

LYAPUNOV INVERSE ITERATION FOR COMPUTING A FEW RIGHTMOST EIGENVALUES OF LARGE GENERALIZED EIGENVALUE PROBLEMS

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Abstract. In linear stability analysis of a large-scale dynamical system, we need to compute the rightmost eigenvalue(s) for a series of large generalized eigenvalue problems. Existing iterative eigenvalue solvers are not robust when no estimate of the rightmost eigenvalue(s) is available. In this study, we show that such an estimate can be obtained from Lyapunov inverse iteration applied to a special eigenvalue problem of Lyapunov structure. Furthermore, we generalize the analysis to a deflated version of this problem, and propose an algorithm that computes a few rightmost eigenvalues for the eigenvalue problems arising from linear stability analysis. Numerical experiments demonstrate the robustness of the algorithm.

1. Introduction. This paper introduces a robust algorithm for computing a few rightmost eigenvalues of generalized eigenvalue problems. In particular, we are concerned with problems of the form

$$\mathcal{J}(\alpha)x = \mu \mathbf{M}x \quad (1.1)$$

arising from linear stability analysis (see [8]) of the dynamical system

$$\mathbf{M}u_t = f(u, \alpha). \quad (1.2)$$

$\mathbf{M} \in \mathbb{R}^{n \times n}$ is called the mass matrix, and the parameter-dependent matrix $\mathcal{J}(\alpha) \in \mathbb{R}^{n \times n}$ is the Jacobian matrix $\frac{\partial f}{\partial u}(\bar{u}(\alpha), \alpha) = \frac{\partial f}{\partial u}(\alpha)$, where $\bar{u}(\alpha)$ is the steady-state solution to (1.2) at α , *i.e.*, $f(\bar{u}, \alpha) = 0$. Let the solution path be the following set: $\mathcal{S} = \{(\bar{u}, \alpha) | f(\bar{u}, \alpha) = 0\}$. We seek the critical point (\bar{u}_c, α_c) associated with transition to instability on \mathcal{S} . Our primary interest is (1.2) arising from spatial discretization of 2- or 3-dimensional, time-dependent partial differential equations (PDEs). Therefore, we assume n to be large and $\mathcal{J}(\alpha), \mathbf{M}$ to be sparse throughout this paper.

The conventional method of locating the critical parameter α_c is to monitor the rightmost eigenvalue(s) of (1.1) while marching along \mathcal{S} using numerical continuation (see [8]). In the stable regime of \mathcal{S} , the eigenvalues μ of (1.1) all lie to the left of the imaginary axis; as (\bar{u}, α) approaches the critical point, the rightmost eigenvalue of (1.1) moves towards the imaginary axis; at (\bar{u}_c, α_c) , the rightmost eigenvalue of (1.1) has real part zero, and finally, in the unstable regime, the rightmost eigenvalue of (1.1) has positive real part. The continuation usually starts from a point (\bar{u}_0, α_0) in the stable regime of \mathcal{S} and the critical point is detected when the real part of the rightmost eigenvalue of (1.1) becomes nonnegative. Consequently, the robustness and efficiency of the eigenvalue solver for the rightmost eigenvalue(s) of (1.1) are crucial for the performance of this method. Direct eigenvalue solvers such as the QR and QZ algorithms (see [11]) compute all the eigenvalues of (1.1), but they are too expensive for large n . Existing iterative eigenvalue solvers (see [11]) are able to compute a small set ($k \ll n$) of eigenvalues of (1.1) near a given shift $\sigma \in \mathbb{C}$ efficiently. For example, they work well when k eigenvalues of (1.1) with smallest modulus are sought, in which case $\sigma = 0$. However, in the computation of the rightmost eigenvalue(s), there is no good way to determine the value of σ .

Meerbergen and Spence [9] proposed the Lyapunov inverse iteration that estimates the critical parameter α_c without computing the rightmost eigenvalue(s) of (1.1). Assume (\bar{u}_0, α_0) is in the stable regime of \mathcal{S} and is also in the neighborhood of the critical point (\bar{u}_c, α_c) . Let $\lambda_c = \alpha_c - \alpha_0$ and $\mathbf{A} = \mathcal{J}(\alpha_0)$. Then the Jacobian matrix $\mathcal{J}(\alpha_c)$ at the critical point can be approximated by $\mathbf{A} + \lambda_c \mathbf{B}$ where $\mathbf{B} = \frac{d\mathcal{J}}{d\alpha}(\alpha_0)$. It is shown in [9] that λ_c is the eigenvalue with smallest modulus of the special eigenvalue problem $\mathbf{A} \mathbf{Z} \mathbf{M}^T + \mathbf{M} \mathbf{Z} \mathbf{A}^T + \lambda(\mathbf{B} \mathbf{Z} \mathbf{M}^T + \mathbf{M} \mathbf{Z} \mathbf{B}^T) = 0$ and that λ_c can be computed by a matrix version of inverse iteration. Estimates of the rightmost eigenvalue(s) of (1.1) at α_c can be obtained as by-products. Elman *et al.* [5] refined the Lyapunov inverse iteration

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proposed in [9] to make it more robust and efficient, and examined its performance on challenging test problems arising from fluid dynamics.

The method proposed in [5, 9], although it allows us to estimate the critical value of the parameter without computing the rightmost eigenvalue of (1.1), only works in the neighborhood of the critical point (\bar{u}_c, α_c) . In [5], for instance, the critical parameter value α_c of all numerical examples is known *a priori*, so that we can pick a point (\bar{u}_0, α_0) close to (\bar{u}_c, α_c) and apply Lyapunov inverse iteration with confidence. In reality, α_c is unknown and we start from a point (\bar{u}_0, α_0) in the stable regime of \mathcal{S} which is distant from the critical point, then the method of [5, 9] cannot be used to estimate α_c , since $\mathcal{J}(\alpha_c)$ cannot be approximated by $\mathbf{A} + \lambda_c \mathbf{B}$ anymore. However, some quantitative information about how far away (\bar{u}_0, α_0) is from the critical point can still be obtained by estimating the distance between the rightmost eigenvalue(s) of (1.1) at (\bar{u}_0, α_0) and the imaginary axis: if the rightmost eigenvalue is far away from the imaginary axis, then it is reasonable to assume that (\bar{u}_0, α_0) is far away from the critical point as well, and therefore we should march along \mathcal{S} using numerical continuation until we are close enough to (\bar{u}_c, α_c) ; otherwise, we can assume that (\bar{u}_0, α_0) is already in the neighborhood of the critical point and the method of [5, 9] can be applied to estimate α_c .

The goal of this paper is to develop a robust method to compute a few rightmost eigenvalues of (1.1) at any point in the stable regime of \mathcal{S} . The plan of this paper is as follows. In section 2, we show that the distance between the rightmost eigenvalue(s) of (1.1) and the imaginary axis is in fact the eigenvalue with smallest modulus of an $n^2 \times n^2$ eigenvalue problem with a special Kronecker structure. This means that this eigenvalue can be computed efficiently by Lyapunov inverse iteration. In section 3, we present numerical results for several examples arising from fluid dynamics. In section 4, we show that the analysis of section 2 can be generalized to a deflated version of the $n^2 \times n^2$ eigenvalue problem, which leads to an algorithm for computing k ($1 \leq k \ll n$) rightmost eigenvalues of (1.1). Finally, we make some concluding remarks in section 5.

2. Computing the distance between the rightmost eigenvalue(s) and the imaginary axis. Let (\bar{u}_0, α_0) be any point in the stable regime of \mathcal{S} and assume \mathbf{M} is nonsingular in (1.1). Let (μ_j, x_j) ($\|x_j\|_2 = 1$, $j = 1, 2, \dots, n$) be the eigenpairs of (1.1) at (\bar{u}_0, α_0) , where the real parts of μ_j , $Re(\mu_j)$, are in decreasing order, i.e., $0 > Re(\mu_1) \geq Re(\mu_2) \geq \dots \geq Re(\mu_n)$. Then the distance between the rightmost eigenvalue(s) and the imaginary axis is $-Re(\mu_1)$. Let $\mathbf{A} = \mathcal{J}(\alpha_0)$ and $S = \mathbf{A}^{-1}\mathbf{M}$. To compute this distance, we first observe that $-Re(\mu_1)$ is the eigenvalue with smallest modulus of the $n^2 \times n^2$ generalized eigenvalue problem

$$\Delta_1 z = \lambda(-\Delta_0)z, \quad (2.1)$$

where $\Delta_1 = S \otimes I + I \otimes S$ and $\Delta_0 = 2S \otimes S$ (I is the identity matrix of order n). We proceed in two steps to prove this assertion. First, we show that $-Re(\mu_1)$ is an eigenvalue of (2.1).

THEOREM 2.1. *The eigenvalues of (2.1) are $\lambda_{i,j} = -\frac{1}{2}(\mu_i + \mu_j)$, $i, j = 1, 2, \dots, n$. The eigenvector of (2.1) associated with $\lambda_{i,j}$ is $z_{i,j} = \alpha_{i,j}x_i \otimes x_j + \beta_{i,j}x_j \otimes x_i$ for any $\alpha_{i,j}, \beta_{i,j} \in \mathbb{C}$ ($\alpha_{i,j}$ and $\beta_{i,j}$ cannot be zero at the same time).*

Proof. Since (μ_j, x_j) ($j = 1, 2, \dots, n$) are the eigenpairs of $\mathbf{A}x = \mu \mathbf{M}x$, (μ_j^{-1}, x_j) are the eigenpairs of S . For any pair (i, j) ($i, j = 1, 2, \dots, n$) and any $\alpha_{i,j}, \beta_{i,j} \in \mathbb{C}$,

$$\begin{aligned} \Delta_1(\alpha_{i,j}x_i \otimes x_j + \beta_{i,j}x_j \otimes x_i) &= \alpha_{i,j}(S \otimes I + I \otimes S)(x_i \otimes x_j) + \beta_{i,j}(S \otimes I + I \otimes S)(x_j \otimes x_i) \\ &= \alpha_{i,j}[(Sx_i) \otimes x_j + x_i \otimes (Sx_j)] + \beta_{i,j}[(Sx_j) \otimes x_i + x_j \otimes (Sx_i)] \\ &= \alpha_{i,j}(\mu_i^{-1} + \mu_j^{-1})(x_i \otimes x_j) + \beta_{i,j}(\mu_j^{-1} + \mu_i^{-1})(x_j \otimes x_i) \\ &= (\mu_i^{-1} + \mu_j^{-1})(\alpha_{i,j}x_i \otimes x_j + \beta_{i,j}x_j \otimes x_i). \end{aligned}$$

Similarly, we can show that

$$\Delta_0(\alpha_{i,j}x_i \otimes x_j + \beta_{i,j}x_j \otimes x_i) = 2(\mu_i\mu_j)^{-1}(\alpha_{i,j}x_i \otimes x_j + \beta_{i,j}x_j \otimes x_i).$$

Therefore, $\lambda_{i,j} = -\frac{1}{2}\mu_i\mu_j(\mu_i^{-1} + \mu_j^{-1}) = -\frac{1}{2}(\mu_i + \mu_j)$ is an eigenvalue of (2.1) and $z_{i,j}$ is the eigenvector of (2.1) associated with $\lambda_{i,j}$. \square

If μ_1 is real, then $-Re(\mu_1) = -\mu_1 = -\frac{1}{2}(\mu_1 + \mu_1) = \lambda_{1,1}$; if μ_1 is not real (*i.e.*, $\mu_1 = \overline{\mu_2}$ and $x_1 = \overline{x_2}$), then $-Re(\mu_1) = -\frac{1}{2}(\mu_1 + \overline{\mu_1}) = -\frac{1}{2}(\mu_1 + \mu_2) = \lambda_{1,2} = \lambda_{2,1}$. In both cases, by Theorem 2.1, $-Re(\mu_1)$ is an eigenvalue of (2.1).

We next show that $-Re(\mu_1)$ is the eigenvalue of (2.1) with smallest modulus.

THEOREM 2.2. *Assume all the eigenvalues of $\mathbf{A}x = \mu\mathbf{M}x$ lie in the left half of the complex plane. Then the eigenvalue of (2.1) with smallest modulus is $-Re(\mu_1)$.*

Proof. Let $\mu_j = a_j + ib_j$. Then $0 > a_1 \geq a_2 \geq \dots \geq a_n$. If the rightmost eigenvalue of $\mathbf{A}x = \mu\mathbf{M}x$ is real, then $-Re(\mu_1) = \lambda_{1,1}$, and since $0 > a_1 \geq a_2 \geq \dots \geq a_n$, it follows that

$$|\lambda_{1,1}|^2 = \frac{1}{4}(a_1 + a_1)^2 \leq \frac{1}{4}[(a_i + a_j)^2 + (b_i + b_j)^2] = |\lambda_{i,j}|^2$$

for any pair (i, j) . Alternatively, if the rightmost eigenvalues of $\mathbf{A}x = \mu\mathbf{M}x$ consist of a complex conjugate pair, then $a_1 = a_2$, $b_1 = -b_2$, $-Re(\mu_1) = \lambda_{1,2} = \lambda_{2,1}$, and similarly,

$$|\lambda_{1,2}|^2 = |\lambda_{2,1}|^2 = \frac{1}{4}[(a_1 + a_1)^2 + (b_1 - b_1)^2] \leq \frac{1}{4}[(a_i + a_j)^2 + (b_i + b_j)^2] = |\lambda_{i,j}|^2$$

for any pair (i, j) . In both cases, $-Re(\mu_1)$ is the eigenvalue of (2.1) with smallest modulus. \square

Assume $\mathbf{A}x = \mu\mathbf{M}x$ has a complete set of eigenvectors $\{x_j\}_{j=1}^n$. Then (2.1) also has a complete set of eigenvectors $\{x_i \otimes x_j\}_{i,j=1}^n$. By Theorem 2.2, the distance between the imaginary axis and the rightmost eigenvalue(s), $-Re(\mu_1)$, can be found by inverse iteration applied to (2.1). Unfortunately, this approach is not suitable for large n because it involves solving linear systems of order n^2 . In [5, 9], an $n^2 \times n^2$ eigenvalue problem similar to (2.1) is dealt with by rewriting the equation of Kronecker sums into an equation of Lyapunov structure. Here, similarly, we can rewrite (2.1) into

$$SZ + ZS^T + \lambda(2SZS^T) = 0. \quad (2.2)$$

Any eigenpair (λ, z) of (2.1) is related to a solution (λ, Z) of (2.2), which we also refer to as an eigenpair of (2.2), by $z = \text{vec}(Z)$. By Theorem 2.1 and the relation between (2.1) and (2.2), $(\lambda_{i,j}, Z_{i,j})$ ($i, j = 1, 2, \dots, n$) with $Z_{i,j} = \alpha_{i,j}x_jx_i^T + \beta_{i,j}x_ix_j^T$ are the eigenpairs of (2.2); in addition, by Theorem 2.2, $-Re(\mu_1)$ is the eigenvalue of (2.2) with smallest modulus. Furthermore, under certain conditions, $-Re(\mu_1)$ is a simple eigenvalue of (2.2) whose associated eigenvector is real, symmetric and of low rank. Assume the following: (a1) for any $1 < i \leq n$, if $Re(\mu_i) = Re(\mu_1)$, then $\mu_i = \overline{\mu_1}$; (a2) μ_1 is a simple eigenvalue of $\mathbf{A}x = \mu\mathbf{M}x$. Consequently, if μ_1 is real, $-Re(\mu_1)$ is a simple eigenvalue of (2.1) with the eigenvector $z = cx_1 \otimes x_1^T$ for any $c \in \mathbb{C}$; otherwise, $-Re(\mu_1)$ is a double eigenvalue of (2.1) with the eigenvector $z = c_1x_1 \otimes \overline{x_1} + c_2\overline{x_1} \otimes x_1$ for any $c_1, c_2 \in \mathbb{C}$. When the eigenvectors of (2.2) are restricted to the symmetric subspace of $\mathbb{C}^{n \times n}$, by Theorem 2.3 from [9], $-Re(\mu_1)$ is a simple eigenvalue of (2.2) that has a unique (up to a scalar multiplier), real and symmetric eigenvector $Z = x_1x_1^T$ (if μ_1 is real), or $Z = x_1x_1^* + \overline{x_1}x_1^T$ (if μ_1 is not real) where x_1^* denotes the conjugate transpose of x_1 . Therefore, we can apply Lyapunov inverse iteration (see [5, 9]) to (2.2) to find $-Re(\mu_1)$, the eigenvalue of (2.2) with smallest modulus:

Algorithm 1 (Lyapunov inverse iteration for computing $-Re(\mu_1)$)

1. Given $V_1 \in \mathbb{R}^n$ with $\|V_1\|_2 = 1$ and $D_1 = 1$, let $Z_1 = V_1D_1V_1^T$ and $m = 1$.
2. For $\ell = 1, 2, \dots$

2.1. Rank reduction: compute $\tilde{S} = V_\ell^T S V_\ell$ and solve for the eigenvalue $\tilde{\lambda}$ of

$$\tilde{S}\tilde{Z} + \tilde{Z}\tilde{S}^T + \tilde{\lambda}(2\tilde{S}\tilde{Z}\tilde{S}^T) = 0 \quad (2.3)$$

with smallest modulus and its eigenvector $\tilde{Z} = \tilde{V}\tilde{D}\tilde{V}^T$, where $\tilde{V} \in \mathbb{R}^{m \times r}$ and $\tilde{D} \in \mathbb{R}^{r \times r}$ with $\|\tilde{D}\|_F = 1$ and $r = 1$ ($\ell = 1$) or 2 ($\ell \geq 2$).

2.2. Set $Z_\ell = V_\ell \tilde{D} V_\ell^T$ and $\lambda_\ell = \tilde{\lambda}$, where $V_\ell = V_\ell \tilde{V}$.

2.3. If (λ_ℓ, Z_ℓ) is accurate enough, then stop.

2.4. Else, solve for Y_ℓ from

$$SY_\ell + Y_\ell S^T = -2SZ_\ell S^T \quad (2.4)$$

in factored form: $Y_\ell = V_{\ell+1} D_{\ell+1} V_{\ell+1}^T$, where $V_{\ell+1} \in \mathbb{R}^{n \times m}$ and $D_{\ell+1} \in \mathbb{R}^{m \times m}$.

As the iteration proceeds, the iterate $(\lambda_\ell, Z_\ell = \mathcal{V}_\ell \tilde{D}_\ell \mathcal{V}_\ell^T)$ will converge to $(-Re(\mu_1), Z = \mathcal{V} \mathcal{D} \mathcal{V}^T)$ where $\|\mathcal{D}\|_F = 1$ and $\mathcal{V} = x_1$ (if μ_1 is real) or $\mathcal{V} \in \mathbb{R}^{n \times 2}$ is an orthonormal basis of $\{x_1, \bar{x}_1\}$ (if μ_1 is not real). Besides an estimate of the distance $-Re(\mu_1)$ between the rightmost eigenvalue(s) of $\mathbf{A}x = \mu \mathbf{M}x$ and the imaginary axis, we can also obtain from Algorithm 1 estimates of the rightmost eigenpair(s) of $\mathbf{A}x = \mu \mathbf{M}x$ as by-products. Consider the generalized eigenvalue problem

$$(I + \lambda S)x = \rho Sx. \quad (2.5)$$

THEOREM 2.3. *If $\lambda = \lambda_{i,j} = -\frac{1}{2}(\mu_i + \mu_j)$ ($i, j = 1, 2, \dots, n$) where μ_i, μ_j are eigenvalues of $\mathbf{A}x = \mu \mathbf{M}x$, then (2.5) has a zero eigenvalue, or a pair of eigenvalues that sum to zero.*

Proof. Since $S = \mathbf{A}^{-1} \mathbf{M}$, (μ_j^{-1}, x_j) ($j = 1, 2, \dots, n$) are the eigenpairs of S . For any pair (i, j) ($i, j = 1, 2, \dots, n$),

$$(I + \lambda_{i,j} S)x_i = x_i + \lambda_{i,j} \mu_i^{-1} x_i = (\mu_i + \lambda_{i,j}) \mu_i^{-1} x_i = (\mu_i + \lambda_{i,j}) Sx_i,$$

and similarly, $(I + \lambda_{i,j} S)x_j = (\mu_j + \lambda_{i,j}) Sx_j$. Therefore, if $\lambda = \lambda_{i,i} = -\mu_i$, then (2.5) has a zero eigenvalue associated with the eigenvector x_i ; if $\lambda = \lambda_{i,j} = -\frac{1}{2}(\mu_i + \mu_j)$ with $i \neq j$, then $(\mu_i + \lambda_{i,j}, \mu_j + \lambda_{i,j})$ is a pair of eigenvalues of (2.5) that sum to zero, and the eigenvectors of (2.5) associated with them are (x_i, x_j) . \square

By Theorem 2.3, if $\lambda = -Re(\mu_1)$, then (2.5) has a zero eigenvalue associated with the eigenvector x_1 (if μ_1 is real), or a conjugate pair of pure imaginary eigenvalues $\mu_1 - Re(\mu_1)$ and $\bar{\mu}_1 - Re(\mu_1)$ associated with the eigenvectors x_1 and \bar{x}_1 (if μ_1 is not real). Since λ_ℓ converges to $-Re(\mu_1)$ and \mathcal{V}_ℓ converges to \mathcal{V} , at each iteration of Algorithm 1, by solving the $r \times r$ ($r = 1$ or 2) generalized eigenvalue problem

$$[\mathcal{V}_\ell^T (I + \lambda_\ell S) \mathcal{V}_\ell] y_\ell = \rho_\ell (\mathcal{V}_\ell^T S \mathcal{V}_\ell) y_\ell, \quad (2.6)$$

we obtain estimates of μ_1 and x_1 : $\mu_\ell = -\lambda_\ell + \rho_\ell$, $x_\ell = \mathcal{V}_\ell y_\ell$. To compute the rightmost eigenpair (μ_1, x_1) more accurately, we can use any iterative eigenvalue solver with $\sigma = \mu_\ell$ as the shift.

At each iteration of Algorithm 1, a large-scale Lyapunov equation (2.4) needs to be solved. We can rewrite (2.4) as

$$SY_\ell + Y_\ell S^T = P_\ell C_\ell P_\ell^T \quad (2.7)$$

(see [5] for details) where P_ℓ is orthonormal and is of rank 1 ($\ell = 1$) or 2 ($\ell > 1$). The solution to (2.7), Y_ℓ , is real and symmetric, and frequently has a low rank (see [1]). Since S is large, direct methods such as [2] are not suitable. An iterative method that solves Lyapunov equations with large coefficient matrix and low-rank right-hand side is needed. The Krylov-type methods for (2.7), such as the Rational Krylov Subspace Method (RKSM) [4], seek approximate solutions of the form WXW^T , where $W \in \mathbb{R}^{n \times m}$ ($m \ll n$) is an orthonormal basis of the Krylov subspace and X is the solution to the m -dimensional, projected Lyapunov equation $(W^T S W)X + X(W^T S W)^T = (W^T P_\ell)C_\ell(W^T P_\ell)^T$, which can be solved using direct methods. The main cost of solving (2.7) using Krylov-type methods is approximately m linear solves with coefficient matrix $a\mathbf{A} + b\mathbf{M}$, where values of the scalars a, b depend on the Krylov method of choice.

In step 2.1 (rank reduction) of Algorithm 1, although it may look like computing the Rayleigh quotient $\tilde{S} = V_\ell^T S V_\ell^T$ requires another m linear solves with coefficient matrix \mathbf{A} , in fact, if a Krylov-type method is used to solve (2.7), \tilde{S} can be obtained from the Arnoldi decomposition computed by the Krylov-type method at no cost when $\ell > 1$.

3. Numerical experiments. In this section, we test Algorithm 1 on several problems arising from fluid dynamics. Note that when (1.2) comes from the finite element discretization of Navier-Stokes equations, the mass matrix \mathbf{M} is singular, leading to the infinite eigenvalues of (1.1) and a singular $S = \mathbf{A}^{-1} \mathbf{M}$. As in [5], we use the matrix transformation proposed in [3] to get a nonsingular mass matrix. This transformation maps the infinite eigenvalues of (1.1) to finite ones away from the imaginary axis, and leaves the finite eigenvalues of (1.1) unchanged. From here on, \mathbf{M} refers to the nonsingular mass matrix after the transformation.

3.1. Example 1: driven-cavity flow. Linear stability analysis of this flow is considered in many papers (see [7], for example). The Q_2 - Q_1 mixed finite element discretization (with a 64×64 mesh) of the Navier-Stokes equations gives rise to a generalized eigenvalue problem (1.1) of order $n = 9539$. The parameter α is the Reynolds number defined by $Re = \frac{1}{\nu}$, where ν is the kinematic viscosity. Figure 3.1a depicts the path traced out by the eight rightmost eigenvalues of (1.1) for $Re = 2000, 4000, 6000, 7800$, at which the steady-state solution to (1.2) is stable. As the Reynolds number increases, the eight rightmost eigenvalues all move towards the imaginary axis. In addition, although the rightmost eigenvalue starts off being real, one conjugate pair of complex eigenvalues (whose imaginary parts are about $\pm 3i$) move faster towards the imaginary axis than the other eigenvalues and eventually become the rightmost. They first cross the imaginary axis at $Re \approx 7929$, causing instability in the steady-state solution of (1.2) (see [5]).

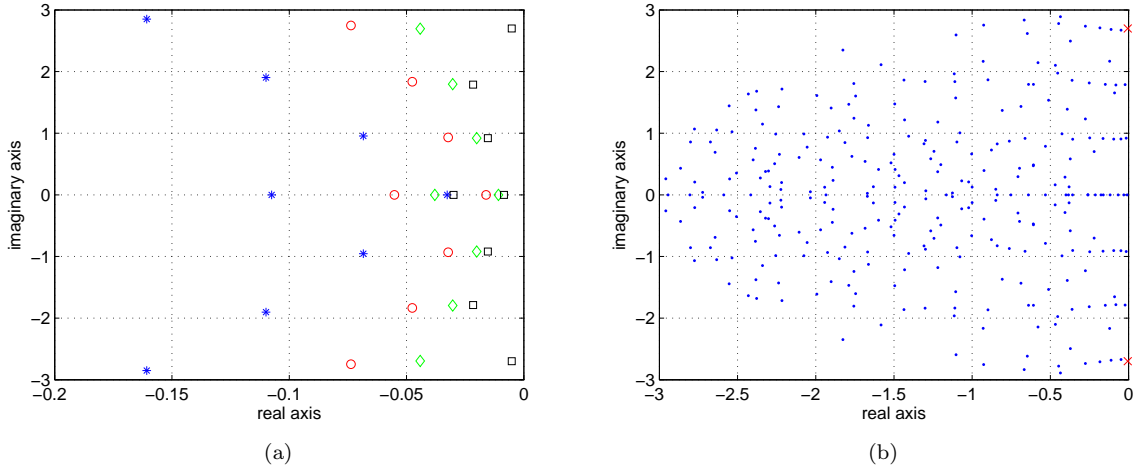


Fig. 3.1: (a) The eight rightmost eigenvalues for driven-cavity flow at different Reynolds numbers (* : $Re = 2000$, o : $Re = 4000$, \diamond : $Re = 6000$, \square : $Re = 7800$). (b) The 300 eigenvalues with smallest modulus at $Re = 7800$ (x: the rightmost eigenvalues).

Finding the conjugate pair of rightmost eigenvalues at a high Reynolds number is difficult in this example. Suppose we are trying to find the rightmost eigenvalues at $Re = 7800$ by conventional methods, such as computing k eigenvalues of (1.1) with smallest modulus using the Implicitly Restarted Arnoldi (IRA) method [10]. If we use the Matlab function ‘eigs’ (which implements IRA) with its default setting, then k has to be as large as 250, since there is a large number of eigenvalues that have smaller modulus than the rightmost pair (see Figure 3.1b). This leads to at least 500 linear solves, and in practice, many more. More importantly, note that the decision $k = 250$ is made based on *a priori* knowledge of where the rightmost eigenvalues lie. In general, we cannot identify a good value for k which guarantees that the rightmost eigenvalues will be found.

For four various Reynolds numbers from 2000 to 7800, we apply Algorithm 1 (with RKSM as the Lyapunov solver) to calculate the distance between the rightmost eigenvalue(s) of (1.1) and the imaginary axis. The results are reported in Table 3.1. At the ℓ^{th} iteration of Algorithm 1, λ_ℓ denotes the estimate of the distance, *i.e.*, the estimate of $-Re(\mu_1)$, (ρ_ℓ, x_ℓ) is the estimated eigenpair of (2.5), $r_\ell = (I + \lambda_\ell S)x_\ell - \rho_\ell Sx_\ell$ is the residual of (2.5), $\mathfrak{R}_\ell = SZ_\ell + Z_\ell S^T + \lambda_\ell(2SZ_\ell S^T)$ is the residual of (2.2), and $R_\ell = SY_\ell + Y_\ell S^T - P_\ell C_\ell P_\ell^T$ is the residual of the Lyapunov solve. Both $\|\mathfrak{R}_\ell\|_F$ and $\|R_\ell\|_F$ are cheap to compute (see [5] for details). The stopping criterion for the Lyapunov solve is $\|R_\ell\|_F < 10^{-9}$, and m_ℓ denotes the dimension of the Krylov subspace needed by RKSM in order to meet this criterion. Therefore, the main cost of each iteration is about m_ℓ linear solves. The initial guess V_1 is chosen to be a random vector (of norm 1) in \mathbb{R}^n and the stopping criterion

for Algorithm 1 is $\|\mathfrak{R}_\ell\|_F < 10^{-8}$. All linear systems are solved using direct methods. Table 3.1 shows that the distances between the rightmost eigenvalue(s) of (1.1) and the imaginary axis at $Re = 2000, 4000, 6000, 7800$ are $3.26410\text{e-}2, 1.60751\text{e-}2, 1.08438\text{e-}2, 5.13509\text{e-}3$, respectively. We also obtain estimates of the rightmost eigenvalue(s) of (1.1), $-\lambda_\ell + \rho_\ell$, at the four Reynolds numbers: $-3.26410\text{e-}2, -1.60751\text{e-}2, -1.08438\text{e-}2$, and $-5.13509\text{e-}3 \pm 2.69845i$.

Table 3.1: Algorithm 1 applied to Example 1 (Lyapunov solver: RKSM)

ℓ	λ_ℓ	ρ_ℓ	$\ r_\ell\ _2$	$\ \mathfrak{R}_\ell\ _F$	$\ R_\ell\ _F$	m_ℓ
Re=2000						
1	8.84383e+2	0	2.41642e+02	1.32049e+02	8.49152e-10	143
2	3.26410e-2	-8.37114e-15	4.48970e-13	2.52377e-11	—	—
Re=4000						
1	-1.77658e+4	0	1.01952e+06	6.58651e+03	9.21268e-10	230
2	1.60751e-2	5.13941e-14	1.94353e-12	4.40201e-10	—	—
Re=6000						
1	1.30124e+3	0	7.46125e+02	8.55652e+02	9.99064e-10	301
2	1.08438e-2	-3.89829e-14	2.18625e-12	7.20713e-10	—	—
Re=7800						
1	6.95951e+2	0	4.78732e+02	6.58622e+02	9.02875e-10	366
2	5.13509e-3	2.69845i	7.60018e-11	3.62567e-11	—	—

3.2. Example 2: flow over an obstacle. For linear stability analysis of this flow, see [5]. The Q_2 - Q_1 mixed finite element discretization (with a 32×128 mesh) of the Navier-Stokes equations gives rise to a generalized eigenvalue problem (1.1) of order $n = 9512$. Figure 3.2a depicts the path traced out by the six rightmost eigenvalues of (1.1) for $Re = 100, 200, 300, 350$ in the stable regime, and Figure 3.2b shows the 300 eigenvalues of (1.1) with smallest modulus at $Re = 350$. (In this example, the Reynolds number $Re = \frac{2}{\nu}$.) As for the previous example, as the Reynolds number increases, the six rightmost eigenvalues all move towards the imaginary axis, and the rightmost eigenvalue changes from being real (at $Re = 100$) to a complex conjugate pair (at $Re = 200, 300, 350$). The rightmost pair of eigenvalues of (1.1) cross the imaginary axis and the steady-state solution to (1.2) loses its stability at $Re \approx 373$.

We again apply Algorithm 1 to estimate the distance between the rightmost eigenvalue(s) of (1.1) and the imaginary axis for the four Reynolds numbers mentioned above. The results are reported in Table 3.2 (see section 3.1 for notation). The stopping criteria for both Algorithm 1 and the Lyapunov solve (2.7) remain unchanged, *i.e.*, $\|\mathfrak{R}_\ell\|_F < 10^{-8}$ and $\|R_\ell\|_F < 10^{-9}$.

Remark. As seen in Tables 3.1 and 3.2, Algorithm 1 converges in just two iterations in many cases. We can show that as long as the first Lyapunov equation $SY_1 + Y_1S^T = P_1C_1P_1^T$ is solved accurately enough, Algorithm 1 will always converge in two iterations (see [6]).

4. Computing k rightmost eigenvalues. In section 2, we have shown that when all the eigenvalues of (1.1) lie in the left half of the complex plane, the distance between the rightmost eigenvalue(s) and the imaginary axis, $-Re(\mu_1)$, is the eigenvalue of (2.2) with smallest modulus. As a result, this eigenvalue can be computed by Lyapunov inverse iteration, which also gives us estimates of the rightmost eigenvalue(s). In section 3, numerical experiments demonstrate the robustness and efficiency of Lyapunov inverse iteration applied to (2.2). As seen in these examples, when we march along the solution path \mathcal{S} , it may be the case that an eigenvalue that is not the rightmost moves towards the imaginary rapidly, becomes the rightmost eigenvalue at some point, and eventually crosses the imaginary axis first, causing instability in the steady-state solution. Therefore, besides the rightmost eigenvalue(s), it is helpful to monitor a few other eigenvalues in the rightmost part of the spectrum as well. In this section, the goal is to discuss how Lyapunov inverse iteration can be applied repeatedly to compute k rightmost eigenvalues of (1.1), where $1 < k \ll n$.

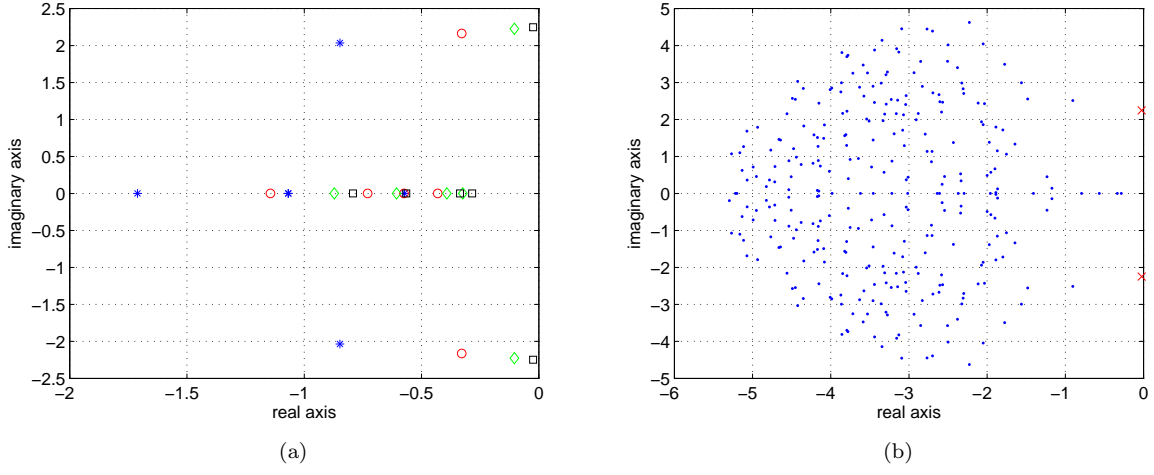


Fig. 3.2: (a) The six rightmost eigenvalues for flow over an obstacle at different Reynolds numbers ($*$: $Re = 100$, \circ : $Re = 200$, \diamond : $Re = 300$, \square : $Re = 350$). (b) The 300 eigenvalues with smallest modulus at $Re = 350$ (\times : the rightmost eigenvalues).

Table 3.2: Algorithm 1 applied to Example 2 (Lyapunov solver: RKSM)

ℓ	λ_ℓ	ρ_ℓ	$\ r_\ell\ _2$	$\ \Re_\ell\ _F$	$\ R_\ell\ _F$	m_ℓ
Re=100						
1	-2.42460e+0	0	5.76523e+0	1.15123e+1	7.07831e-10	48
2	5.72856e-1	-2.01081e-14	8.87207e-6	2.19026e-5	1.44423e-10	20
3	5.72852e-1	-8.48302e-16	2.10538e-7	5.19760e-7	2.59670e-10	12
4	5.72852e-1	1.30404e-15	6.37589e-8	1.57403e-7	6.49978e-10	10
5	5.72852e-1	-1.85924e-15	7.50147e-9	1.85191e-8	6.16387e-10	4
6	5.72852e-1	1.44773e-15	1.23444e-9	3.04748e-9	—	—
Re=200						
1	-2.45074e+0	0	5.87186e+0	1.16834e+1	8.20904e-10	66
2	3.28838e-1	2.16393i	1.61772e-5	7.96948e-6	9.79193e-10	74
3	3.28838e-1	2.16393i	6.04017e-8	2.97889e-8	9.91143e-10	40
4	3.28838e-1	2.16393i	8.89769e-9	4.37230e-9	—	—
Re=300						
1	-2.47804e+0	0	5.97742e+00	1.18371e+01	7.09501e-10	80
2	1.04049e-1	2.22643i	2.04448e-07	9.38438e-08	9.59921e-10	70
3	1.04049e-1	2.22643i	9.30321e-10	4.28600e-10	—	—
Re=350						
1	-2.49317e+0	0	6.04038e+0	1.19385e+1	8.85599e-10	89
2	2.410711e-2	2.24736i	1.39467e-8	6.26715e-9	—	—

We continue to assume the following: we are at a point (\bar{u}_0, α_0) in the stable regime of the solution path \mathcal{S} and the eigenvalue problem $\mathbf{A}x = \mu\mathbf{M}x$ with $\mathbf{A} = \mathcal{J}(\alpha_0)$ has a complete set of eigenvectors. Let $E_k = \{\mu_1, \mu_2, \dots, \mu_k\}$ be the set containing k rightmost eigenvalues of $\mathbf{A}x = \mu\mathbf{M}x$ such that if $\mu_j \in E_k$, then $\bar{\mu}_j \in E_k$ as well. In addition, let $X_k = [x_1, x_2, \dots, x_k] \in \mathbb{C}^{n \times k}$ be the matrix that holds the k corresponding eigenvectors. Assume both E_k and X_k are known and we are

interested in computing $-Re(\mu_{k+1})$, the distance between the $(k+1)^{st}$ rightmost eigenvalue and the imaginary axis. We will show that we can use the same methodology described in section 2, that is, that $-Re(\mu_{k+1})$ is the eigenvalue with smallest modulus of a certain $n^2 \times n^2$ eigenvalue problem with the same Kronecker structure as (2.1) and it can be computed by Lyapunov inverse iteration.

Let $\hat{S} = (I - Q_k Q_k^T) S$, where $Q_k \in \mathbb{R}^{n \times k}$ is an orthonormal basis of X_k . We claim that the distance between μ_{k+1} and the imaginary axis, $-Re(\mu_{k+1})$, is the eigenvalue of

$$\hat{\Delta}_1 z = \lambda \left(-\hat{\Delta}_0 \right) z, \quad z \in \mathcal{R} \left(\hat{\Delta}_0 \right), \quad (4.1)$$

with smallest modulus, where $\hat{\Delta}_1 = \hat{S} \otimes I + I \otimes \hat{S}$, $\hat{\Delta}_0 = 2\hat{S} \otimes \hat{S}$, and $\mathcal{R}(\mathcal{M})$ denotes the range of a matrix \mathcal{M} . To prove this claim, we first study the eigenvalues and eigenvectors of \hat{S} .

LEMMA 4.1. *Let $\hat{x}_j = x_j$ for $j \leq k$ and $\hat{x}_j = (I - Q_k Q_k^T) x_j$ for $j > k$. The eigenpairs of \hat{S} are $(0, \hat{x}_j)$ with $j \leq k$, and (μ_j^{-1}, \hat{x}_j) with $j > k$.*

Proof. The proof is quite straightforward and is omitted here. \square

Under the assumption that $\mathbf{A}x = \mu \mathbf{M}x$ has a complete set of eigenvectors, we can show that $\{\hat{x}_i \otimes \hat{x}_j\}_{i,j=1}^n$ are linearly independent and $\mathcal{R}(\hat{\Delta}_0) = \text{span}\{\hat{x}_i \otimes \hat{x}_j | i, j > k\}$. Now we will show that $-Re(\mu_{k+1})$ is the eigenvalue of (4.1) with smallest modulus.

THEOREM 4.2. *Let $\hat{z}_{i,j} = \hat{\alpha}_{i,j} \hat{x}_i \otimes \hat{x}_j + \hat{\beta}_{i,j} \hat{x}_j \otimes \hat{x}_i$ for any pair (i, j) ($i, j = 1, 2, \dots, n$) and any $\hat{\alpha}_{i,j}, \hat{\beta}_{i,j} \in \mathbb{C}$ ($\hat{\alpha}_{i,j}$ and $\hat{\beta}_{i,j}$ cannot be zero at the same time). The eigenpairs of (4.1) are $(\lambda_{i,j}, \hat{z}_{i,j})$ for $i, j > k$.*

Proof. With the help of Lemma 4.1, the proof is very similar to that of Theorem 2.1. \square

If μ_{k+1} is real, $-Re(\mu_{k+1}) = \lambda_{k+1,k+1}$; otherwise, $-Re(\mu_{k+1}) = \lambda_{k+1,k+2} = \lambda_{k+2,k+1}$. In either case, by Theorem 4.2, $-Re(\mu_{k+1})$ is an eigenvalue of (4.1).

THEOREM 4.3. *Assume all the eigenvalues of $\mathbf{A}x = \mu \mathbf{M}x$ lie in the left half of the complex plane. Then the eigenvalue of (4.1) with smallest modulus is $-Re(\mu_{k+1})$.*

Proof. See the proof of Theorem 2.2. \square

Let $\mathbb{P}_k = \{Z \in \mathbb{C}^{n \times n} | Z = (I - Q_k Q_k^T) X (I - Q_k Q_k^T) \text{ where } X \in \mathbb{C}^{n \times n}\}$. If $Z \in \mathbb{P}_k$, then $z = \text{vec}(Z) \in \mathcal{R}(\hat{\Delta}_0)$, and vice versa. Therefore, (4.1) can be rewritten in the form of a matrix equation,

$$\hat{S}Z + Z\hat{S}^T + \lambda \left(2\hat{S}Z\hat{S}^T \right) = 0, \quad Z \in \mathbb{P}_k. \quad (4.2)$$

By Theorem 4.3, $-Re(\mu_{k+1})$ is the eigenvalue of (4.2) with smallest modulus. Let $\mathbb{P}_k^s = \{Z \in \mathbb{P}_k | Z = Z^T\}$ be the symmetric subspace of \mathbb{P}_k . Assume the following (similar to assumptions (a1) and (a2) in section 2): (b1) for any $k+1 < i \leq n$, if $Re(\mu_i) = Re(\mu_{k+1})$, then $\mu_i = \overline{\mu_{k+1}}$; (b2) μ_{k+1} is a simple eigenvalue of $\mathbf{A}x = \mu \mathbf{M}x$. As a result, when the eigenspace of (4.2) is restricted to \mathbb{P}_k^s , $-Re(\mu_{k+1})$ is a simple eigenvalue of (4.2) that has the unique (up to a scalar multiplier), real and symmetric eigenvector $Z = (I - Q_k Q_k^T) x_{k+1} x_{k+1}^T (I - Q_k Q_k^T)$ (if μ_{k+1} is real), or $Z = (I - Q_k Q_k^T) (x_{k+1} x_{k+1}^* + \overline{x_{k+1}} x_{k+1}^T) (I - Q_k Q_k^T)$ (if μ_{k+1} is not real). Therefore, if we can restrict the search space for the target eigenvector of (4.2) to \mathbb{P}_k^s , Lyapunov inverse iteration can be applied to (4.2) to compute $-Re(\mu_{k+1})$. This implies that in Algorithms 1, we should seek a solution to the Lyapunov equation

$$\hat{S}Y_\ell + Y_\ell \hat{S}^T = P_\ell C_\ell P_\ell^T \quad (4.3)$$

in \mathbb{P}_k^s , where $P_\ell C_\ell P_\ell^T = -2\hat{S}Z_\ell \hat{S}^T$. In general, solutions to (4.3) are not unique: any matrix of the form $Y_\ell + Q_k X Q_k^T$ where $X \in \mathbb{C}^{n \times n}$ is also a solution, since $\hat{S}Q_k = \mathbf{0}$ by Lemma 4.1. However, in the designated search space \mathbb{P}_k^s , the solution to (4.3) is indeed unique. The Lyapunov solver RKSM can be modified to compute the unique solution to (4.3) in \mathbb{P}_k^s .

By Theorem 2.3 and Lemma 4.1, the eigenvalue problem

$$(I + \lambda \hat{S}) x = \rho \hat{S} x \quad (4.4)$$

has a zero eigenvalue or a conjugate pair of pure imaginary eigenvalues $\mu_{k+1} - Re(\mu_{k+1})$ and $\overline{\mu_{k+1}} - Re(\mu_{k+1})$ if $\lambda = -Re(\mu_{k+1})$. Therefore, using the method of computing estimates for (μ_1, x_1) described in section 2, we can obtain estimates for $(\mu_{k+1}, \hat{x}_{k+1})$ here as well.

The analysis above leads to the following algorithm for computing k rightmost eigenvalues of $\mathbf{A}x = \mu\mathbf{M}x$:

Algorithm 2 (compute k rightmost eigenvalues of $\mathbf{A}x = \mu\mathbf{M}x$)

1. Initialization: $i = 0$, $E_i = \emptyset$, $X_i = \emptyset$, $Q_i = \mathbf{0}$, and $\hat{S} = S = \mathbf{A}^{-1}\mathbf{M}$.
2. While $i < k$, compute the $(i+1)^{st}$ rightmost eigenpair:
 - 2.1. Solve (4.2) for the eigenvalue with smallest modulus, $-Re(\mu_{i+1})$, and its corresponding eigenvector in \mathbb{P}_i^s using Algorithm 1. Obtain an estimate $\tilde{\mu}_{i+1}$ for μ_{i+1} .
 - 2.2. Compute (μ_{i+1}, x_{i+1}) accurately using an iterative eigenvalue solver with $\sigma = \tilde{\mu}_{i+1}$.
 - 2.3. Update:
 - if μ_{i+1} is real:
$$E_{i+1} \leftarrow \{E_i, \mu_{i+1}\}, X_{i+1} \leftarrow [X_i, x_{i+1}], i \leftarrow i + 1;$$
 - else:
$$E_{i+2} \leftarrow \{E_i, \mu_{i+1}, \overline{\mu_{i+1}}\}, X_{i+2} \leftarrow [X_i, x_{i+1}, \overline{x_{i+1}}], i \leftarrow i + 2.$$
 - 2.4. Let $Q_i \in \mathbb{R}^{n \times i}$ be an orthonormal basis of X_i and let $\hat{S} = (I - Q_i Q_i^T) S$.

At each iteration of Algorithm 2, the next rightmost eigenvalue μ_{i+1} or the next pair of rightmost eigenvalues $(\mu_{i+1}, \mu_{i+2} = \overline{\mu_{i+1}})$ are computed. We test Algorithm 2 on the two examples considered in section 3 to compute a few rightmost eigenvalues of (1.1) at a certain Reynolds number (the target eigenvalues are marked by ‘ \square ’ in Figures 3.1a and 3.2a). The results of Algorithm 1 at each iteration of Algorithm 2 are reported in Tables 4.1 and 4.2, where λ_ℓ denotes the estimate of $-Re(\mu_{i+1})$, ρ_ℓ denote the estimated eigenvalue of (4.4), r_ℓ is the residual of (4.4), \Re_ℓ is the residual of the eigenvalue problem (4.2), and R_ℓ denotes the residual of the Lyapunov solve (4.3). For example, when we use Algorithm 2 to find eight rightmost eigenvalues of (1.1) for the cavity flow at $Re = 7800$, as shown in Table 4.1: in the first iteration, the rightmost pair of eigenvalues $\mu_{1,2} = -5.13509e - 3 \pm 2.69845i$ are found; in the second iteration, Algorithm 2 finds the third rightmost eigenvalue $\mu_3 = -8.44960e - 3$; the fourth and fifth rightmost eigenvalues, $\mu_{4,5} = -1.53097e - 2 \pm 0.91037i$, are found in iteration 3; in the following iteration, Algorithm 2 picks up the sixth and seventh rightmost eigenvalues $\mu_{6,7} = -2.16259e - 2 \pm 1.78863i$; and at last, in the fifth iteration, the eighth rightmost eigenvalue $\mu_8 = -2.99634e - 2$ gets computed.

Table 4.1: Algorithm 2 ($k = 8$) applied to Example 1 ($Re = 7800$, Lyapunov solver: RKSM)

ℓ	λ_ℓ	ρ_ℓ	$\ r_\ell\ _2$	$\ \Re_\ell\ _F$	$\ R_\ell\ _F$	m_ℓ
Iteration 1						
1	6.95951e+2	0	4.78732e+02	6.58622e+02	9.02875e-10	366
2	5.13509e-3	2.69845i	7.60018e-11	3.62567e-11	—	—
Iteration 2						
1	7.32044e+2	0	5.03483e+02	6.92569e+2	9.55688e-10	365
2	8.44960e-3	5.86661e-14	5.06015e-12	1.80579e-9	—	—
Iteration 3						
1	6.70701e+1	0	3.15116e+01	2.96177e+01	9.50232e-10	364
2	1.53097e-2	0.91937i	6.19001e-11	7.12215e-11	—	—
Iteration 4						
1	6.82490e+1	0	3.18706e+01	2.97730e+01	9.92182e-10	362
2	2.16259e-2	1.78863i	8.03894e-11	4.59443e-11	—	—
Iteration 5						
1	5.58888e+1	0	2.59430e+01	2.40938e+01	9.76190e-10	362
2	2.99634e-2	-3.85945e-14	3.03416e-12	1.89975e-10	—	—

Table 4.2: Algorithm 2 ($k = 6$) applied to Example 2 ($Re = 350$, Lyapunov solver: RKSM)

ℓ	λ_ℓ	ρ_ℓ	$\ r_\ell\ _2$	$\ \Re_\ell\ _F$	$\ R_\ell\ _F$	m_ℓ
Iteration 1						
1	-2.49317e+0	0	6.04038e+0	1.19385e+1	8.85599e-10	89
2	2.410711e-2	2.24736i	1.39467e-8	6.26715e-9	—	—
Iteration 2						
1	-2.49284e+0	0	6.03899e+00	1.19362e+01	7.82734e-10	86
2	2.84079e-1	4.59280e-14	3.00574e-12	1.30693e-11	—	—
Iteration 3						
1	-2.40435e+0	0	5.66951e+00	1.13265e+01	9.69285e-10	84
2	3.35708e-1	-2.92636e-12	2.25745e-11	1.10909e-10	—	—
Iteration 4						
1	-3.07840e+0	0	7.87471e+0	1.32487e+1	7.92390e-10	85
2	5.64849e-1	-1.11057e-12	1.20581e-9	3.01907e-9	—	—
Iteration 5						
1	-3.05288e+0	0	7.76816e+0	1.31121e+1	4.29111e-10	87
2	7.91958e-1	1.97705e-11	5.18047e-9	9.25097e-9	—	—

5. Conclusion. In this paper, we developed a robust method of computing a few rightmost eigenvalues of (1.1) at any point in the stable regime. We show that the distance between the rightmost eigenvalue of (1.1) and the imaginary axis is the eigenvalue with smallest modulus of an $n^2 \times n^2$ eigenvalue problem (2.1). Since (2.1) has the same Kronecker structure as the one considered in previous work [5, 9], this distance can be computed by Lyapunov inverse iteration as well, which also produces estimates of the rightmost eigenvalue(s) as by-products. Furthermore, assuming k rightmost eigenpairs are known, we show that all the main theoretical results proven for (2.1) can be generalized to the deflated problem (4.1), whose eigenvalue with smallest modulus is the distance between the $(k + 1)^{st}$ rightmost eigenvalue and the imaginary axis. Finally, an algorithm that computes a few rightmost eigenvalues of (1.1) are proposed. The method developed in this study together with the method proposed in [5, 9] constitute a robust way of detecting the transition to instability in the steady-state solution of a large-scale dynamical system.

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