

THE GENERALIZED EIGENVALUE PROBLEM FOR NONSQUARE PENCILS USING A MINIMAL PERTURBATION APPROACH*

GREGORY BOUTRY[†], MICHAEL ELAD[‡], GENE H. GOLUB[†], AND
PEYMAN MILANFAR[§]

Abstract. This work focuses on nonsquare matrix pencils $A - \lambda B$, where $A, B \in \mathcal{M}^{m \times n}$ and $m > n$. Traditional methods for solving such nonsquare generalized eigenvalue problems $(A - \lambda B)\underline{v} = \underline{0}$ are expected to lead to no solutions in most cases. In this paper we propose a different treatment: We search for the minimal perturbation to the pair (A, B) such that these solutions are indeed possible. Two cases are considered and analyzed: (i) the case when $n = 1$ (vector pencils); and (ii) more generally, the $n > 1$ case with the existence of one eigenpair. For both, this paper proposes insight into the characteristics of the described problems along with practical numerical algorithms toward their solution. We also present a simplifying factorization for such nonsquare pencils, and some relations to the notion of pseudospectra.

Key words. nonsquare pencils, generalized eigenvalue, pseudospectra

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1. Introduction.

1.1. Pencils and nonsquare pencils. The term “pencil” used in linear algebra is well known and refers to the expression $A - \lambda B$, where both A and B are typically square $n \times n$ matrices, and λ is a complex scalar. Of special interest are the values that reduce the pencil rank, namely, the λ values satisfying $(A - \lambda B)\underline{v} = \underline{0}$ for some nonzero vector \underline{v} . Then the problem is defined as the generalized eigenvalue problem, where the scalars λ are the generalized eigenvalues, and their corresponding vectors \underline{v} are the generalized eigenvectors.¹

In recent years several different fields of research have led to the generalized eigenvalue problem involving a nonsquare pencil, where A and B are rectangular $m \times n$ matrices and $m > n$ [2, 12, 22, 25]. In many of these applications, the pencil involved becomes rectangular due to additional measurements—each new set of measurements constructs a new row in the pencil. Clearly, more measurements (and thus more rows) imply better possible estimation, though it is not clear how this additional information can be exploited. Also, in most applications the content of the pencil involves noisy measurements. Theoretically, in the noiseless case it is known that n (or possibly fewer) solutions reducing the pencil rank exist. However, after the perturbation these solutions may be elusive. It is this very property of the noiseless solvable case that leads us to a different perspective in treating the nonsquare generalized eigenvalue problem.

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[†]Faculté Libre des Sciences et Technologies, Institut Catholique de Lille, 41 rue du Port, 59046 Lille Cedex, France (gregory.boutry@icl-lille.fr).

[‡]Computer Science Department, The Technion - Israel Institute of Technology, Haifa, 32000 Israel (elad@cs.technion.ac.il).

[§]Department of Electrical Engineering, University of California, Santa Cruz, CA 95064 (milanfar@ee.ucsc.edu).

¹If B is invertible, one immediately sees the relation to the regular eigenvalue problem because $(A - \lambda B)\underline{v} = \underline{0}$ implies $B^{-1}A\underline{v} = \lambda\underline{v}$.

1.2. Problem formulation. Removing the application details, we can cast the eventual problem in the following form: Given the matrix pair $(A, B) \in \mathcal{M}^{m \times n}$ where $m > n$, we assume that these matrices originated from the pair $(A_0, B_0) \in \mathcal{M}^{m \times n}$ by perturbation (additive noise). We further assume that for the original pair there exist n distinct eigenpairs of the form $(A_0 - \lambda_k B_0)v_k = 0$, $k = 1, 2, \dots, n$. Therefore, given the measured pair (A, B) we search for both the eigenpairs $\{\lambda_k, v_k\}_{k=1}^n$ and the original pair (A_0, B_0) . Clearly, even if $m = n$, there may be some situations when there are not n solutions. Similarly, in the general case of $m > n$, there may not be any solution to the pencil $(A - \lambda B)v = 0$, and we are searching for the minimal perturbation such that a rank-reducing solution exists. We will assume hereafter that the perturbed matrices A and B are full rank (i.e., n). More formally, we are interested in solving the following optimization problem:

$$(1) \quad \text{Given } A, B, \text{ find } \min_{A_0, B_0, \{\lambda_k, v_k\}_{k=1}^n} \|A_0 - A\|_F^2 + \|B_0 - B\|_F^2 \\ \text{subject to } \{(A_0 - \lambda_k B_0)v_k = 0, \|v_k\|_2^2 = 1\}_{k=1}^n.$$

The Frobenius norm is used to measure the perturbation, entrywise, between the original pair and the estimated pair. This proposed formulation coincides with the maximum-likelihood description if the perturbation is assumed to originate from an additive white and zero mean Gaussian noise.

It should be noted that in many cases there is a need to constrain the solution to have a specific structure (e.g., Hankel/Toeplitz). In this work we neglect this option and leave this topic for future research. We note, however, that exploiting such additional information should lead to a more satisfactory solution. Similarly, in the spirit of generalizing the above problem we might be interested in adding weights to the computed Frobenius norm in order to emphasize some of the entries, or to cover cases when some of the entries are exact (e.g., fixed zeros). Again, we leave this weighted form of the problem for future research.

1.3. Relation to previous work. Several previous papers already addressed the treatment of perturbed rectangular pencils. However, all these contributions concentrate on theoretical analysis, proposing extensions based on perturbation theory, and forming bounds on the error measure we defined in (1) as our minimization goal. In contrast, this paper discusses a numerical algorithm for finding the eigenvalues and the matrix pair (A_0, B_0) .

Demmel and Kågström [4] suggested a treatment for nonsquare pencils based on the Kronecker canonical form (KCF). Under the assumption on the regularity of the KCF, the spectrum of the perturbed pencil $(A + E) - \lambda(B + F)$ is considered and compared to the spectrum of the original pencil $A - \lambda B$. Later work by Edelman, Elmroth, and Kågström and Elmroth, Johansson, and Kågström extends this work, suggesting a geometric interpretation of the above perturbation results [6, 8, 9]. Bounds are obtained for the distance from the pencil $A - \lambda B$ to $A_0 - \lambda B_0$. A similar approach and treatment is found in [2, 22]. Again, lower and upper bounds on the distance to a solvable pair of matrices are developed.

Another line of research relevant to this work is the study of pseudospectra for rectangular pencils (see the paper by Wright and Trefethen [25] on this topic). Most of the contributions in this field refer to the square pencil case [23, 11, 24]. When treating a rectangular nonsolvable pencil, we see that its pseudospectra is most likely to be empty for very small distances. As this distance grows, at some point the pseudospectra becomes nonempty. This is exactly the distance to which our solution

should point. More on the relation of pencils to pseudospectra will be mentioned in section 5.

In this work we focus on the minimal perturbation that guarantees a solution. However, we concentrate on a practical numerical scheme that finds the optimal (in the maximum-likelihood sense) eigenpairs, and also leads to the perturbed pair that guarantees a solution. We find a set of eigenvalues that minimizes the distance and we find the matrices that are the closest.

1.4. This paper's contribution and content. Solving the optimization problem in (1) is the challenge of this paper. We open the discussion with an effective method for visualizing the problem at hand. Then we present an analysis and insight for the following two simplified variations of the problem posed in (1):

1. We assume $n = 1$, so that $A = \underline{a}$ and $B = \underline{b}$. For this case we show that the defined problem leads to a closed form solution. We also show equivalence to the total least squares (TLS) method (cf. [13, p. 595]).
2. We assume $n > 1$ and search for a single eigenpair $\{\lambda, \underline{v}\}$. For this more complicated problem, a stable and convergent numerical algorithm is proposed.

This paper is organized as follows. In the next section we present a method for visualizing the behavior of such nonsquare pencils as a function of the scalar λ , and this way get a better understanding of the features of the problem at hand. In section 3 we show how the nonsquare pencil is solved analytically for the case of $n = 1$; i.e., the matrices A and B are single vectors. Through this solution we obtain a better understanding of the solution mechanism for the more general case. Section 4 treats the more general case with $n > 1$, but with the simplifying assumption that only one eigenpair is sought. A highly effective numerical method is proposed and analyzed. In section 5, we discuss the relationship between our work and the notion of pseudospectra, showing the similarities and the differences between these two approaches toward the issue of analyzing rectangular pencils. In section 6, we present a new factorization for the rectangular pencil, and through it an analysis of our initialization choice in the numerical algorithm. We conclude this paper in section 7 and summarize its contribution, list some open questions we have not treated, and outline future research directions.

The problem is wide and complicated. We regard this contribution as a first stage in a sequence of activities made to encompass its various aspects.

2. Visualizing nonsquare pencils. In order to gain insight into the treatment of such nonsquare pencils, let us look at a related function

$$(2) \quad f(\lambda) = \sigma_{\min}(A - \lambda B) = \min_{\underline{v} \mid \|\underline{v}\|^2=1} \|(A - \lambda B)\underline{v}\|_2.$$

The notation $\sigma(X)$ designates the singular values of the matrix X and σ_{\min} is the smallest singular value. It is interesting to note that this function is used often for the construction of the pseudospectra of square matrices [25, 23]. This function describes the constraints in (1) as a penalty term, and it has several interesting properties that may help us visualize the behavior of the nonsquare pencil. This function is a mapping from the complex plane (values of λ) to the real and nonnegative numbers, because $f(\lambda)$ is nonnegative by the definition of the singular values. For a solvable pair of matrices A and B (i.e., a pair that has a rank-reducing solution λ_0), the value of the function at this λ_0 value is exactly zero. This is trivial since, if the pencil $A - \lambda_0 B$ is rank deficient, it must have zero as its smallest singular value (and may have more than one zero singular value). For such a solvable pair the eigenvalues are the local

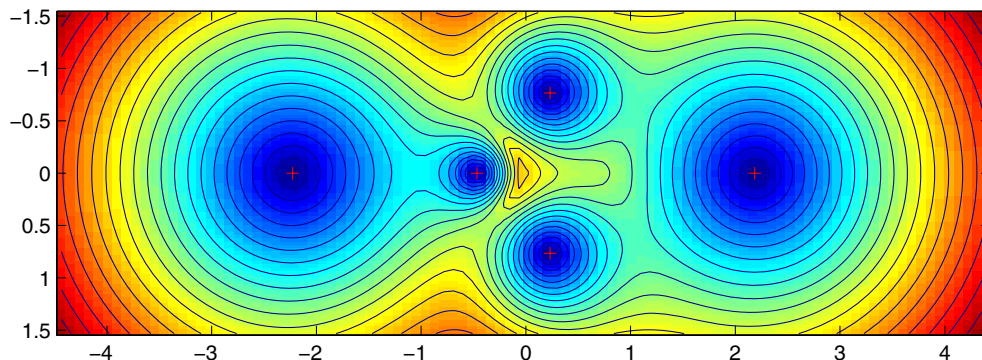


FIG. 1. A plot of the level curves of $f_0 = \sigma_{\min}(A_0 - \lambda B_0)$, built using the unperturbed pair (A_0, B_0) .

minimum points of this function. This is easily seen since, if λ_0 is perturbed, we get a full rank pencil that leads to a strictly positive minimal singular value and, in the case of a nonsolvable pair A and B , the function is strictly positive for all λ . However, the local minimum of this function may still help in finding a solution to (1).

Due to the first property, it is quite easy for us to visualize this function and learn about its behavior. Let us describe a simple example: We start by creating a pair of 5×5 random matrices, denoted as \tilde{A} and \tilde{B} . The entries are drawn from a zero mean Gaussian distribution with standard deviation $\sigma = 1$. We verify that this pair has five distinct generalized eigenvalues denoted as $\{\alpha_k\}_{k=1}^5$. Let Q be an arbitrary full rank matrix of size 50×5 ; we create the pair $A_0 = Q\tilde{A}$ and $B_0 = Q\tilde{B}$. This pair of matrices is made up of rectangular 50×5 matrices. It is clear that they represent a solvable pair since, for all k ,

$$\begin{aligned} \text{Rank}(\tilde{A} - \alpha_k \tilde{B}) &= 4 \\ \implies \text{Rank}(A_0 - \alpha_k B_0) &= \text{Rank}(Q\tilde{A} - \alpha_k Q\tilde{B}) = \text{Rank}(Q(\tilde{A} - \alpha_k \tilde{B})) = 4. \end{aligned}$$

Given this rectangular pair, Figure 1 shows the 2D function $f_0(\lambda) \equiv \sigma_{\min}(A_0 - \lambda B_0)$. The exact eigenvalues $\{\alpha_k\}_{k=1}^5$ are overlaid (represented by “+” signs), and the minimum points of f_0 match exactly the location of the eigenvalues.

We proceed and define $A = A_0 + N_A$ and $B = B_0 + N_B$, where both N_A and N_B are of size 50×5 with entries drawn from a Gaussian white noise distribution with $\sigma = 0.1$. In Figure 2 we describe the function $f(\lambda) = \sigma_{\min}(A - \lambda B)$ for the noisy version of the original pair. As can be seen, there are still five local minima. However, relative to the location of the true eigenvalues, the local minima points are slightly deviated.

To conclude this experiment, we present in Figure 3 yet another function $f(\lambda)$, built using a perturbed pair A and B but with much stronger noise $\sigma = 5$. We see that all the local minima points vanished and there is a single minimum point near the origin. This demonstrates the difficulty we will be facing when the perturbation is relatively great.

Figure 4 shows an intersection of these functions with the real axis. As can be seen, for f_0 the values at the minimum are exactly zero, as expected.² As we go to the

²Since this function was sampled uniformly, near zero values are obtained.

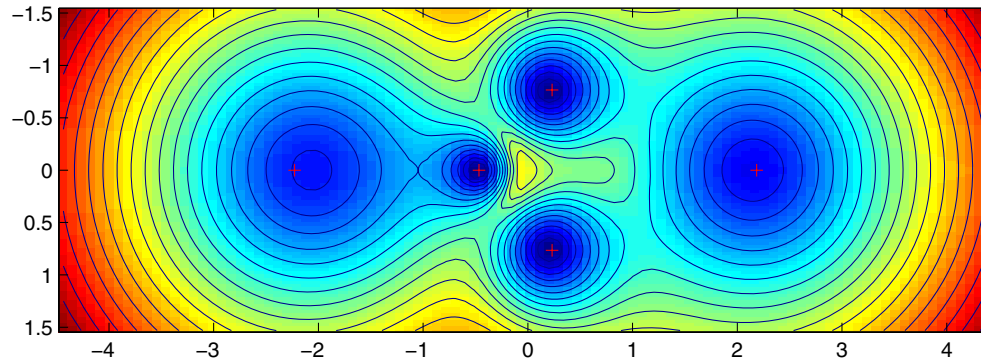


FIG. 2. A plot of the level curves of $f = \sigma_{\min}(A - \lambda B)$, built using a moderately perturbed pair (A, B) ($\sigma = 0.1$).

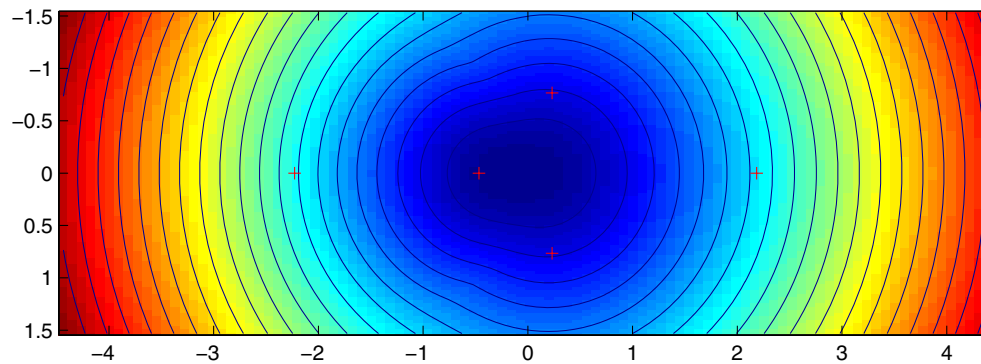


FIG. 3. A plot of the level curves of $f = \sigma_{\min}(A - \lambda B)$, built using a strongly perturbed pair (A, B) ($\sigma = 5$).

function f with the moderate noise, we get that the minimum points' height is above zero, though they exist and are close to the true points. The case of strong perturbation seems to appear as a unimodal function with one minimal point at the origin.

From this experiment it is clear that the function $f(\lambda) = \sigma_{\min}(A - \lambda B)$ could be beneficial in obtaining a good guess for the required eigenvalues. In the small perturbation case this idea seems to work quite well. We also see that in solving the problem presented in (1) we actually create a new pair of matrices that reduce the height of the function $f(\lambda)$ to zero at the local minima. It is not clear how we can refine the eigenvalues to compensate for the induced shift due to the perturbation. Lastly, we see that strong perturbations may lead to numerical problems if n distinct eigenvalues are sought.

3. Solving the $n = 1$ case. In this section, we redefine the problem described in (1) while assuming $n = 1$, and show that this case is analytically solvable.

3.1. Analysis.

THEOREM 1. *Given any pair of vectors \underline{a} and \underline{b} , a unique global solution of the minimization problem given (1) always exists, and is given by*

$$(3) \quad \underline{a}_0 = \underline{a} - \frac{(\underline{a} - \lambda \underline{b})}{1 + |\lambda|^2}, \quad \underline{b}_0 = \underline{b} + \frac{\lambda^*(\underline{a} - \lambda \underline{b})}{1 + |\lambda|^2},$$

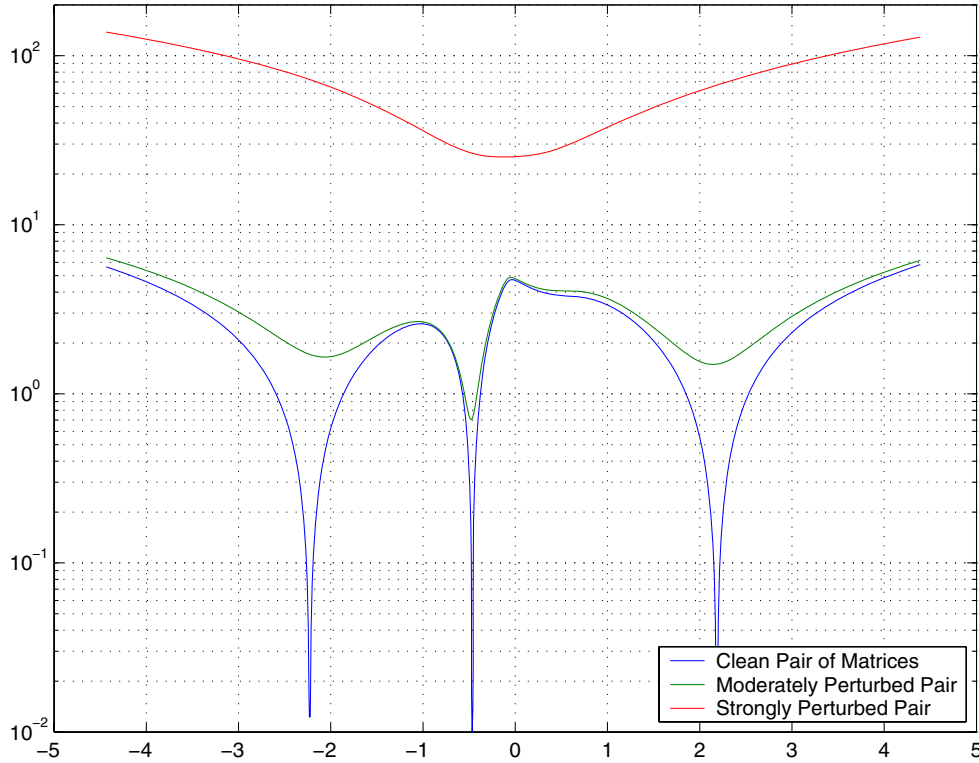


FIG. 4. A 1D intersection along the center horizontal axis (the real values) of the 2D functions described in Figures 1, 2, and 3.

where λ is the (+)-root³ of the quadratic equation

$$(4) \quad 0 = \lambda^2 \underline{a}^H \underline{b} + \lambda (\underline{b}^H \underline{b} - \underline{a}^H \underline{a}) - \underline{b}^H \underline{a}.$$

Proof. As this theorem is a particular case of a more general theorem presented in the next section, the proof will be given in section 4. \square

Next, we find an equivalent constraint-free optimization problem that eases the overall solution. Notice the close resemblance to the objective function used in the previous section for visualization.

THEOREM 2. *The optimization problem posed in (1) is equivalent to the optimization problem*

$$(5) \quad \min_{\{\lambda\}} \frac{\|\underline{a} - \lambda \underline{b}\|_2^2}{1 + |\lambda|^2}.$$

The optimal solutions are given by the former theorem.

Proof. This theorem is also a particular case of a more general theorem presented in the next section, and again, the proof will be given later in section 4. \square

It is interesting to note that the observation made above, about the equivalence between the original optimization problem and the one posed in (5), implies that a function closely related to the one presented in the previous section (see (2)) is

³For a quadratic equation $\alpha x^2 + \beta x + \gamma = 0$, the (+)-root is given by $(-\beta + \sqrt{\beta^2 - 4\alpha\gamma})/(2\alpha)$.

minimized, but there is an additional term that moves the eigenvalue solution away from the origin. From Figures 2 and 3, it is clear that such a force is desired to better allocate the eigenvalues as the local minimum points of the treated function. As it turns out, this term in the denominator is quite commonly seen with respect to TLS (cf. [13, p. 595]). We next show that there is a close relation between our problem and TLS.

3.2. Relation to TLS. Here we show that the case of $n = 1$ actually forms a classic TLS problem. This strengthens our claim about the existence of a closed form solution for the $n = 1$ nonsquare pencil. However, as we shall see, this equivalence to TLS does not generalize to the $n > 1$ pencils.

THEOREM 3. *Given any pair of nonzero vectors \underline{a} and \underline{b} , a unique global solution of the minimization problem posed in (1) is given by the singular value decomposition (SVD) of the matrix $[\underline{a} \ \underline{b}]$ by replacing the smaller, second singular value by zero.*

Proof. Writing (1) differently, we obtain a classic TLS formation

$$(6) \quad \min_{\underline{a}_0, \underline{b}_0} \ \|[\underline{a}_0, \underline{b}_0] - [\underline{a}, \underline{b}]\|_F^2 \quad \text{subject to} \quad \text{Rank}([\underline{a}_0, \underline{b}_0]) = 1.$$

The optimal solution for this problem can be obtained by the SVD on $[\underline{a}, \underline{b}]$ (cf. [13, p. 70]). Writing $UDV^T = [\underline{a}, \underline{b}]$, we have that U is an $m \times 2$ unitary matrix, V is a 2×2 unitary matrix, and D is a diagonal 2×2 matrix containing the singular values of $[\underline{a}, \underline{b}]$ in descending order. The optimal solution is obtained by replacing the second singular value by zero, and the solution becomes $[\underline{a}_0, \underline{b}_0] = d_{1,1} \underline{U}_1 \underline{V}_1^H$, where \underline{U}_1 and \underline{V}_1 are the first columns of U and V , respectively, and $d_{1,1}$ is the larger singular value. \square

This analogy between the pencil problem and the TLS holds only for $n = 1$ and cannot be employed for larger n . An attempt to rewrite (1) as a TLS problem appears as

$$\min_{A_0, B_0, V} \ \| [A_0, B_0] - [A, B] \|_F^2 \quad \text{subject to} \quad \left\{ \begin{array}{l} \text{Rank}([A_0 V, B_0 V]) = n, \\ \text{Rank}(V) = n \end{array} \right\},$$

where V is a matrix containing all the eigenvectors. Clearly, this is not a classic TLS formulation and its solution can no longer be applied using the SVD since V is involved. This explains our interest in the simpler solution for $n = 1$.

3.3. Squaring effect. Looking back at (3) and (4), it can be shown that

$$(7) \quad \underline{b}_0^H (\underline{a} - \lambda \underline{b}) = \left(\underline{b} + \frac{\lambda^* (\underline{a} - \lambda \underline{b})}{1 + |\lambda|^2} \right)^H (\underline{a} - \lambda \underline{b}) = \frac{(\underline{b}^H + \lambda \underline{a}^H)(\underline{a} - \lambda \underline{b})}{1 + |\lambda|^2} = 0.$$

This implies that

$$(8) \quad \lambda = \frac{\underline{b}_0^H \underline{a}}{\underline{b}_0^H \underline{b}}.$$

Similarly, if we repeat all the above analysis starting with (1) and using the constraint $\underline{b}_0 - \alpha \underline{a}_0 = 0$, where α plays the role of $1/\lambda$, we get a dual solution

$$(9) \quad \underline{a}_0^H \frac{\underline{b} - \alpha \underline{a}}{1 + |\alpha|^2} = 0 \implies \lambda = \frac{1}{\alpha} = \frac{\underline{a}_0^H \underline{a}}{\underline{a}_0^H \underline{b}}.$$

These two results imply that to find the optimal eigenvalue we square the rectangular pencil by multiplication on both sides by either \underline{a}_0 or \underline{b}_0 . Of course, these vectors are not known and we have to go through a process as described above to find them. However, an approximate alternative to the above process could be an application of these squaring processes using the measured matrices instead of the estimated ones, that is,

$$(10) \quad \hat{\lambda} = \frac{\underline{b}^H \underline{a}}{\underline{b}^H \underline{b}} \quad \text{or} \quad \hat{\lambda} = \frac{\underline{a}^H \underline{a}}{\underline{a}^H \underline{b}}.$$

Then two different candidate solutions may be obtained as before. To choose between them, the corresponding \underline{a}_0 and \underline{b}_0 need to be computed. This could be done by solving the optimization problem given by (1), while assuming that λ is known. It is not hard to see that the solution is the one proposed in (3). As before, after computing \underline{a}_0 and \underline{b}_0 for the solutions of λ we may choose the one which leads to the smallest perturbation.⁴ Note that this approximate solution is expected to be close to the optimal solution if a small perturbation is assumed. We shall use this squaring idea for the general ($n > 1$) case.

3.4. Examples. We now give several examples to see the behavior of the above results.

Example 1. Assume $\underline{a} = \underline{b} \neq \underline{0}$. This case is solvable without any perturbation and it is clear that the proper eigenvalue should be 1.

The quadratic equation (4) becomes $\lambda^2 \underline{a}^H \underline{a} - \underline{a}^H \underline{a} = 0$, leading to the possible solutions $\{\lambda_1 = 1, \lambda_2 = -1\}$. Using (3) we get, for $\lambda_1 = 1$, $\underline{a}_0 = \underline{a}$ and $\underline{b}_0 = \underline{b}$, and thus the perturbation is $\underline{0}$. For the other solution $\lambda_1 = -1$, we obtain $\underline{a}_0 = \underline{0}$ and $\underline{b}_0 = \underline{0}$, and the perturbation is $\|\underline{a}\|^2 + \|\underline{b}\|^2$, and so clearly the (+)-root is the desired solution.

Using the approximate method in (10) we get that the two solutions are equal: $\lambda = \underline{b}^H \underline{a} / \underline{b}^H \underline{b} = \underline{a}^H \underline{a} / \underline{a}^H \underline{b} = 1$. Using (3), we obtain the optimal results that lead to no perturbation.

Example 2. Assume that $\underline{a}^H \underline{b} = \epsilon^2 \rightarrow 0$, $\|\underline{a}\|_2^2 = 1$, and $\|\underline{b}\|_2^2 = 0.5$. In this case the minimal perturbation zeros one of the vectors, and replaces the vector of smallest norm by zero. This leads to the optimal result (in our case it is \underline{b} that should be nulled).

The quadratic equation in (4) becomes $0 = \lambda^2 \epsilon^2 - 0.5\lambda - \epsilon^2$, and the solutions are $\{\lambda_1 = \infty, \lambda_2 = 0\}$ for $\epsilon \rightarrow 0$. The (+)-solution leads to $\underline{a}_0 = \underline{a}$ and $\underline{b}_0 = \underline{0}$ as required, and the second solution is similar but nulls \underline{a} instead, which is incorrect.

Approximating the solution by $\lambda = \underline{b}^H \underline{a} / \underline{b}^H \underline{b} = 0$ gives the wrong solution, and using $\lambda = \underline{a}^H \underline{a} / \underline{a}^H \underline{b} = \infty$ leads to the optimal solution.

Example 3. Assume that for $\epsilon \rightarrow 0$ we have $\underline{a} = [1, 0]^T$ and $\underline{b} = [1, \epsilon]^T$. Clearly, if we replace ϵ by zero, we get the case described in Example 1. Thus, a perturbation of ϵ^2 in the ℓ^2 norm could lead to a possible solution. However, moving an $\epsilon/2$ from \underline{b} to \underline{a} also causes $\underline{a} = \underline{b}$ and leads to a better solution since the perturbation in this case is $0.5\epsilon^2$.

From (4) we get $0 = \lambda^2 + \lambda\epsilon^2 - 1$. The solutions are $\{\lambda_1 \approx 1, \lambda_2 \approx -1\}$. The first result is the correct one and the perturbed solution is given by (3):

⁴In this approximate approach we found that there is no solution that was consistently better.

$\underline{a}_0 = [1, \epsilon/2]^T$ and $\underline{b}_0 = [1, \epsilon/2]^T$, as required, and the obtained perturbation is $\epsilon^2/2$.

Using the squaring approximation, one solution is given by λ being $\underline{b}^H \underline{a} / \underline{b}^H \underline{b} = 1/(1 + \epsilon^2)$. Then the minimal perturbation is roughly $3\epsilon^2$. The other solution $\lambda = \underline{a}^H \underline{a} / \underline{a}^H \underline{b} = 1$ leads to the optimal solution as before.

Example 4. Since in all the previous examples the approximate method gave the optimal solution, this might lead to a wrong conjecture that it is always equivalent to the optimal procedure. We give a counterexample, where this approximation fails. Assume $\underline{a} = [0.5, 0.5]^T$ and $\underline{b} = [0.5, -0.25]^T$. In this case, by using the exact solver (or the TLS approach) it is easily verified that the optimal solution is $\lambda_1 = 2$, which is the (+)-root $\underline{a}_0 = [0.6, 0.3]^T$ and $\underline{b}_0 = [0.3, 0.15]^T$. Thus, the minimal perturbation is 0.25. The second solution leads to $\lambda_2 = -1/2$ and the implied perturbation turns out to be bigger.

Using the approximation method, we get two possible solutions $\lambda_1 = 0.4$, $\lambda_2 = 4$, and clearly, both are wrong. It turns out that using the first, the perturbation is 0.3879, and using the second, the perturbation is 0.2647, and so we see that for both solutions the result is indeed suboptimal.

4. $n > 1$. The one-eigenvalue case.

4.1. Analysis. We analyze the $n > 1$ case by discussing a simplified problem, where indeed $n > 1$ but only one eigenvalue is known to exist. The optimization problem given in (1) simplifies in this case to

$$(11) \quad \min_{A_0, B_0, \lambda, \underline{v}} \|A_0 - A\|_F^2 + \|B_0 - B\|_F^2$$

$$\text{subject to } (A_0 - \lambda B_0)\underline{v} = 0 \quad \text{and} \quad \|\underline{v}\|_2^2 = 1,$$

where A, B are given.

As we shall see, this case corresponds to the assumption that the perturbation on the pair (A, B) is rank-one. Similar to the analysis for $n = 1$, we find an equivalent constraint-free optimization problem that simplifies the overall solution.

THEOREM 4. *The optimization problem posed in (11) is equivalent to the optimization problem*

$$(12) \quad \min_{\{\lambda, \underline{v}\}} \frac{\|(A - \lambda B)\underline{v}\|_2^2}{1 + |\lambda|^2} \quad \text{subject to } \|\underline{v}\|_2^2 = 1.$$

The optimal solution for A_0 and B_0 is obtained by a rank-one perturbation to the original pair A and B :

$$(13) \quad A_0 = A - \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H \quad \text{and} \quad B_0 = B + \lambda^* \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H.$$

Proof. To solve the optimization problem in (11), we express it by distinguishing the real part (x-part) and the imaginary part (y-part) of each variable. We solve the problem by the Lagrange multipliers method. We define a Lagrangian function

$$(14) \quad \mathcal{L}\{A_x^0, A_y^0, B_x^0, B_y^0\}$$

$$= \frac{1}{2}(\|A_x^0 - A_x\|_F^2 + \|A_y^0 - A_y\|_F^2 + \|B_x^0 - B_x\|_F^2 + \|B_y^0 - B_y\|_F^2)$$

$$+ \gamma_1^T [(A_x^0 - \lambda_x B_x^0 + \lambda_y B_y^0)\underline{v}_x - (A_y^0 - \lambda_y B_x^0 - \lambda_x B_y^0)\underline{v}_y]$$

$$+ \gamma_2^T [(A_x^0 - \lambda_x B_x^0 + \lambda_y B_y^0)\underline{v}_y + (A_y^0 - \lambda_y B_x^0 - \lambda_x B_y^0)\underline{v}_x]$$

$$+ \delta(\|\underline{v}_x\|_2^2 + \|\underline{v}_y\|_2^2 - 1).$$

The vectors $\underline{\gamma}_x, \underline{\gamma}_y$ and the scalar δ are the Lagrange multipliers of the constraints. Taking derivatives with respect to A_x^0, A_y^0, B_x^0 , and B_y^0 , we get

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial A_x^0} &= A_x^0 - A_x + \underline{\gamma}_1 \underline{v}_x^T + \underline{\gamma}_2 \underline{v}_y^T = 0, \\ \frac{\partial \mathcal{L}}{\partial A_y^0} &= A_y^0 - A_y - \underline{\gamma}_1 \underline{v}_y^T + \underline{\gamma}_2 \underline{v}_x^T = 0, \\ \frac{\partial \mathcal{L}}{\partial B_x^0} &= B_x^0 - B_x - \lambda_x \underline{\gamma}_1 \underline{v}_x^T + \lambda_y \underline{\gamma}_1 \underline{v}_y^T - \lambda_x \underline{\gamma}_2 \underline{v}_y^T - \lambda_y \underline{\gamma}_2 \underline{v}_x^T = 0, \\ \frac{\partial \mathcal{L}}{\partial B_y^0} &= B_y^0 - B_y + \lambda_y \underline{\gamma}_1 \underline{v}_x^T + \lambda_x \underline{\gamma}_1 \underline{v}_y^T + \lambda_y \underline{\gamma}_2 \underline{v}_y^T - \lambda_x \underline{\gamma}_2 \underline{v}_x^T = 0.\end{aligned}$$

From this equation, we can deduce that

$$(15) \quad A_0 = A - \underline{\gamma} \underline{v}^H, \quad B_0 = B + \lambda^* \underline{\gamma} \underline{v}^H,$$

with $\gamma = \gamma_1 + i\gamma_2$. These expressions validate our claim regarding the rank-one update. Using the constraint $(A_0 - \lambda B_0) \underline{v} = \underline{0}$, we obtain

$$\begin{aligned}0 &= (A_0 - \lambda B_0) \underline{v} = (A - \lambda B) \underline{v} - (\underline{\gamma} \underline{v}^H + |\lambda|^2 \underline{\gamma} \underline{v}^H) \underline{v} \\ &= (A - \lambda B) \underline{v} - (1 + |\lambda|^2) \underline{\gamma},\end{aligned}$$

where we have used the constraint $\|\underline{v}\|^2 = 1$. Thus,

$$(16) \quad \underline{\gamma} = \frac{(A - \lambda B) \underline{v}}{1 + |\lambda|^2}.$$

Using this in (15), we get

$$(17) \quad A_0 = A - \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H \quad \text{and} \quad B_0 = B + \lambda^* \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H.$$

For an eigenpair $\{\lambda, \underline{v}\}$ we may compute A_0 and B_0 using this equation, and the perturbation can be derived easily, leading to

$$(18) \quad \begin{aligned}\|A_0 - A\|_F^2 + \|B_0 - B\|_F^2 &= \left\| \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H \right\|_F^2 + \left\| \lambda^* \frac{A - \lambda B}{1 + |\lambda|^2} \underline{v} \underline{v}^H \right\|_F^2 \\ &= \frac{\|(A - \lambda B) \underline{v} \underline{v}^H\|_F^2}{1 + |\lambda|^2} = \frac{\|(A - \lambda B) \underline{v}\|_2^2}{1 + |\lambda|^2}.\end{aligned}$$

Here we used the property $\|\underline{u} \underline{z}^H\|_F^2 = \|\underline{u}\|_2^2 \cdot \|\underline{z}\|_2^2$ and the fact that $\|\underline{v}\|_2^2 = 1$. Note that, as in the $n = 1$ case, we get a similar relation to the heuristic function $\|(A - \lambda B) \underline{v}\|_2$ described in section 2, but there is an additional force that moves the eigenvalue away from the origin.

Finally, it is clear that minimizing this function with respect to $\lambda_x, \lambda_y, \underline{v}_x, \underline{v}_y$ leads to the optimal solution of both problems posed in (11) and (12), as claimed.

For $n = 1$ we have that \underline{v} is a scalar of unit norm. Thus $\underline{v} \underline{v}^H = \underline{v}^H \underline{v} = 1$, and from (13) and (12) we obtained the results stated in (3) and (5). \square

This suggests that, instead of solving the problem given by (11), finding optimal A_0, B_0, λ , and \underline{v} , one can solve the problem presented in (12) and find optimal values

for λ and \underline{v} only. These optimal values can be used in (13) to obtain optimal A_0 and B_0 as well.

An interesting consequence of the above result is that evaluation of pseudospectra for nonsquare pencils can be performed using the function $\sigma_{\min}(A - \lambda B)/\sqrt{1 + |\lambda|^2}$. This is a generalization of the function $\sigma_{\min}(A - \lambda I)$ used for the square pseudospectra case.

In case there are several such candidate eigenpair solutions, one could check each by computing the perturbation obtained and choose the solution that leads to the smallest value. This perturbation is given simply by $\|(A - \lambda B)\underline{v}\|_2/\sqrt{1 + |\lambda|^2}$. In fact, multiple solutions for (12) may lead to the solution of the more general case of having more than one eigenpair.

The problem of finding the optimal eigenpair remains. We next show the necessary conditions on $\{\lambda, \underline{v}\}$ for both optimization problems.

THEOREM 5. *The necessary conditions on $\{\lambda, \underline{v}\}$ to solve both optimization problems posed in (11) and (12) are given by*

$$(19) \quad \underline{v}^H (B^H + \lambda A^H)(A - \lambda B)\underline{v} = 0,$$

$$(20) \quad (A - \lambda B)^H (A - \lambda B)\underline{v} = \alpha \underline{v}$$

for the real and positive scalar $\alpha = \underline{v}^H (A - \lambda B)^H (A - \lambda B)\underline{v}$.

Proof. Returning to the Lagrangian function in (14) and taking derivatives with respect to λ_x, λ_y , we get

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \lambda_x} &= -\gamma_1^T B_x^0 \underline{v}_x + \gamma_1^T B_y^0 \underline{v}_y - \gamma_2^T B_x^0 \underline{v}_y - \gamma_2^T B_y^0 \underline{v}_x = 0, \\ \frac{\partial \mathcal{L}}{\partial \lambda_y} &= \gamma_1^T B_y^0 \underline{v}_x + \gamma_1^T B_x^0 \underline{v}_y + \gamma_2^T B_y^0 \underline{v}_y - \gamma_2^T B_x^0 \underline{v}_x = 0. \end{aligned}$$

In fact, we have

$$\begin{aligned} \underline{v}^H B_0^H \underline{\gamma} = 0 \text{ or } 0 &= \underline{v}^H \left(B^H + \underline{v} \underline{v}^H \lambda \frac{A^H - \lambda^* B^H}{1 + |\lambda|^2} \right) \frac{(A - \lambda B) \underline{v}}{1 + |\lambda|^2} \\ (21) \quad &= \underline{v}^H \frac{(B^H + \lambda A^H)(A - \lambda B)}{(1 + |\lambda|^2)^2} \underline{v}. \end{aligned}$$

The denominator may be discarded since $1 + |\lambda|^2 \geq 1$. The resemblance to (4) is evident. Note also that for $n = 1$ this immediately leads to (4). To validate our claim in Theorem 1 that the (+)-root is the proper solution, we take the second derivative of (5) with respect to λ (done properly, with real and imaginary parts separated) and show that this derivative is negative for the (+)-root. The function we refer to is

$$(22) \quad f(\lambda) = \frac{\|\underline{a} - \lambda \underline{b}\|_2^2}{1 + |\lambda|^2} = \frac{\|\underline{a}_x - \lambda_x \underline{b}_x + \lambda_y \underline{b}_y\|_2^2 + \|\underline{a}_y - \lambda_x \underline{b}_y - \lambda_y \underline{b}_x\|_2^2}{1 + |\lambda_x|^2 + |\lambda_y|^2}.$$

We skip the algebraic steps of the derivative, as those are elementary (and tedious). It can be shown that the second derivative is indeed negative. Equation (4) will be shown as a consequence of the next theorem.

Returning to the $n > 1$ case, we see that any nontrivial solution (i.e., $\|\underline{v}\|_2^2 = 1$) for the equation

$$(23) \quad \underline{v}^H [\lambda^2 A^H B + \lambda(B^H B - A^H A) - B^H A] \underline{v} = \underline{v}^H (B^H + \lambda A^H)(A - \lambda B) \underline{v} = 0$$

is a candidate for the minimum point of the problem in (11). Another constraint on the solution is given by taking a derivative of the Lagrangian in (14) with respect to $\underline{v}_x, \underline{v}_y$. In this way we get

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \underline{v}_x} &= (A_x^0 - \lambda_x B_x^0 + \lambda_y B_y^0)^T \underline{\gamma}_1 + (A_x^0 - \lambda_y B_x^0 - \lambda_x B_y^0)^T \underline{\gamma}_2 + 2\delta \underline{v}_x = \underline{0}, \\ \frac{\partial \mathcal{L}}{\partial \underline{v}_y} &= -(A_y^0 - \lambda_y B_x^0 - \lambda_x B_y^0)^T \underline{\gamma}_1 + (A_x^0 - \lambda_x B_x^0 + \lambda_y B_y^0)^T \underline{\gamma}_2 + 2\delta \underline{v}_y = \underline{0}. \end{aligned}$$

Joining these together, we obtain

$$\begin{aligned} (24) \quad \underline{0} &= (A_0 - \lambda B_0)^H \underline{\gamma} + 2\delta \underline{v} \\ &= \left[(A - \lambda B) - (1 + |\lambda|^2) \frac{(A - \lambda B)}{1 + |\lambda|^2} \underline{v} \underline{v}^H \right]^H \frac{(A - \lambda B) \underline{v}}{1 + |\lambda|^2} + 2\delta \underline{v} \\ &= \frac{(I - \underline{v} \underline{v}^H) (A - \lambda B)^H (A - \lambda B) \underline{v}}{1 + |\lambda|^2} + 2\delta \underline{v}. \end{aligned}$$

Multiplying both sides by \underline{v}^H from the left and exploiting again the unit norm of \underline{v} yields

$$(25) \quad 0 = (\underline{v}^H - \underline{v}^H) (A - \lambda B)^H (A - \lambda B) \underline{v} + 2(1 + |\lambda|^2)\delta = 2(1 + |\lambda|^2)\delta,$$

implying that $\delta = 0$. Thus (24) becomes

$$0 = (I - \underline{v} \underline{v}^H) (A - \lambda B)^H (A - \lambda B) \underline{v}.$$

The matrix $(I - \underline{v} \underline{v}^H)$ is a projection matrix with a null space spanned by the vector \underline{v} . Thus, this leads to the requirement

$$(26) \quad (A - \lambda B)^H (A - \lambda B) \underline{v} = \alpha \underline{v}$$

for the real and positive scalar $\alpha = \underline{v}^H (A - \lambda B)^H (A - \lambda B) \underline{v}$. To conclude this part, the optimal eigenpair λ, \underline{v} should satisfy (23) and (26), as claimed by Theorem 5. Note that these two requirements could be derived directly from (12). \square

The two proposed requirements on the optimal λ and \underline{v} cannot be solved analytically. Instead, we propose a numerical algorithm for their solution, leading to the minimization of the function given in (12).

4.2. Numerical algorithm. From our understanding gained in Theorem 4, and the necessary conditions on λ and \underline{v} in Theorem 5, we propose a numerical algorithm to minimize (12). The algorithm requires a proper initialization guess for λ . Using (21), we obtain $\underline{v}^H B_0^H (A - \lambda B) \underline{v} = \underline{0}$. This equation can be approximated by the solution of $B^H (A - \lambda B) \underline{v} = \underline{0}$, which is a square generalized eigenvalue problem and equivalent to the problem $(B^\dagger A - \lambda I) \underline{v} = \underline{0}$, and this can serve for the computation of the initial values.

Given an initial λ , the optimal \underline{v} is obtained by the right singular vector corresponding to the smallest singular value of $(A - \lambda B)^H (A - \lambda B)$, as suggested above. Using this updated vector, from (19) we obtain a quadratic equation with respect to λ . In the spirit of our discussion in section 3, we choose the (+)-root, leading to the minimum of the function with respect to λ . This process is repeated, alternating between an updated λ and an updated \underline{v} until convergence. Algorithm A is a pseudocode description of this algorithm.

ALGORITHM A. *Numerical algorithm for the minimization of the $n > 1$ case with one eigenpair.*

Task: Minimize $\|(A - \lambda B)\underline{v}\|_2^2 / (1 + |\lambda|^2)$ with respect to λ and \underline{v} .

Initialization: Choose initial λ from $(B^H A - \lambda B^H B)\underline{v} = 0$.

Repeat until convergence:

- Update \underline{v} : Compute \underline{v} as the right singular vector corresponding to the smallest singular value of the matrix $A - \lambda B$.
- Update λ : Choose λ as the (+)-root of the scalar quadratic equation $\underline{v}^H (B^H + \lambda A^H) (A - \lambda B) \underline{v}$.

Finalize: With λ and \underline{v} compute A_0 and B_0 using (17).

THEOREM 6. *Algorithm A is guaranteed to converge to a local minimum of the function $f(\lambda, \underline{v}) = \|(A - \lambda B)\underline{v}\|_2^2 / (1 + |\lambda|^2)$.*

Proof. For the case $n = 1$, the convergence is established in one step, since the update of \underline{v} is unnecessary, and the solution is given by solving the quadratic equation for λ .

Let us look at the function $f(\lambda, \underline{v})$ at the k th iteration and treat the general $n > 1$ case. For a current solution \underline{v}_k , we have two candidate solutions for λ_{k+1} by solving the quadratic equation (23). The solutions are

$$\lambda_{k+1}^{\pm} = \frac{-\underline{v}_k B^H B \underline{v}_k + \underline{v}_k A^H A \underline{v}_k \pm \sqrt{(\underline{v}_k B^H B \underline{v}_k - \underline{v}_k A^H A \underline{v}_k)^2 + 4(\underline{v}_k A^H B \underline{v}_k)^2}}{2\underline{v}_k A^H B \underline{v}_k}.$$

It can be shown that the second derivative of $f(\lambda, \underline{v})$ for fixed \underline{v}_k and the two solutions for λ_{k+1} are proportional to

$$\mp \sqrt{(\underline{v}_k B^H B \underline{v}_k - \underline{v}_k A^H A \underline{v}_k)^2 + 4(\underline{v}_k A^H B \underline{v}_k)^2}.$$

Thus the (+)-root is the minimizer of $f(\lambda, \underline{v})$, and we get that

$$f(\lambda_{k+1}, \underline{v}_k) \leq f(\lambda_k, \underline{v}_k).$$

Given λ_{k+1} , we update \underline{v}_{k+1} by choosing the rightmost singular vector of the matrix $A - \lambda_{k+1} B$, and it immediately follows that

$$\|(A - \lambda_{k+1} B)\underline{v}_{k+1}\|_2^2 \leq \|(A - \lambda_{k+1} B)\underline{v}_k\|_2^2.$$

Thus we obtain

$$0 \leq f(\lambda_{k+1}, \underline{v}_{k+1}) \leq f(\lambda_{k+1}, \underline{v}_k) \leq f(\lambda_k, \underline{v}_k),$$

which guarantees convergence. \square

4.3. Example. Theoretical analysis of the rate of convergence is difficult. Extensive experiments consistently show successful convergence at a rate similar to that shown in the examples below. In those experiments we see a linear rate of convergence. We define the rate of convergence as

$$r(k) = \frac{f(\lambda_{k+1}, \underline{v}_{k+1}) - f(\lambda_{\infty}, \underline{v}_{\infty})}{f(\lambda_k, \underline{v}_k) - f(\lambda_{\infty}, \underline{v}_{\infty})}.$$

Figure 5 presents a graph of $r(k)$ as a function of k for a specific yet representative

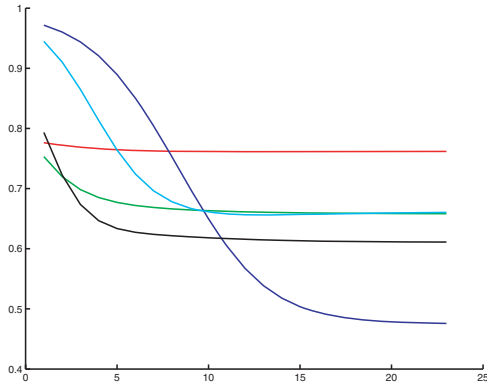


FIG. 5. Convergence of $r(k)$ as a function of k for a 15×5 matrix with $\sigma = 0.1$.

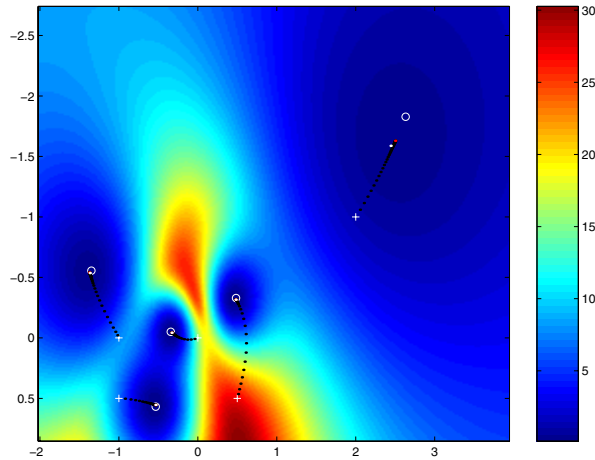


FIG. 6. The function $f(\lambda) = \sigma_{\min}(A - \lambda B)$ using $\sigma = 0.1$.

example. The pencil was chosen to be of size 15×5 , generated similarly to those described in section 2 and with $\sigma = 0.1$. We plotted the five different curves obtained with different initial values chosen manually (such that they are far worse than the ones found by the proposed squaring approach). As can be seen, $r(k)$ tends to stabilize to a constant value, indicating linear convergence.

In Figure 6, the function

$$f(\lambda) = \min_{\underline{v}} \frac{\|(A - \lambda B)\underline{v}\|_2^2}{1 + |\lambda|^2}$$

is visualized, along with the iterative process using the same experiment mentioned above with $\sigma = 0.1$ (note that this time we used complex entries so that the function is no longer symmetric). The +’s mark the manually chosen initial points, and the white points are the initial points that could have been obtained by the squaring method (those points are much closer to the steady-state solution). The o’s mark the true eigenvalues of the clear matrix pair (A_0, B_0) . The black dots present the iterative

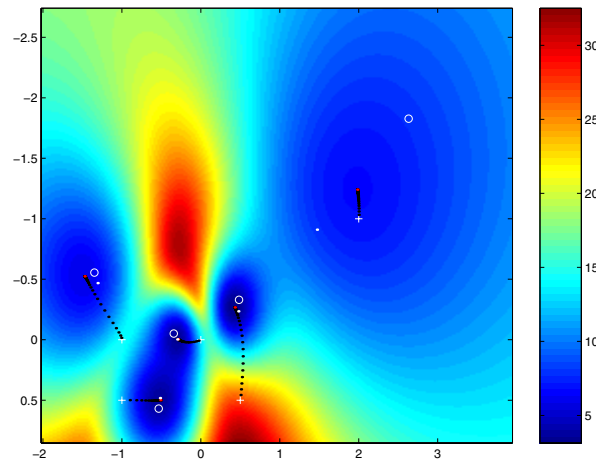


FIG. 7. The function $f(\lambda) = \sigma_{\min}(A - \lambda B)$ using $\sigma = 0.5$.

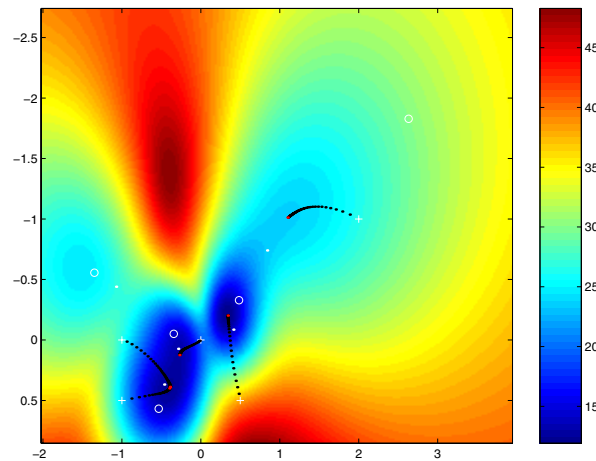


FIG. 8. The function $f(\lambda) = \sigma_{\min}(A - \lambda B)$ using $\sigma = 1.0$.

algorithm results. We can see that convergence to near optimal values is obtained, especially for those eigenvalues near the origin.

Figures 7 and 8 present a similar simulation for stronger noise. Figure 7 corresponds to $\sigma = 0.5$ and Figure 8 to $\sigma = 1$. As can be seen, the analyzed function's local minima points deviate gradually from the true values. As the noise gets stronger, some local minima may vanish altogether.

The simulations of the proposed algorithm and the creation of all the figures were performed using MATLAB. A typical run-time of the algorithm for the matrix sizes involved takes approximately 1–2 seconds for 20 iterations.

5. Relation to pseudospectra. For the regular eigenvalue problem with a square matrix A , we define λ as the eigenvalues of A satisfying the condition $(A - \lambda I)\underline{v} = \underline{0}$ for some nonzero n -vector \underline{v} . We write also that $\lambda \in \Lambda(A)$. Similarly, $\lambda \in \Lambda(A, B)$ refers to the generalized eigenvalues of the (possibly nonsquare) pencil $A - \lambda B$. A pseudospectra of a matrix extends the concept of eigenvalues and

generalized eigenvalues and considers their location due to perturbation of the matrices involved [23] (see also [3, 15, 19, 18] for a relation of this concept to stability). The notion of pseudospectra in general, and for rectangular pencils in particular, is a relatively recent subject of research. The definition of pseudospectra for the square case is given in [23]:

$$\Lambda_\epsilon(A) = \{z \in \Lambda(A + E) : \|E\|_F \leq \epsilon\}.$$

Many papers treat the square case [2, 11, 10, 24, 25]. For a comprehensive survey see [23]. A treatment of the nonsquare pencil is addressed in [25, 11] by generalizing the definition of Van Dorsselaer for pencils to⁵

$$\Lambda_\epsilon(A, B) = \{z : \exists \underline{u} \neq 0, (A + E)\underline{u} = z(B + F)\underline{u} \quad \forall \|E\|_F^2 + \|F\|_F^2 \leq \epsilon\}.$$

Clearly, the resemblance to our problem is evident. Analysis of the pseudospectra is primarily concerned with the patterns of eigenvalue location due to perturbation of the involved matrices. The above definition creates a cloud of points that correspond to all possible perturbation matrices E and F in the permissible range.

Referring to the above definition, our approach is similar and closely related. If we apply this definition to a nonsquare pencil with more rows than columns, it is most likely that this pseudospectra set will be empty. As we increase the perturbation energy ϵ , at some point we hit a solvable pair for which there are eigenvalues and the pseudospectra set is no longer empty. This is the solution of our proposed approach, since we seek the closest solvable pair. Thus, for a given starting pair of matrices A, B our method finds the minimal ϵ that leads to a nonempty pseudospectra. Moreover, our approach yields the exact perturbation that gets such a set of eigenvalues, and the eigenvalues themselves. In a way, we may refer to our approach as an *inverse pseudospectra* analysis of the treated pencil.

As a last comment in this discussion, we note that pseudospectra for a square matrix A is practically computed by studying the function $f(\lambda) = \sigma_{\min}(A - \lambda I)$ [23]. When we are working with matrix pencils, and allowing perturbation in both A and B , this function needs to be changed to $f(\lambda) = \sigma_{\min}(A - \lambda B) / \sqrt{1 + |\lambda|^2}$. The close relation between these two choices can be easily explained if one returns to Theorem 3 and discusses the maximum likelihood estimation of A_0 in the case when B is chosen to be fixed. Then, with the constraint $B_0 = B$, we obtain a target function without the denominator $\sqrt{1 + |\lambda|^2}$. Indeed, in the case of $B = I$, we return to the original function used by the pseudospectra.

6. A simplifying factorization. There are several ways to prefactorize the involved matrices A and B to simplify their structure, prior to the application of the numerical algorithm proposed here (see, for example, [21]). In this section we present one such way, which serves two different objectives: (i) requiring less computation in the iterative algorithm, and (ii) obtaining a bound on the error of the squaring initialization method. The proposed algorithm is a combination of the QR transformation and the GSVD due to Van Loan (cf. page 465 in [13] and [20]). A similar decomposition was given in [16, 17].

⁵The definition of pseudospectra used in [25] is actually slightly different, using separate and independent bounds on the perturbation of each of the two matrices involved. We chose to describe here a variant of their definition that aligns well with our point of view.

6.1. The factorization. We start our description with the assumption that $m \geq 2n$ (there are at least twice as many rows as there are columns in the pencil). The general case will be treated later.

THEOREM 7. *Consider a rectangular matrix pencil, defined by the two matrices $A, B \in \mathcal{M}^{m,n}$. An $m \times m$ unitary matrix W and an $n \times n$ invertible matrix X can be found such that*

$$A = W \begin{pmatrix} A_n \\ 0 \\ 0 \end{pmatrix} X^H, \quad B = W \begin{pmatrix} G \\ B_n \\ 0 \end{pmatrix} X^H,$$

with A_n, B_n two diagonal matrices with nonnegative terms such that $A_n^T A_n + B_n^T B_n = I_n$, and G is a full square matrix.⁶

Proof. First, apply a QR decomposition to the matrix $[A \ B]$. Consider the obtained upper triangular matrices $A_1 = QA$ and $B_1 = QB$. Applying the GSVD to the matrices $A_1(1 : n, :)$ and $B_1(n + 1 : 2n, :)$, we obtain two $n \times n$ unitary matrices U, V and an $n \times n$ invertible matrix X such that

$$A_1 = UA_n X^H, \quad B_1 = VB_n X^H,$$

with $A_n^T A_n + B_n^T B_n = I_n$. Defining the $m \times m$ unitary matrix $W := Q(U \oplus V \oplus I_{m-2n})$, we obtain the desired result. \square

The next theorem extends the above result for the case $n < m < 2n$.

THEOREM 8. *Consider a rectangular matrix pencil, built of the two matrices $A, B \in \mathcal{M}^{m,n}$. An $m \times m$ unitary matrix U and an $n \times n$ invertible matrix X can be found such that*

$$A = Q \begin{pmatrix} A_{m-n} \oplus I_{2n-m} \\ 0_{m-n,n} \end{pmatrix} X^H, \quad B = Q \begin{pmatrix} G \\ [B_{m-n} \ O_{m-n,2n-m}] \end{pmatrix} X^H,$$

where A_{m-n}, B_{m-n} are two $(m - n) \times (m - n)$ diagonal matrices with nonnegative terms such that $A_{m-n}^T A_{m-n} + B_{m-n}^T B_{m-n} = I_{m-n}$, and G is a full square matrix.

The proof of this theorem is omitted, as it immediately follows from the application of the GSVD to two matrices with different number of rows. We should note that we have found a speed-up factor of 2–3 for large matrices when using the factorization before iterating.

6.2. Squaring method for initialization. As a last point in our discussions in this section, we show that based on the factorization algorithm we are able to bound the error induced by the squaring initialization algorithm, as presented in previous sections.

THEOREM 9. *Consider a rectangular matrix pencil, built of the two full rank matrices $A, B \in \mathcal{M}^{m,n}$, and assume $m > 2n$. We denote the pair $\{\lambda_s, \underline{v}_s\}$ as the initialization pair, obtained by solving the square generalized eigenvalue problem $B^H(A - \lambda B)\underline{v} = \underline{0}$. Then, our target function*

$$f(\lambda, \underline{v}) = \frac{\|(A - \lambda B)\underline{v}\|_2^2}{1 + |\lambda|^2}$$

⁶Note that X is the product of an upper triangular matrix with a unitary matrix, which is also easily invertible.

satisfies

$$f(\lambda_s, \underline{v}_s) \leq \|A_n X\|_2^2,$$

where A_n and X are matrices obtained by the factorization given by applying it on the pair $[B, A]$.

Proof. Using the factorization (note that we replaced the order of the treated matrices) we get

$$A = W \begin{pmatrix} G \\ A_n \\ 0 \end{pmatrix} X^H, \quad B = W \begin{pmatrix} B_n \\ 0 \\ 0 \end{pmatrix} X^H.$$

Thus,

$$(27) \quad f(\lambda, \underline{v}) = \frac{\|(A - \lambda B)\underline{v}\|_2^2}{1 + |\lambda|^2} = \frac{\|(G - \lambda B_n)X^H \underline{v}\|_2^2 + \|A_n X^H \underline{v}\|_2^2}{1 + |\lambda|^2}.$$

On the other hand, when using the squaring method, we solve $B^H(A - \lambda B)\underline{v} = 0$. Using again the factorization, we get

$$(28) \quad B^H(A - \lambda B)\underline{v} = X B_n^H (G - \lambda B_n) X^H \underline{v} = 0.$$

Since X is invertible, and since B is full rank, it implies that the multiplication by $X B_n^H$ can be omitted from the above equation without affecting the solution. Thus, the squaring method finds the pair $\{\lambda_s, \underline{v}_s\}$ that solves $(G - \lambda_s B_n) X^H \underline{v}_s = 0$. Substituting this relation in (27), we obtain

$$(29) \quad \begin{aligned} f(\lambda_s, \underline{v}_s) &= \frac{\|(G - \lambda_s B_n)X^H \underline{v}_s\|_2^2 + \|A_n X^H \underline{v}_s\|_2^2}{1 + |\lambda_s|^2} = \frac{\|A_n X^H \underline{v}_s\|_2^2}{1 + |\lambda_s|^2} \\ &\leq \|A_n X^H \underline{v}_s\|_2^2 \leq \|A_n X^H\|_2^2 \leq \|A_n\|_2^2 \|X\|_2^2 \leq \|X\|_2^2, \end{aligned}$$

where we have used $\|\underline{v}_s\|_2 = 1$ and $A_n^T A_n + B_n^T B_n = I_n$. \square

Based on the above theorem we have that for the function $f(\lambda, \underline{v}) = \|A - \lambda B\|_2^2 / (1 + |\lambda|^2)$, we get the relation

$$(30) \quad 0 \leq f(\lambda_{opt}, \underline{v}_{opt}) \leq f(\lambda_s, \underline{v}_s) \leq \|A_n X^H\|_2^2.$$

This implies that from the computable bound we are able to evaluate the proximity of our pencil pair (A, B) to a solvable pair. This result also implies that, while the squaring method does not minimize our penalty function, it performs near-optimal evaluation of the solution by concentrating on the easier part of the penalty, as can be seen in (27).

7. Conclusions and future work. This work has addressed the nonsquare generalized eigenvalue problem. In its general form, the problem we aimed to solve was

$$\begin{aligned} \min_{A_0, B_0, \{\lambda_k, \underline{v}_k\}_{k=1}^n} & \|A_0 - A\|_F^2 + \|B_0 - \mathbf{B}\|_F^2 \\ \text{subject to} & \{(A_0 - \lambda_k B_0)\underline{v}_k = 0, \quad \|\underline{v}_k\|_2^2 = 1\}_{k=1}^n. \end{aligned}$$

In this paper we treated two simplified variations of this problem. Starting with the $n = 1$ case, we showed that it leads to a closed form solution. Then we treated the $n > 1$ case with one eigenpair. For this more general problem we proposed a numerical algorithm and demonstrated its behavior. We presented a new factorization of such rectangular pencils, leading to a simplified implementation.

Work is underway to extend these results and treat the general problem with n eigenpairs as proposed above. Our final goal is to propose a reliable numerical method that can be extended to treat the structured pencil problem.

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