expansion as $u = [u_1, \ldots, u_{n_1}, u_{12}, \ldots, u_{n_1n_2}]^T$ results in

$$
(4.4) \quad \left( \sum_{i=0}^{m} G_i \otimes K_i \right) u = g_0 \otimes f_0,
$$

where the system matrices are defined as

$$
[G_0]_{st} = \langle \psi_s(\xi) \psi_t(\xi) \rangle_{\rho}, \quad [K_0]_{kt} = \int_{D} a_0(x) \nabla \phi_k(x) \cdot \nabla \phi_t(x) dx,
$$

$$
[G_i]_{st} = \langle \psi_s(\xi) \psi_t(\xi) \rangle_{\rho}, \quad [K_i]_{kt} = \int_{D} a_i(x) \nabla \phi_k(x) \cdot \nabla \phi_t(x) dx,
$$

for $i = 1, \ldots, m$, $s, t = 1, \ldots, n_s$ and $k, \ell = 1, \ldots, n_x$. Due to the deterministic forcing term $f(x) \equiv 1$, the right-hand side has a rank-one structure (i.e., $r = 0$ in (1.1)), with $[f_0]_k = \int_{D} f(x) \phi_k(x) dx$, and $[g_0]_s = \langle \psi_s(\xi) \rangle_{\rho}$. Matricizing (4.4) gives the multi-term matrix equation as shown in (1.2) with $n_1 = n_x$ and $n_2 = n_s$, and now we can apply the AEM methods to compute an approximate solution of the equation.

\(^{3}\text{Our implementation uses the Incompressible Flow & Iterative Solver Software (IFISS) [10, 35].}\)
4.2. Benchmark problem 1: separable exponential covariance. In this problem, we assume that the random field $a(x, \xi)$ is a truncated KL expansion

$$a(x, \xi) = \mu + \sigma \sum_{i=1}^{m} \sqrt{\lambda_i} \varphi_i(x) \xi_i,$$

where $\mu$ is the mean of $a(x, \xi)$, $\{(\varphi_i(x), \lambda_i)\}_{i=1}^{m}$ are eigenpairs of the integral operator associated with the separable covariance kernel $C(x, y) \equiv \exp\left(-\frac{|x_1-y_1|}{c} - \frac{|x_2-y_2|}{c}\right)$, $c$ is the associated correlation length, and $\sigma^2$ is the variance of the untruncated random field. In addition, each $\xi_i \sim U(-\sqrt{3}, \sqrt{3})$ and so has mean zero and variance one.

In the following sections, we compare the five AEM variants, Stage-$p$ (Algorithm 2.1), S-rank-1 (Algorithm 2.2), PGD-updated (Algorithm 3.4), PGD/GS-updated (Algorithm 3.5), and reduced stage-$p$ (Algorithm 3.6). For orthonormalization in PGD-updated (Algorithm 3.4) and reduced stage-$p$ (Algorithm 3.6), we use MATLAB’s qr function. For assessing performances, we explore two key aspects. The first is the accuracy of the computed solutions, which we assess by computing two error metrics: cosines of angles between the truth singular vectors and the columns of the computed factors (Section 4.2.1), and errors between the truth solution and the computed solution measured in three different norms (Section 4.2.2). The second aspect is timings and scalability (Section 4.2.3). As the assessment of the first aspect requires the ground truth solution of (4.4), which is computed using MATLAB’s backslash operator, and its singular vectors, we choose small-sized problems in Sections 4.2.1–4.2.2. When making comparisons with the truth solution, we set the maximum number of outer iterations for all the AEM methods to be $p_{\text{max}} = \min(n_x, n_{\xi}) = 56$. Larger problems are considered in Section 4.2.3, where scalability matters and finding the truth solution is impossible with the available resources.

4.2.1. Relation to singular vectors. We begin by exploring how the factors in the approximate solutions constructed by each of the methods compare with the left and right singular vectors of the true solution matrix $U$. This is important because (i) singular vectors represent the most effective choice with respect to the Frobenius norm for approximating a matrix $U$. That is, the minimum error over all rank-$p$ approximations is $\|U - \hat{V}_p \Sigma_p \hat{W}_p^T\|_F$, where $U = V \Sigma W^T$ is the singular value decomposition [7], and (ii) in some applications such as collaborative filtering for recommendation systems, computing singular vectors accurately is very important for precise predictions [16, 17, 40]. For these tests, the diffusion coefficient is given by (4.5) with $(\mu, \sigma) = (1, 1)$ and $c = 2$. We use a spatial discretization with grid level 4 (i.e., grid spacing $\frac{1}{4}$, and $n_x = 225$) and we truncate the expansion (4.5) at $m = 5$. For the stochastic Galerkin approximation, we choose $d_{\text{tot}} = 3$ which gives $n_{\xi} = 56$.

For any approximation of the form (1.3), let $\hat{V}_p$ and $\hat{W}_p$ be normalized versions of the factors, i.e., each column of $\hat{V}_p$ and $\hat{W}_p$ is scaled to have unit norm. From the ground truth solution $U$, the matrices $V^*$ and $W^*$ of left and right singular vectors are computed. The entries of $V^* \hat{V}_p^T$, the cosines of the angles between the left singular vectors of the true solution and the left vectors defining the approximate solution, together with the analogous angles for the right vectors, $W^* \hat{W}_p^T$, give insight into the quality of the approximate solution. Figures 1a and 1f and Figures 1b and 1g depict the cosines of the angles between the singular vectors and the columns of $\hat{V}_p$ and $\hat{W}_p$ computed using the Stage-$p$ AEM and S-rank-1 AEM methods discussed in Section 2. It can be seen from these results (in Figures 1a and 1f) that the Stage-$p$ AEM method does a good job of approximating the singular vectors of the solution.
Fig. 1. Cosines of angles (plotted in log scale) between the left singular vectors $V^*$ and $\tilde{V}_p$, and the right singular vectors $W^*$ and $\tilde{W}_p$, where $V_p$ and $W_p$ are computed using the Stage-$p$ and S-rank-$1$ AEM methods, and the EnhancedAEM methods with PGD-update, PGD/GS, and R-stage-$p$ enhancements.

That is, the values of the diagonal entries are close to one and the values of the off-diagonal entries are close to zero. On the other hand, the S-rank-$1$ AEM method (see Figures 1b and 1g) is far less effective. The $2 \times 2$ blocks on the diagonals in Figures
1a and 1f reflect the presence of equal singular values.

Figures 1c–1e and 1h–1j show analogous results for EnhancedAEM with PGD-update (Algorithm 3.4), PGD/GS (Algorithm 3.5), and R-stage-p (Algorithm 3.6). Since we attempt to see each method’s best possible results without considering the computational costs, we set $k_{\text{max}} = 5$ and $n_{\text{update}} = 1$ (i.e., enhancements are performed at every outer iteration) in Algorithm 3.1. For the same reason, we set PGD/GS to update all the solution pairs and, for R-stage-p, we set $\tau = .001$. With PGD-update, the spatial component gets reduced (i.e., we form $\tilde{K}_i = \tilde{V}_p^T K_i \tilde{V}_p$) and $W_p$ is updated. Figures 1c and 1h show that this computation improves the quality of the resulting factor $W_p$ (and $V_p$ as well) as approximate singular vectors, compared to those obtained with the S-rank-1 method. It is evident that PGD/GS further improves the quality of $\tilde{V}_p$ and $\tilde{W}_p$ (Figures 1d and 1i) as approximate singular vectors, and R-stage-p is nearly as effective as the Stage-p AEM approach (Figures 1e and 1j).

### 4.2.2. Assessment of solution accuracy

We now compare the convergence behavior of the variants of the AEM methods introduced in Sections 2 and 3. We use two different settings for the stochastic diffusion coefficient: $[\exp1] (\mu, \sigma) = (1, .1), c = 2$ and $[\exp2] (\mu, \sigma) = (1, .2), c = .5$. We again truncate the series (4.5) at $m = 5$ and, for the Legendre basis polynomials, we consider $d_{\text{tot}} = 3$ which gives $\eta_5 \approx 56$. We deliberately keep the same value for $m$ and $d_{\text{tot}}$ for both settings so that we can keep the dimensions of the problem the same and, thus, directly compare the behavior of each method in different problem settings. We also use the same parameters for the EnhancedAEM methods as before (i.e., $k_{\text{max}} = 5$, $n_{\text{update}} = 1$, and $\tau = .001$).

For each method, the approximate solution $U_p$ is computed and we measure the accuracy compared to the reference solution $U$. We did this using three different metrics: the energy norm error $\|U - U_p\|_A$, the error in the Frobenius norm $\|U - U_p\|_F$, and the residual in the Frobenius norm $\|B - A(U_p)\|_F$. Here, we only report the energy norm errors (in Figure 2), as behavior for the other two metrics is virtually identical.

For comparison, a rank-$p$ reference solution (referred to as “full” in Figure 2) is also obtained directly from the first $p$ singular values and singular vectors of $U$.

For both settings, as expected, the convergence behavior of the S-rank-1 AEM method is significantly worse than that of the rank-$p$ reference solution, whereas that of the Stage-$p$ AEM method is virtually the same as for the full direct solver.
The EnhancedAEM method with PGD-update converges well until a certain level of accuracy is achieved, but it fails to achieve a high level of accuracy. In both experiments, the EnhancedAEM methods with PGD/GS and R-stage-\(p\) are more effective than with the PGD-update. The accuracy that those two methods achieve is virtually the same as that of the Stage-\(p\) AEM method and the full direct solver.

4.2.3. Computational timings. The above results do not account for computational costs; we now investigate timings under various experimental settings. This is important for large-scale applications, and so we now consider a finer spatial grid, with grid level 6 (i.e., grid spacing \(\frac{1}{2^n}\), and \(n_x = 3969\)), as well as larger parameter spaces, with \(m = \{20, 24\}\) (the number of random variables in (4.5)) and \(d_{tot} = 4\), which results in \(n_\xi = \{10626, 20475\}\). We use the same settings for the stochastic diffusion coefficient [exp1] \((\mu, \sigma) = (1, 1.1), c = 2\) and [exp2] \((\mu, \sigma) = (1, 2), c = .5\). Again, we set \(m\) and \(d_{tot}\) to be the same for both problems, as we want to keep the dimensions fixed so that we can make direct and fair comparisons.

Before we present these results, we summarize the systems of equations to be solved for each of the EnhancedAEM methods and the adjustable parameters that affect the performances of the methods.\(^4\) We first describe how we solve the systems arising at the \(p\)th outer iteration when the condition for applying the enhancement is met, as well as the systems arising in RANKONECORRECTION (Algorithm 3.2). We use PCG to solve each system of equations using mean-based preconditioners [30], where \(X\) is a quantity to be updated, \(\bar{K}_i\) and \(\bar{G}_i\) are reduced matrices, and \(M_x\) and \(M_{\xi}\) are the preconditioner factors. Table 1 summarizes each system matrix and preconditioner.\(^5\)

\footnotesize
\begin{table}[h]
\centering
\caption{System matrices and preconditioners for each Enhancement procedure}
\begin{tabular}{|c|c|c|c|c|c|c|}
\hline
Name & \(X\) & \(K_i\) & \(G_i\) & \(M_x\) & \(M_{\xi}\) & Eqs \\
\hline
S-rank-1 & \(v_p\) & \(K_i\) & \(w_p^T G_i w_p\) & \(K_0\) & 1 & (2.14) \\
(Alg. 3.2) & & & & & & (2.15) \\
PGD-update & \(V_p\) & \(K_i\) & \(W_p^T G_i W_p\) & \(K_0\) & \(W_p^T G_0 W_p\) & (3.2) \\
(Alg. 3.4) & & & & & & (3.3) \\
PGD/GS & \(V_{i(p)}\) & \(K_i\) & \(w_i^T G_i w_i\) & \(K_0\) & 1 & (3.4) \\
(Alg. 3.5) & & & & & & (3.5) \\
R-stage-\(p\) & \(V_{i(p)}\) & \(K_i\) & \(W_{i(p)}^T G_i W_{i(p)}\) & \(K_0\) & \(W_{i(p)}^T G_0 W_{i(p)}\) & (3.6) \\
(Alg. 3.6) & & & & & & \\
\hline
\end{tabular}
\end{table}

\(^4\)The results of using the Stage-\(p\) and S-rank-1 AEM methods are not reported because the Stage-\(p\) AEM method is computationally too expensive and the S-rank-1 AEM method exhibits poor convergence behavior and, indeed, fails to satisfy the given convergence criterion.

\(^5\)Note that, for PGD-update, one can always choose the smallest solution component to update. In practice, however, updating the \(W_p\) component (i.e., reduction in \(\{K_i\}_{i=0}^m\)) always requires the smallest computational costs and, thus, we only report the result of updating \(W_p\).
Now, we discuss adjustable parameters. The EnhancedAEM methods (Algorithms 3.1–3.3) require parameters $p_{\text{max}}$, $k_{\text{max}}$, $n_{\text{update}}$, and $\epsilon$. We set $p_{\text{max}} = 1000$ to prevent excessive computations. We found that choosing $k_{\text{max}} > 2$ results in negligible difference in accuracy, but requires extra computations and, thus, we use $k_{\text{max}} = \{1, 2\}$. For $n_{\text{update}}$, which determines how often the enhancement procedure is called, we vary $n_{\text{update}}$ as $\{5, 10, 20, 30\}$. Next, we use $\epsilon$ to check the convergence (as in Algorithm 3.3), and we vary $\epsilon$ as $\{10^{-10}, 10^{-9}, 10^{-8}, 10^{-7}\}$. Finally, for PGD/GS and R-stage-$p$, we empirically found that choosing $\tau > 0.05$ results in decreased accuracy in the approximate solution and, thus, we set $\tau = 0.05$.

Next, we set parameters for the PCG method. For all systems, the stopping criterion uses the relative residual in the Frobenius norm. We use two different tolerances: $\tau_{\text{basis}}$ for solving systems that arise in RankOneCorrection and PGD/GS, and $\tau_{\text{coupled}}$ for solving systems that arise in PGD-update and R-stage-$p$. We choose the values of $\tau_{\text{basis}}$ and $\tau_{\text{coupled}}$ based on results of preliminary numerical experiments with the EnhancedAEM methods for $(\tau_{\text{basis}}, \tau_{\text{coupled}}) = \{10^{-8}, 10^{-7}, 10^{-6}, 10^{-5}\}$: (i) setting $\tau_{\text{basis}} < 10^{-5}$ does not result in improved accuracy of approximate solutions and, thus, we set $\tau_{\text{basis}} = 10^{-5}$, and (ii) for a given outer iteration tolerance $\epsilon$, having too mild PCG tolerance $\tau_{\text{coupled}} > 10^2\epsilon$ results in poor performance and having stringent tolerance $\tau_{\text{coupled}} < 10^2\epsilon$ results in negligible difference in accuracy; thus, we use $\tau_{\text{coupled}} = 10^2\epsilon$. Table 2 summarizes the parameters used for the experiments.

| Parameter | Value |
|-----------|-------|
| $p_{\text{max}}$ | 1000 |
| $k_{\text{max}}$ | $\{1, 2\}$ |
| $n_{\text{update}}$ | $\{5, 10, 20, 30\}$ |
| $\epsilon$ | $\{10^{-10}, 10^{-9}, 10^{-8}, 10^{-7}\}$ |
| $\tau_{\text{basis}}$ | $10^{-5}$ |
| $\tau_{\text{coupled}}$ | $10^2\epsilon$ |

In Figure 3, we plot elapsed time (in seconds) against relative residual error for both [exp1] and [exp2]. Note that the relative residual is computed afterwards in a post-processing step. Recall that the stopping condition for the outer iteration (see Algorithm 3.3) is not based on the relative residual (as this is expensive to compute). The values of $\epsilon$ used for the stopping test for these results (see Algorithm 3.3) are shown in the figure. Note that for these experiments, the relative residual error is approximately three orders of magnitude larger than $\epsilon$. Results obtained with the EnhancedAEM methods with PGD-update, PGD/GS, and R-stage-$p$ are marked in red, green, and blue, respectively, and each configuration of $n_{\text{update}}$ and $k_{\text{max}}$ is marked with a different symbol. It can be seen from the figures that

- the costs of R-stage-$p$ and PGD/GS are less sensitive to $n_{\text{update}}$ and $k_{\text{max}}$ than those of PGD-update;
- R-stage-$p$ is more efficient for smaller values of $n_{\text{update}}$ whereas PGD/GS and PGD-update are better with larger $n_{\text{update}}$;
- for PGD-update and PGD/GS, relatively large $n_{\text{update}} > 10$ and $k_{\text{max}} = 2$ results in better performances, and, for R-stage-$p$, relatively small $n_{\text{update}} \leq 10$ and $k_{\text{max}} = 1$ results in better performances.

Table 3 reports the number of outer iterations $p$ required to achieve the stopping tolerance $\epsilon$ for problems [exp1] and [exp2] when PGD-update, PGD/GS, and R-stage-$p$
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Fig. 3. Computational timings (in seconds) of three EnhancedAEM methods for varying $k_{\text{max}}$ and $n_{\text{update}}$. Timings of each method with each parameter set-up are averaged over 5 testing runs.

are used. The benefit of using R-stage-$p$ becomes more pronounced as we seek highly accurate solutions with smaller $\epsilon$. Our general observation is that among the three enhancement approaches, the R-stage-$p$ method is less sensitive to choice of algorithm parameter inputs, scales better for larger problem sizes, and is the most effective of the three approaches.

We now briefly consider a second benchmark problem whose solution matrix has different rank characteristics and for which low-rank solvers ought to perform well.
Table 3

The number of outer iterations \( p \) required to achieve the stopping tolerance \( \epsilon \) for solving the problems \([\text{exp}1]\) and \([\text{exp}2]\) when PGD-update, PGD/GS, and R-stage-\( p \) are used. The reported values of \( p \) are computed by averaging values of \( p \) obtained with the eight different combinations of \( n_{\text{update}} \) and \( k_{\text{max}} \) shown in the legend of Figure 3.

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
&m=20&m=24\\
\hline
\epsilon=10^{-7} & 163.8 & 152.9 & 184.9 & 173.0 \\
\epsilon=10^{-8} & 264.6 & 259.5 & 306.6 & 296.7 \\
\epsilon=10^{-9} & 356.3 & 340.1 & 415.0 & 397.3 \\
\epsilon=10^{-10} & 531.1 & 486.0 & 609.4 & 563.9 \\
\hline
\end{array}
\]

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
&m=20&m=24\\
\hline
\epsilon=10^{-7} & 293.1 & 282.1 & 344.0 & 330.6 \\
\epsilon=10^{-8} & 414.6 & 397.7 & 492.8 & 478.3 \\
\epsilon=10^{-9} & 569.8 & 511.6 & 673.7 & 616.7 \\
\epsilon=10^{-10} & 821.6 & 677.1 & 933.1 & 810.1 \\
\hline
\end{array}
\]

4.3. Benchmark problem 2: fast decay coefficients. We define the random field \( a(x, \xi) \) as in (4.2) but now we choose \( \xi_i \sim U(-1, 1) \) and the functions \( a_i(x) \) have coefficients that decay more rapidly than in the first benchmark problem. The details of this problem can be found in [8]. Specifically, the coefficients of the expansion are

\[
a_0 = 1, \quad a_i(x) = \alpha_i \cos(2\pi \varrho_1(i)x_1) \cos(2\pi \varrho_2(i)x_2), \quad i = 1, 2, \ldots, m
\]

where \( \alpha_i = \bar{\alpha} i^{-\sigma} \) with \( \sigma > 1 \) and \( \bar{\alpha} \) satisfies \( 0 < \bar{\alpha} < 1/\zeta(\sigma) \), where \( \zeta \) is the Riemann zeta function. Furthermore, \( \varrho_1(i) = i - k(i)(k(i)+1)/2 \) and \( \varrho_2(i) = k(i) - \varrho_1(i) \) where \( k(i) = \lfloor -1/2 + \sqrt{1/4 + 2i} \rfloor \). Our implementation is based on the MATLAB software package S-IFISS [34]. In the following experiment, we choose \( \sigma = 4 \) and \( \bar{\alpha} = 0.832 \). The parameter \( \sigma \) controls the rate of algebraic decay of the coefficients. The specific choice \( \sigma = 4 \) leads to fast decay and this causes the true solution matrix to have a lower rank than in the first benchmark problem.

We investigate computational timings of the EnhancedAEM methods with the same experimental settings used in Section 4.2.3. Here, we vary the stopping tolerance for the outer iterations as \( \epsilon = \{10^{-9}, 10^{-8}, 10^{-7}, 10^{-6}\} \) and we choose the same values of \( n_{\text{update}} \) and \( k_{\text{max}} \) as before. Figure 4 reports elapsed time (in seconds) against relative residual error. In nearly all cases, our observations agree with the findings in Figure 3. However, the impact of \( n_{\text{update}} \) is slightly less clear for these tests. The R-stage-\( p \) method is generally still less sensitive than the other two methods to the choices of \( n_{\text{update}} \) and \( k_{\text{max}} \), with one exception, indicated by the blue triangle marker, which is located to the far right in Figure 4. With \( n_{\text{update}} = 30, k_{\text{max}} = 2, \) and \( \epsilon = 10^{-9} \) (giving the right-most blue triangle), the R-stage-\( p \) method does not meet the stopping criterion until \( p \approx 125 \), which is larger than the value \( p \approx 90 \) needed for the other choices of algorithm inputs. We attribute this to the large number of steps (30) between enhancements; in this case, the method fell just short of the stopping criterion after 90 steps. Finally, we report the number of outer iterations \( p \) required to achieve the stopping tolerance \( \epsilon \) in Table 4. As the true solution matrix has an
intrinsic low-rank structure, the reported values of $p$ are much smaller than those shown in Table 3.

### 4.4. Further Extensions
We also tested all the AEM methods on matrix equations obtained from stochastic Galerkin finite element discretizations of stochastic convection-diffusion problems [23, Section 5.2], where the randomness is in the diffusion coefficient as in Section 4.2. Although the energy norm cannot be defined for this problem because it has a non-symmetric operator, the same projection framework described herein can be applied to compute approximate solutions. Experiments (not reported here) were conducted similar to the ones in Sections 4.2.1–4.2.2. We observed that the proposed R-stage-p method produces qualitatively better approximate factors $V_p$ and $W_p$, as measured in the error metrics used in Sections 4.2.1–4.2.2, than the S-rank-1 AEM method and the other two EnhancedAEM methods.

### 5. Conclusions
In this study, we have investigated several variants of alternating minimization methods to compute low-rank solutions of linear systems that arise from stochastic Galerkin finite element discretizations of parameterized elliptic PDEs. Using a general formulation of alternating energy minimization methods derived from the well-known general projection method, our starting point was a variant of the stagewise ALS method, a technique for building rank-$p$ approximate solutions developed for matrix completion and matrix sensing. Our main contribution

![Fig. 4. Computational timings (in seconds) of three EnhancedAEM methods for varying $k_{\text{max}}$ and $n_{\text{update}}$. Timings of each method with each parameter set-up are averaged over 5 testing runs.](image-url)
consists of a combination of this approach with so-called enhancement procedures of the type used for PGD methods [26, 27] in which rank-one approximate solutions are enhanced by adaptive use of higher-rank quantities that improve solution quality but limit costs by adaptively restricting the rank of updates. Experimental results demonstrate that the proposed PGD/GS and R-stage-p methods produce accurate low-rank approximate solutions built from good approximations of the singular vectors of the matricized parameter-dependent solutions. Moreover, the results show that the R-stage-p method scales better for larger problems, is less sensitive to algorithm inputs, and produces approximate solutions in the fastest times.

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