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The dynamical functional particle method for the generalized Sylvester equation*

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Recent years have seen a renewal of interest in the study of generalized Sylvester equations, which have come to play a role in a number or applications. Here we consider the solution of such equations by means of the dynamical functional particle method, an iterative technique that relies on the construction and numerical integration of a damped second order dynamical system. We develop a new algorithm for the solution of a large class of these equations, a class that includes, among others, all generalized Sylvester equations with Hermitian positive definite coefficients. Our numerical experiments show that the new implementations outperform existing methods for the solution of generalized Sylvester equations, and can be faster and more accurate than the Bartels–Stewart algorithm for the solution of the Sylvester equation AX - XB = C, when A and B are well conditioned and have very different order.

Key words. Generalized Sylvester equation, discrete functional particle method, Sylvester equation, Lyapunov equation, Stein equation.

AMS subject classifications. 15A24, 65F30

1 Introduction

The matrix equation AX + XB = C, where $A \in \mathbb{C}^{m \times m}$, $B \in \mathbb{C}^{n \times n}$, and $X, C \in \mathbb{C}^{m \times n}$, is named after Joseph J. Sylvester, who was the first to investigate the homogeneous case [23]. Many similar equations appear in various branches of science and have been extensively investigated. Here we are interested in numerical algorithms for the solution of the so-called "generalized" Sylvester equation

$$\sum_{i=1}^{\ell} A_i X B_i = C, \qquad A_1, \dots, A_{\ell} \in \mathbb{C}^{m \times m}, \qquad B_1, \dots, B_{\ell} \in \mathbb{C}^{n \times n}, \qquad X, C \in \mathbb{C}^{m \times n}.$$
(1)

Stating conditions for the existence and uniqueness of solutions to (1) in terms of the coefficients A_i and B_i is a difficult problem in the general case, although well-known results are available

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for special cases [19, Ch. 9, 10, and 11]. As suggested by Lancaster [20], by using the Kronecker product one can recast (1) as the $mn \times mn$ linear system

$$M \operatorname{vec}(X) = \operatorname{vec}(C), \qquad M := \sum_{i=1}^{\ell} (B_i^T \otimes A_i),$$
(2)

where $\cdot \otimes \cdot$ and vec denote the Kronecker product and the operator that stacks the columns of a matrix into a column vector, respectively. In the following, we denote by $\operatorname{unvec}_{m,n}$ the operator that reshapes a vector of length mn into an $m \times n$ matrix, so that $\operatorname{unvec}_{m,n}(\operatorname{vec}(X)) = X$ for $X \in \mathbb{C}^{m \times n}$. As it is customary, we will omit the subscript and not specify the dimensions of the reshaped matrix when these are clear from the context. The linear system (2) has a unique solution if and only if $\det M \neq 0$, that is, if the coefficient matrix M is full rank. If $\det M = 0$ then (1) has infinitely many solutions if M has the same rank as the augmented matrix $[M \operatorname{vec}(C)] \in \mathbb{C}^{mn \times (mn+1)}$ and no solution otherwise.

Some special cases of (1) are well known, and have been extensively studied in the literature. The most obvious example is that of a linear system with multiple right-hand sides. Here we will discuss, in particular, the following:

• the two-sided linear equation

$$AXB = C, (3)$$

• the generalized inverse

$$AXA = A, (4)$$

• the continuous-time Lyapunov equation

$$AX + XA^* = C, (5)$$

• the discrete-time Lyapunov equation

$$AXA^* - X = C, (6)$$

• the Sylvester equation

$$AX + XB = C, (7)$$

• the Stein equation

$$AXB + X = C. \tag{8}$$

A couple of decades ago, the generalized equation (1) was considered to be mainly of theoretical interest [17, sect. 16.5]. In recent years, however, it has come to play an important role in a variety of applications [22] such as the numerical study of certain bilinear dynamical systems [2], [12], [16, sect. 2.2], or uncertainty quantification in PDEs with random inputs [7], [8], [21]. In many of these applications, the matrix coefficients show a special structure, and in particular are often Hermitian and positive definite or semi-definite.

Here we adapt the dynamical functional particle method [5] to the numerical solution of (1). The algorithm we develop requires the eigenvalues of the coefficient matrix M in (2) to be real and have same sign. The class of equations that satisfy this requirements is of particular interest as it includes, among others, all the generalized Sylvester equations with Hermitian

positive definite coefficients, which are of great interest in applications. The general technique we develop can be tailored to the special cases (3)-(8), in order to obtain a reduction of the computational cost and therefore of the execution time.

In its basic form, the algorithm involves only matrix-matrix multiplications, and a more refined variant can exploit the availability of routines for the solution of linear systems. This simplicity translates into ease of implementation, which makes the approach very suitable for all those frameworks, such as multiprecision libraries, in which only a few linear algebra kernels are typically available. The technique developed by Bartels and Stewart for the solution of (5) and (7), for example, requires the Schur factorization of the coefficients of the matrix equation [1]. This factorization is computed by means of Francis's algorithm [26], also known as QR algorithm [24], [25], which is one of the most complex algorithms in matrix computation [11, Chap. 13], and is not always available in a multiprecision computing environment [9].

Moreover, the iterative nature of the new method allows for a finer control of the accuracy of the computed solution, as it allows the user to stop the iteration as soon as the target precision has been reached, which would not be possible if the Bartels–Stewart method were used. We remark that ours is not the only iterative method for the solution of generalized Sylvester equations of the form (1). Ding and Chen have developed several gradient-based algorithms for the solution of generalized Sylvester equations [3], which can be adapted to the case of coupled Sylvester equations [4].

The next section summarizes the main features of the dynamical functional particle method, upon which our technique for the solution of the generalized Sylvester equation (1) is built. In view of the equivalent formulation (2), particular emphasis is given to the theoretical aspects specific to the solution of linear systems. In Section 3 we describe how the method can be adapted to the solution of generalized Sylvester equations of the form (1), and discuss how the algorithm can be tailored to the solution of (3)–(8). In Section 4 we compare our implementation of the new algorithms with the built-in MATLAB function sylvester, and with an implementation of the gradient-based iterative algorithm of Ding and Chen [3], [4]. Finally in Section 5 we draw our conclusion and outline possible directions for future work.

2 The dynamical functional particle method

Edvardsson, Gulliksson, and Persson originally introduced the dynamical functional particle method as a technique for the solution of boundary value problems arising in quantum chemistry [5], but the use of this technique has been investigated for a number of applications, including constrained optimization and linear eigenvalue problems [13], and linear least squares and ill-posed linear systems [14].

Our iterative method for the solution of (1) builds upon the corresponding method for the solution of linear systems of equations [6], which we now briefly recall. Let $G \in \mathbb{C}^{n \times n}$ be a matrix with positive real eigenvalues, let $b \in \mathbb{C}^n$, and let $x : \mathbb{R}^+ \to \mathbb{C}^n$, where \mathbb{R}^+ denotes the closed positive real axis, be a function of the dummy time variable t. In order to solve the linear system Gx = b, consider the second order dynamical system

$$\ddot{x}(t) + \mu \dot{x}(t) = b - Gx(t), \qquad \mu > 0,$$
(9)

which can equivalently be written as the first order system

$$\begin{cases} \dot{x}(t) = v\\ \dot{v}(t) = -\mu \dot{x}(t) + b - Gx(t). \end{cases}$$
(10)

The system (10) can be integrated efficiently in time using the symplectic Euler algorithm [15, Chap. VI], which for $\Delta t > 0$ yields

$$\begin{cases} v_{k+1} = v_k - \mu \Delta t \, v_k + \Delta t (b - G x_k) \\ x_{k+1} = x_k + \Delta t \, v_{k+1}. \end{cases}$$
(11)

For the initial conditions, x(0) is initialized to a random vector and $\dot{x}(0)$ is set to 0 for simplicity. It is easy to see that if (11) converges, then $\tilde{x} := x(t_s)$ satisfies $G\tilde{x} = b$ for some $t_s > 0$.

The convergence of the symplectic scheme (11) is governed by the damping coefficient $\mu > 0$ in the dissipation term and by the discretization step Δt . The optimal choice of these two parameters is [6]

$$\mu^* = \frac{2\sqrt{\lambda_{\min}(G)\lambda_{\max}(G)}}{\sqrt{\lambda_{\min}(G)} + \sqrt{\lambda_{\max}(G)}}, \qquad \Delta t^* = \frac{2}{\sqrt{\lambda_{\min}(G)} + \sqrt{\lambda_{\max}(G)}}, \tag{12}$$

where $\lambda_{\min}(G)$ and $\lambda_{\max}(G)$ denote the smallest and largest eigenvalue of the matrix G, respectively. This method is shown to be stable and convergent for positive definite matrices in [14, Cor. 1].

3 Solving the generalized Sylvester equation

The dynamical functional particle method for the solution of the generalized Sylvester equation (1) can readily be formulated by using the alternative expression (2). For efficiency's sake, the coefficient matrix M in (2) is never explicitly computed, and the matrix-vector product Gx in (11) is performed implicitly, as we now explain.

Let $\widetilde{X}_0 \in \mathbb{C}^{mn}$ be a vector with randomly generated entries, and let $\widetilde{Y}_0 \in \mathbb{C}^{mn}$ be vector of length mn with all entries set to 0. Then we can apply the symplectic Euler scheme in (11) to (2) and write

$$\begin{cases} \widetilde{R}_k = \operatorname{vec}(C) - M \operatorname{vec}\left(\widetilde{X}_k\right), \\ \widetilde{Y}_{k+1} = \widetilde{Y}_k + \Delta t \cdot \left(\widetilde{R}_k - \mu \widetilde{Y}_k\right), \\ \widetilde{X}_{k+1} = \widetilde{X}_k + \Delta t \cdot \widetilde{Y}_{k+1}, \end{cases}$$
(13)

where the matrix M is the sum of Kronecker products defined in (2). The approximate solution to (1) at step k' will be $\operatorname{unvec}_{m,n}(\widetilde{X}_{k'})$.

The iterative scheme (13) is not practical, as at each step it requires the evaluation of the matrix-vector product $M \operatorname{vec}(X)$. As M is a matrix of order mn, this matrix computation requires $2m^2n^2 + o(m^2n^2)$ floating-point operations (flops), and can become unduly expensive even for moderate values of m and n. The computation of the residual R_k , however, can equivalently be written

$$\widetilde{R}_k = \operatorname{vec}\left(C - \sum_{i=1}^{\ell} A_i X_k B_i\right),\tag{14}$$

so that one step of the iteration now requires only $2\ell(m^2n + mn^2) + o(\ell(m^2n + mn^2))$ flops. In view of this observation, we can rewrite (13) in the more natural form

$$\begin{cases} R_k = C - \sum_{i=1}^{\ell} A_i X_k B_i, \\ Y_{k+1} = Y_k + \Delta t \cdot (R_k - \mu Y_k), \\ X_{k+1} = X_k + \Delta t \cdot Y_{k+1}, \end{cases}$$
(15)

Matrix equation	Coefficient M	$\lambda_{\min}(M)$	$\lambda_{\max}(M)$
AXB = C	$B^T\otimes A$	$\lambda_{\min}(A)\lambda_{\min}(B)$	$\lambda_{\max}(A)\lambda_{\max}(B)$
AXA = C	$A^T\otimes A$	$\lambda_{\min}(A)^2$	$\lambda_{\max}(A)^2$
$AX + XA^* = C$	$I_m \otimes A + \overline{A} \otimes I_m$	$2\lambda_{\min}(A)$	$2\lambda_{\max}(A)$
$AXA^* - X = C$	$\overline{A} \otimes A - I_m \otimes I_m$	$\lambda_{\min}(A)^2 - 1$	$\lambda_{\max}(A)^2 - 1$
AX + XB = C	$I_m \otimes A + B^T \otimes I_m$	$\lambda_{\min}(A) + \lambda_{\min}(B)$	$\lambda_{\max}(A) + \lambda_{\max}(B)$
AXB + X = C	$B^T\otimes A + I_m\otimes I_m$	$\lambda_{\min}(A)\lambda_{\min}(B) + 1$	$\lambda_{\max}(A)\lambda_{\max}(B) + 1$

Table 1: The spectrum of the Kronecker form of some special cases of the generalized Sylvester equation in (1).

where $X_k, Y_k, R_k \in \mathbb{C}^{m \times n}$.

In order to obtain the optimal damping and time step for this scheme we still need an efficient way of estimating the extreme eigenvalues of M in (2), which are real by assumption. In the most general case, the most efficient way of estimating $\lambda_{\max}(M)$ is the power method [27, Ch. 10], an iteration that approximates an eigenvector corresponding to the largest eigenvalue in absolute value. At each step, this algorithm requires only one matrix-vector product, which can be implemented implicitly without ever forming the matrix M explicitly. The power method could also be used to efficiently estimate $\lambda_{\min}(M) = \lambda_{\max}(M^{-1})$ if a routine for solving linear system having M as coefficient is available. To the best of our knowledge, no such routine exists for the general matrix M in (2) for ℓ greater than 2, but the extreme eigenvalues of M can be computed efficiently for some special cases, as we now explain.

For the one-term and two-terms linear equations in (3)-(8) we can use the following well-know result.

Proposition 3.1. [18, Theorem 4.2.12 and Exercise 19, p. 251] Let $\lambda_1, \ldots, \lambda_m$ be the eigenvalues of $A \in \mathbb{C}^{m \times m}$ and ξ_1, \ldots, ξ_n be the eigenvalues of $B \in \mathbb{C}^{n \times n}$. Then for $i = 1, \ldots, n$ and $j = 1, \ldots, m$, the mn eigenvalues of $A \otimes B$ and $A \otimes I_n + I_m \otimes B$ have the form $\lambda_i \xi_j$ and $\lambda_i + \xi_j$, respectively.

Combining this result with the fact that a matrix and its transpose have the same characteristic polynomial and thus the same eigenvalues, allows us to obtain formulae for the extreme eigenvalues of M which only require knowledge of the extreme eigenvalues of the coefficient matrices appearing on the left-hand side of the matrix equation. We summarize the results for the special cases of interest in Table 1.

The method described in this section inherits the convergence behavior and the stability of the algorithm for linear systems described in Section 2.

4 Numerical experiments

Now we compare the algorithm discussed in Section 3 with existing methods for the solution of Sylvester and generalized Sylvester equations. The results in this section were obtained by running the experiments in MATLAB 9.8.0 (R2020a) on a machine equipped with an Intel I5-5287U running at 2.9 GHz and 16 GiB of RAM. We compared the following five codes.

• gs_kron solves the linear system in (2) by explicitly constructing the matrix M and then using the MATLAB backslash operator.

- gs_dfpm_opt solves (1) by using the dynamical functional particle method described in Section 3 with optimal damping and time step computed according to (12) for G = M. The quantities $\lambda_{\min}(M)$ and $\lambda_{\max}(M)$ are computed by constructing the matrix M explicitly, with the exception of the special cases in Table 1.
- gs_dfpm_app solves (1) by using the dynamical functional particle method described in Section 3 with parameters chosen according to (12) for G = M, but using the estimates

$$\lambda_{\min}(A) \approx \sum_{i=1}^{\ell} \lambda_{\min}(B_i^T \otimes A_i), \qquad \lambda_{\max}(A) \approx \sum_{i=1}^{\ell} \lambda_{\max}(B_i^T \otimes A_i),$$

which do not require the explicit computation of the matrix M.

- gs_gbia solves (1) by using the gradient based iterative algorithms for solving generalized Sylvester matrix equations developed by Ding and Chen [3], [4].
- sylvester solves the continuous-time Lyapunov equation (5) and the Sylvester equation (7) by means of the MATLAB function sylvester, which implements the algorithm of Bartels and Stewart [1].

For the iterative algorithms, we set the maximum number of iterations to 50 000 and keep iterating until the 1-norm difference between two successive iterates is below $2^3 u$, where $u = 2^{-53} \approx 1.11 \times 10^{-16}$ denotes the unit roundoff of binary64 floating-point arithmetic.

In our tests, the superscript notation $A^{(\eta)} \in \mathbb{R}^{m \times m}$ denotes the real non-symmetric matrix generated as

$$A^{(\eta)} = PD^{(\eta)}P^{-1},\tag{16}$$

where the $P \in \mathbb{R}^{m \times m}$ is such that $\kappa_2(P) = 2$ and is generated using the randsvdfast function [10], whereas D_η is a diagonal matrix with extreme eigenvalues $\sqrt{\eta}^{-1}$ and $\sqrt{\eta}$ and remaining diagonal elements uniformly distributed in $[\sqrt{\eta}^{-1}, \sqrt{\eta}]$. This choice of P and $D^{(\eta)}$ ensures that $\kappa_2(A^{(\eta)}) \leq 4\eta$, and in practice provide a matrix $A^{(\eta)}$ such that $\kappa_2(A^{(\eta)}) \approx \eta$.

4.1 The Sylvester equation

In this first experiment we consider the solution of the Sylvester equation

$$A^{(\eta)}X - XB^{(\eta)} = C, (17)$$

where $A^{(\eta)} \in \mathbb{R}^{m \times m}$ and $B^{(\eta)} \in \mathbb{R}^{n \times n}$ are as in (16) and $C \in \mathbb{R}^{m \times n}$ is generated using a matrix $X \in \mathbb{R}^{m \times n}$ with entries from the Gaussian distribution.

In Figure 1 we report the execution time required by sylvester and gs_dfpm_opt to solve (17) and the forward error of the solutions the two algorithms computed. In the plots we consider two moderate values of η , namely 10 (top row) and 100 (bottom row), and we fix n = 500 and allow m to vary. For both values of η , gs_dfpm_opt is more accurate than sylvester for all the test matrices. The forward error of gs_dfpm_opt is of the order of $\kappa_1(M)u$ for $\eta = 10$ and about one order of magnitude smaller than the accuracy reference for $\eta = 100$.

We now discuss the timings of the two algorithms. As gs_dfpm_opt is an iterative algorithm, its execution time depends not only on the total number of iterations the algorithm requires to converge, but also on the computational cost of each iteration. As discussed above, the most



Figure 1: Left: execution time, in seconds, required by gs_dfpm_opt and sylvester to solve the matrix equation in (17) for n = 500. Right: relative forward error of the computed solution.

expensive operation of each iteration of gs_dfpm_opt is the computation of the residual, thus each iteration asymptotically requires $2(m^2n + mn^2)$ flops. Therefore, we should expect the timings of this algorithm to grow with the order of $A^{(\eta)}$ and $B^{(\eta)}$, which is confirmed by the plots in the left column of Figure 1.

The total number of iteration required by gs_dfpm_opt is proportional to the conditioning of the matrix M in (2), which in turn roughly depend on the parameter η . This is consistent with previous findings in the literature on the dynamical functional particle method for the solution of linear systems with positive definite coefficients. In our experiments, the algorithm required 44 and 64 iterations for the matrices in the top row and between 201 and 948 for those in the bottom row.

In our experimental setup, for $\eta = 10 \text{ gs_dfpm_opt}$ is faster than sylvester when the order of $A^{(\eta)}$ is at most 20% of that of $B^{(\eta)}$, a percentage that reduces to about 5% when $\eta = 100$. For larger values of η , gs_dfpm_opt is typically slower but still more accurate than sylvester. Similar results obtained for larger values of n suggest that gs_dfpm_opt is typically marginally but consistently more accurate than sylvester, but is faster than the latter only when the coefficients of the matrix equation (17) are well conditioned and differ considerably in size.

4.2 The generalized Sylvester equation

Now we consider the solution of the more general matrix equation

$$\sum_{i=1}^{5} A_i^{(\eta)} X B_i^{(\eta)} = C.$$
(18)

In our experiments, the $m \times m$ matrices $A_1^{(\eta)}, \ldots, A_5^{(\eta)}$ are simultaneously diagonalizable, and so are the $m \times m$ matrices $B_1^{(\eta)}, \ldots, B_5^{(\eta)}$, although the eigenvectors of $A_i^{(\eta)}$ and $B_i^{(\eta)}$ are in general different. We resort to this technique to ensure that the matrix M in (2) has positive real eigenvalues. As in the previous experiment, the matrix $C \in \mathbb{R}^{m \times m}$ is computed by using a matrix $X \in \mathbb{R}^{m \times m}$ with entries from the Gaussian distribution.

In Figure 2 we compare the performance and accuracy of gs_kron, gs_dfpm_opt, gs_dfpm_app, and gs_gbia for the solution of (18) as m varies. As we are mainly interested in well-conditioned matrices, as in the previous experiment we consider the two cases $\eta = 10$ and $\eta = 100$.

Our results suggest that gs_kron is the most accurate of the four algorithms, and is the only one that achieves a forward error of the magnitude of $\kappa_1(M)u$. The two implementations based on the dynamical functional particle method achieve a similar level of accuracy, whereas gs_gbia is always the least accurate of the algorithms we test, and for three of our test matrices it fails to satisfy our stopping criterion within 50 000 iterations.

We now compare the four algorithms in terms of execution time. For matrix equations of small size, gs_kron is typically the most efficient algorithm, followed by gs_dfpm_opt , gs_dfpm_app , and finally gs_gbia . For these small matrices, the approximation of the extreme eigenvalues of M in (2) is inexpensive, and the cost of the three iterative algorithms depends mostly on the number of iterations that are necessary to achieve convergence. As gs_dfpm_opt requires considerably fewer iterations than the other two methods, it is the fastest for m below 40.

We note that, in our implementations, gs_dfpm_opt cannot achieve an execution time lower than that of gs_kron . In fact, estimating $\lambda_{\min}(M)$ requires the solution of at least one—but typically several—linear systems with coefficient matrix M. Therefore the computation that gs_kron performs is, in a sense, just a pre-processing step for gs_dfpm_opt . In order for this method to be competitive, an alternative technique for estimating the smallest eigenvalue of M is necessary. We do not investigate this further, as the choice of said technique is likely to depend on the problem being solved and on a priori knowledge of the properties of the coefficient matrices.

As the size of the matrix coefficients of the equations grows, estimating the extreme eigenvalues of M becomes more expensive, and the lower number of iterations that the optimal



Figure 2: Left: execution time, in seconds, required by gs_kron , gs_dfpm_opt , gs_dfpm_app and gs_gbia to solve the matrix equation in (18) m = n between 1 and 100. Right: relative forward error of the computed solution.

choice of parameters produces is not sufficient to offset the time spent estimating $\lambda_{\min}(M)$. Thus for larger matrices the crude choice of parameters of gs_dfpm_app pays off, leading to an execution time two order of magnitudes smaller for m as small as 100.

5 Conclusion

We have developed a family of algorithms for the solution of a class of generalized Sylvester equations in the form (1), and we have explained how these methods can be tailored to tackle some special cases of particular importance in applications. The new techniques build upon the dynamical functional particle method for the solution of linear systems, and exploit the equivalence between the two formulations (1) and (2).

Numerical results show that our implementations are typically capable of outperforming existing methods for the solution of (1) in terms of both accuracy and execution speed. In order to show the potential of our new techniques, we compared the algorithm for the Sylvester equation (7) to the built-in MATLAB function sylvester. We found that if the matrix coefficients on the left-hand side are sufficiently well conditioned and have very different size, then our implementation of the discrete functional particle method can outperform sylvester in terms of both accuracy and speed.

As the dynamical functional particle method has been successfully applied to nonlinear optimization problems, it is natural to ask whether similar techniques for the solution of nonlinear matrix equations can be derived. This nontrivial problem will be the subject of future work.

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