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COUNTING EIGENVALUES IN DOMAINS OF THE COMPLEX FIELD*

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Abstract. A procedure for counting the number of eigenvalues of a matrix in a region surrounded by a closed curve is presented. It is based on the application of the residual theorem. The quadrature is performed by evaluating the principal argument of the logarithm of a function. A strategy is proposed for selecting a path length that insures that the same branch of the logarithm is followed during the integration. Numerical tests are reported for matrices obtained from conventional matrix test sets.

Key words. eigenvalue, resolvent, determinant, complex logarithm

AMS subject classifications. 65F15,65F40,65F50,65E05

1. Introduction. The localization of eigenvalues of a given matrix A in a domain of the complex plane is of interest in scientific applications. When the matrix is real symmetric or complex Hermitian, a procedure based on computations of Sturm sequences allows to safely apply bisections on real intervals to localize the eigenvalues [19]. The problem is much harder for real non-symmetric or complex non-Hermitian matrices and especially for non-normal ones. This latter case is the main concern of this work. Proceeding by trying to compute the eigenvalues of the matrix may not always be appropriate for two reasons.

First, most of the iterative methods frequently used to calculate eigenvalues of large and sparse matrices may miss some of them, since only a part of the spectrum is computed, and as such there is no guarantee to localize all the eigenvalues in a selected domain. When a shift-and-invert transformation is used, the eigenvalues are obtained in an order more or less dictated by their distance from the shift, and if one eigenvalue is skipped over, there is no easy strategy that can be used to recover it.

Second, the entries of the matrix may be known with some uncertainty and, consequently the eigenvalues cannot be exactly known. They can only be localized in some domains of $\mathbb{C}$.

Many authors have defined regions in the complex plane that include the eigenvalues of a given matrix; one of the main tool is the Geršgorin theorem. Since a straight application of the theorem often leads to large disks, some authors have extended the family of inequalities for obtaining smaller regions with the use of intersections which include eigenvalues (see e.g., [9, 10, 16, 23, 24]). Other techniques consist of considering bounds involving the singular values (see [6]), the eigenvalues of the Hermitian part and the skew-Hermitian part of the matrix (see [2]), or the field of values of inverses of the shifted matrices (see [15]). When taking into account possible perturbations of the matrix, Godunov [13] and Trefethen [22] have independently defined the notion of the of ϵ-spectrum or pseudospectrum of a matrix to address the problem. The problem can then be reformulated as that of determining level curves of the 2-norm of the resolvent $R(z) = (zI - A)^{-1}$ of the matrix A.

The previous approaches determine a priori enclosures of the eigenvalues. A dual approach can be considered: given some curve Γ in the complex plane, count the number of eigenvalues of the matrix A that are surrounded by Γ. This problem was considered in [7]

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where several procedures were proposed. The number of surrounded eigenvalues is determined by evaluating the integral $\frac{1}{2i\pi}\int_\Gamma \frac{d}{dz}\log\det(zI-A)dz$. This integral is also considered in works devoted to the non-linear eigenvalue problems [8, 18].

In this paper, we make some progress with respect to the work in [7]. Our work is mainly concerned with the control of the integration path so as to stay on the same branch along an interval when evaluating the principal argument of a logarithm.

In Section 2, we present some previous works on the subject. In Section 3, we present the basis of our strategy for following a branch of the logarithm function and conditions for controlling the path length. Section 4 deals with the implementation of our method: we show how to safely compute the determinant and how to include new points along the boundary. In Section 5 we present numerical results carried out on some test matrices and in Section 6, we conclude with some few remarks and future work.

2. Mathematical tool and previous works. In this section we present the Cauchy's argument principle and some previous works on counting eigenvalues in regions of the complex field.

2.1. Use of the argument principle. The localization of the eigenvalues of matrix A involves the calculation of determinants. Indeed let Γ be a closed piecewise regular Jordan curve (piecewise C^1 and of winding number 1) in the complex plane which does not contain eigenvalues of A. By application of the Cauchy's integral formula [21, p. 172], the number N_Γ of eigenvalues surrounded by Γ can be expressed by :

$$N_\Gamma = \frac{1}{2i\pi}\int_\Gamma \frac{f'(z)}{f(z)}dz, \tag{2.1}$$

where $f(z)=\det(zI-A)$ is the characteristic polynomial of A.

If $\gamma(t)_{0\le t\le 1}$ is a parametrization of Γ, equation (2.1) can be rewritten as

$$N_\Gamma = \frac{1}{2i\pi}\int_0^1 \frac{f'(\gamma(t))}{f(\gamma(t))}\gamma'(t)dt. \tag{2.2}$$

The primitive φ defined by

$$\varphi(u) = \int_0^u \frac{f'(\gamma(t))}{f(\gamma(t))}\gamma'(t)dt, u\in[0,1],$$

is a continuous function which is a determination of $\log(f\circ\gamma)$ (see [21]):

$$\log f(\gamma(t)) = \log|f(\gamma(t))| + i\arg(f(\gamma(t))),\ \ t\in[0,1].$$

It then follows that

$$N_\Gamma = \frac{1}{2\pi}\varphi_I(1),$$

where $\varphi_I(1)$ is the imaginary part of $\varphi(1)$ since its real part vanishes.

2.2. Counting the eigenvalues in a region surrounded by a closed curve. In [7], two approaches were proposed for counting the eigenvalues in a domain surrounded by a closed curve.

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The first method is based on the series expansion of $\log(I + hR(z))$, where $R(z) = (zI - A)^{-1}$, combined with a path-following technique. The method uses a scheme with an adaptive step size satisfying the constraint

$$|\varphi_I(z + \Delta z) - \varphi_I(z)| < \pi,$$

for a discrete list of points z. The implementation of the algorithm requires the computation of a few of the smallest singular values of $(zI - A)$.

In the second approach, the domain is surrounded by a parameterized user-defined curve $z = \gamma(t)$ and thus

$$N_\Gamma = \frac{1}{2i\pi} \int_{\gamma(0)}^{\gamma(1)} \frac{\frac{d}{dt}\det(\gamma(t)I - A)}{\det(\gamma(t)I - A)} dt. \tag{2.3}$$

Since $\gamma(0) = \gamma(1)$, the function $\gamma(t)$ defined on $[0, 1]$, can be extended onto $\mathbb{R}$ by

$$\gamma_{\text{ext}}(t) = \gamma(t \bmod 1).$$

By subdividing the interval $[0, 1]$ into subintervals of equal length, and by assuming that $\gamma_{\text{ext}} \in \mathcal{C}^\infty$, a fundamental result from quadrature of periodic functions is used to prove an exponential convergence of the integral [7]. In that paper, the method is compared to other integrators with adaptive step sizes.

Each of these methods makes use of the computation of

$$u(t) = \frac{\det(\gamma(t)I - A)}{|\det(\gamma(t)I - A)|},$$

which is efficiently computed through a LU factorization of the matrix $(\gamma(t)I - A)$ with partial pivoting. In order to avoid underflow or overflow, the quantity is computed by

$$\frac{\det(\gamma(t)I - A)}{|\det(\gamma(t)I - A)|} = \prod_{i=1}^{n} \frac{u_{ii}}{|u_{ii}|}$$

where u_{ii} is the i-th diagonal element of U in the LU factorization. The product is computed using the procedure that will be described later on in Section 4.

Our work is a follow-up of the second method with an adaptive stepsize introduced in [7]. The new method given in this paper and implemented in the procedure `EIGENCNT` (see Algorithm 4.1), defines a reliable stepsize control strategy whereas the corresponding former method can sometimes select inappropriate stepsizes which cannot guaranty an accurate eigenvalue count.

3. Integrating along a curve. In this section, we describe strategies for the integration of the function $g(z) = \frac{f'(z)}{f(z)}$, where $f(z) = \det(zI - A)$, along the boundary of a domain limited by a user-defined curve Γ that does not include eigenvalues of A. Let us assume that $\Gamma = \bigcup_{i=0}^{N-1} [z_i, z_{i+1}]$ is a polygonal curve where $[z_i, z_{i+1}] \subset \mathbb{C}$ denotes the line segment with end points z_i and z_{i+1}. This is a user-defined curve which approximates the initial Jordan curve within the desired precision.

3.1. Following a branch of log(f(z)) along the curve. Let $\text{Arg}(z) \in (-\pi, \pi]$ denote the principal determination of the argument of a complex number z, and $\arg(z) \equiv \text{Arg}(z)\ (2\pi)$, be any determination of the argument of z. In this section, we are concerned with the problem of following a branch of $\log(f(z))$ when z runs along (Γ). The branch (i.e. a determination

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$\arg_0$ of the argument), which is to be followed along the integrating process, is fixed by selecting an origin $z_0 \in \Gamma$ and by insuring that

$$\arg_0(f(z_0)) = \mathrm{Arg}(f(z_0)). \tag{3.1}$$

Let z and $z+h$ be two points of Γ. Since

$$\begin{aligned}(z+h)I - A &= (zI - A) + hI \\ &= (zI - A)(I + hR(z)),\end{aligned}$$

where $R(z) = (zI - A)^{-1}$, it then follows that

$$f(z+h) = f(z)\det(I + hR(z)). \tag{3.2}$$

Let $\Phi_z(h) = \det(I + hR(z))$, then

$$\begin{aligned}\int_z^{z+h} \frac{f'(z)}{f(z)}dz &= \log(f(z+h)) - \log(f(z)) \\ &= \log\left(\frac{f(z+h)}{f(z)}\right) \\ &= \log(\Phi_z(h)) \\ &= \log|\Phi_z(h)| + i\arg(\Phi_z(h)).\end{aligned}$$

In the previous approach [7], given z, the step h is chosen such that the condition

$$|\arg(\Phi_z(h))| < \pi, \tag{3.3}$$

is satisfied. In [7], the condition expressed in (3.3) is only checked at point $z+h$ but we want the condition to be satisfied at all the points $s \in [z, z+h]$, so as to guarantee that we stay on the same branch along the interval $[z, z+h]$. We therefore need a more restrictive condition which is mathematically expressed by the following lemma:

LEMMA 3.1 (*Condition A*). *Let z and h be such that $[z, z+h] \subset \Gamma$.*
If

$$|\mathrm{Arg}(\Phi_z(s))| < \pi, \quad \forall s \in [0, h], \tag{3.4}$$

then,

$$\arg_0(f(z+h)) = \arg_0(f(z)) + \mathrm{Arg}(\Phi_z(h)), \tag{3.5}$$

where $\arg_0$ is the determination of the argument determined as in (3.1) by an a priori given $z_0 \in \Gamma$.

Proof. We prove it by contradiction. Let us assume that there exists $k \in \mathbb{Z} \setminus \{0\}$ such that

$$\arg_0(f(z+h)) = \arg_0(f(z)) + \mathrm{Arg}(\Phi_z(h)) + 2k\pi.$$

By continuity of the branch, there exists $s \in [0, h]$ such that $|\mathrm{Arg}(\Phi_z(s))| = \pi$, which contradicts (3.4). ∎

Condition (3.4) will be called *Condition A*.

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3.2. Step size control. In our approach, given z, the step h is chosen such that the conditions of Lemma 3.1 are satisfied. *Condition A* is equivalent to

$$\Phi_z(s) \notin (-\infty, 0], \forall s \in [0, h].$$

In order to find a practical criterion that will insure it, we look for a more severe condition by requiring that $\Phi_z(s) \in \Omega$, where Ω is an open convex set neighborhood of 1, and $\Omega \subset \mathbb{C} \setminus (-\infty, 0]$. A possible choice for Ω is the positive real half-plane, or any disk included in it and centered in 1.

Since $\Phi_z(0) = 1$, let

$$\Phi_z(s) = 1 + \delta, \text{ with } \delta = \rho e^{i\theta}.$$

A sufficient condition for (3.4) to be satisfied is $\rho < 1$, i.e.

$$|\Phi_z(s) - 1| < 1, \quad \forall s \in [0, h]. \tag{3.6}$$

This condition will be referred to as *Condition B* and, when only verified at $z + h$, i.e.

$$|\Phi_z(h) - 1| < 1, \tag{3.7}$$

it will be referred to as *Condition B'*. This last condition is the one used in [7]. It is clear that *Condition B* implies *Condition A* whereas *Condition B'* does not.

Since it is very difficult to check (3.6), we approximate $\Phi_z(s)$ in the neighborhood of 0 by its tangent $\Psi_z(s) = 1 + s\Phi'_z(0)$, and, substituting it in (3.6), we obtain

$$|\Psi_z(s) - 1| < 1, \quad \forall s \in [0, h], \tag{3.8}$$

which is equivalent to the following condition, referred to as *Condition C*:

$$|h| < \frac{1}{|\Phi'_z(0)|}. \tag{3.9}$$

In the following, we give three examples to illustrate the possible behaviors of the three conditions. Example 3.1 illustrates the most common situation where *Condition B* is well covered by *Condition C*.

EXAMPLE 3.1. Let $A = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$. It then follows that

$$\begin{aligned} f(z) &= z(z-1), \\ \Phi_z(h) &= \left(1 + \frac{h}{z}\right)\left(1 + \frac{h}{z-1}\right), \\ \Phi'_z(0) &= \frac{1}{z} + \frac{1}{z-1}. \end{aligned}$$

Let us assume that we are integrating along the segment ranging from $z = 2$ to $z = 1 + i$. In order to see if intermediate points are needed to insure that the branch of the logarithm is correctly followed, we consider the previously introduced conditions with $h = t(-1 + i)$ where $t \in [0, 1]$.

Condition A: $\Phi_2(h) = 1 + \frac{3h}{2} + \frac{h^2}{2}$ is a non-positive real number if and only if $h \in [-2, -1] \bigcup (-\frac{3}{2} + i\mathbb{R})$. From that, it can easily be seen that the segment $[0, -1 + i]$ does not intersect the forbidden region. Therefore no intermediate points are needed.

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Condition B: this condition is equivalent to $|h||3+h| < 2$. By studying the function $\phi(t) = |h||3+h| = \sqrt{2}t|3-t+it|$, the parameter t must remain smaller than $\alpha \approx 0.566$.
Condition B': in this example, this condition is equivalent to the previous one, since the function $\phi(t)$ is increasing with t.
Condition C: since $\Phi_2'(h) = \frac{3}{2} + h$, this condition limits the extent of the interval to $|h| < \frac{2}{3}$ or equivalently $t < \frac{\sqrt{2}}{3} \approx 0.471$.

In the second example, we illustrate the lack of reliability of *Condition B'*.

EXAMPLE 3.2. Let $A = \lambda I_n$, where $\lambda \in \mathbb{R}$ and I_n is the identity matrix of order n. It then follows that

$$f(z) = (z-\lambda)^n,$$
$$\Phi_z(h) = \left(1 + \frac{h}{z-\lambda}\right)^n,$$
$$\Phi_z'(0) = \frac{n}{z-\lambda}.$$

Let us assume that we are willing to integrate from $z = \lambda+1$ to $z+h = \lambda+e^{i\theta}$. We consider the previously introduced conditions on h.
Condition A: $|\theta| < \frac{\pi}{n}$.
Condition B: $|\theta| < \frac{\pi}{3n}$.
Condition B': $\cos n\theta > \frac{1}{2}$ which is satisfied for values that violate *Condition B*.
Condition C: $|\frac{\theta}{2}| < \arcsin \frac{1}{2n}$, which is guaranteed by $|\theta| < \frac{1}{n}$.

In this example, if Γ is the circle with center λ and radius 1, the step size must be reduced in such a way that more than $2n$ intervals are needed to satisfy *Condition A*, and even $6n$ and $2\pi n$ intervals for *Condition B* and *Condition C* respectively.

Practically, we consider that *Condition C* implies *Condition A*, as long as the linear approximation is valid. Problems may occur when Φ_z' vanishes. The following example illustrates such a situation.

EXAMPLE 3.3 (Critical situation). Let us consider the matrix of Example 3.1. For $z = 1/2$, $\Phi_{1/2}(h) = 1 - 4h^2$, and $\Phi_{1/2}'(0) = 0$, and the conditions become
Condition A: $h \notin \mathbb{R}$ or $|h| < 1/2$,
Condition B: $|h| < 1/2$,
Condition B': $|h| < 1/2$,
Condition C: is satisfied for all $h \in \mathbb{C}$.

This pathological example exhibits an undesired situation, since it may lead to adopt a stepsize that is too large . However, in Section 4.3, we explain how to overcome this flaw by using the second bound of the interval.

4. Implementation. In this section, we describe the numerical implementation of our method. Strategies for including new points and a procedure for safely computing the determinants are given.

4.1. Avoiding overflows and underflows. The implementation of our method requires the computation of

$$\Phi_z(h) = \frac{\det((z+h) - A)}{\det(zI - A)}.$$

In order to avoid underflow or overflow, we proceed as follows.

For any non-singular matrix $M \in \mathbb{C}^{n\times n}$, let $PM = LU$ be its LU factorization where P is a permutation matrix of signature σ. Then $\det(M) = \sigma \prod_{i=1}^n (u_{ii})$ where $u_{ii} \in \mathbb{C}$ are

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the diagonal entries of U. If the matrix M is not correctly scaled, the product $\prod_{i=1}^{n}(u_{ii})$ may generate an overflow or an underflow. To avoid this, the determinant is represented by the triplet (ρ, K, n) so that

$$\det(A) = \rho K^n \tag{4.1}$$

where:

$$\rho = \sigma \prod_{i=1}^{n} \frac{u_{ii}}{|u_{ii}|}, \quad (\rho \in \mathbb{C} \text{ with } |\rho| = 1), \text{ and}$$

$$K = \sqrt[n]{\prod_{i=1}^{n} |u_{ii}|} \quad (K > 0).$$

The quantity K is computed through its logarithm:

$$\log(K) = \frac{1}{n} \sum_{i=1}^{n} \log(|u_{ii}|).$$

In this way, the value of the determinant is not computed, when the matrix is not properly scaled.

In Section 3, it was indicated that our algorithm will heavily be based on the computation of $\Phi_z(h) = \det(I + hR(z))$. For an h with a moderate modulus, the determinant does not overflow. This can be verified since

$$\Phi_z(h) = \frac{\det((z+h)I - A)}{\det(zI - A)} = \frac{K_2^n \rho_2}{K_1^n \rho_1},$$

where $\det(zI - A)$ and $\det((z + h)I - A)$ are respectively represented by the triplets (ρ_1, K_1, n) and (ρ_2, K_2, n). To protect from under- or overflow, before raising to power n, the ratio K_2/K_1 must be in the interval $[\frac{1}{\sqrt[n]{M_{fl}}}, \sqrt[n]{M_{fl}}]$ where M_{fl} is the largest floating point number. When this condition is violated, intermediate points must be inserted between z and $z + h$.

4.2. Estimating the derivative. It can be shown that the derivative $\Phi'_z(0)$ can be expressed as :

$$\Phi'_z(0) = \operatorname{trace}(R(z)). \tag{4.2}$$

The computation of this simple expression however involves many operations, as shown in the following. By using the LU factorization $P(zI - A) = LU$ which is available at z, and by using (4.2), we may compute $\Phi'_z(0) = \sum_{i=1}^{n} u_i^* l_i$, where $l_i = L^{-1}e_i$ and $u_i = (U^*)^{-1}e_i$, with e_i being the i-th column of the identity matrix. When A is a sparse matrix, the factors L and U are sparse but not the vectors u_i and l_i. Therefore, the whole computation involves solving $2n$ triangular systems. However the number of operations can be reduced as shown by Duff et al. in [12, pp. 273–275] since the diagonal entries of $R(z)$ can be computed by recursion which only involves the entries of $R(z)$ corresponding to the patterns of L or U.

Approximations of the trace of the inverse of a matrix have been investigated. They involve less operations than using the LU factorization but they are mostly valid for symmetric or Hermitian matrices [5, 14]. However Bai et al. also considered the non-symmetric case in [4]. Since a precise estimation of $|\Phi'_z(0)|$ is not needed but only its order of magnitude,

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such approaches might be of interest. The same approach is considered by Maeda et al. in [18] in a close but more general context (estimation of the eigenvalue density of a non-linear eigenvalue problem). The authors consider the quadrature of a function but without stepsize control. A review of methods is also presented by Saad [20].

If the derivative is approximated by its first order approximation, sparsity helps. More specifically, given z and $z+h$, the derivative of Φ_z at 0 is estimated by

$$\Phi_z'(0) \approx \frac{\Phi_z(s)-1}{s},$$

where $s=\alpha h$ with $\alpha = \min(10^{-6}\mu/|h|, 1)$, and $\mu = \max_{z\in\Gamma}|z|$. Therefore, the computation imposes an additional LU factorization for evaluating the quantity $\Phi_z(s)$. It is known that, for a sparse matrix, the sparse LU factorization involves much less operations that its dense counterpart. We make use of this approximation in the sequel.

4.3. Test for including new points. In this subsection, we describe a procedure for including new points in the interval $[z, z+h]$. In Section 3, we introduced *Condition B* which is more severe than *Condition A* but might be easier to verify, and we proposed to test its linear approximation called *Condition C*. Unfortunately Example 3.3 has exhibited that *Condition C* may be satisfied while *Condition B'* and therefore *Condition B* are violated. To accept the interval $[z, z+h]$, we simultaneously check *Condition C* and *Condition B'*.

In addition, we insist that *Condition C* be satisfied at each bound of the segment $[z, z+h]$. Therefore, on exit, the condition $|h| < \frac{1}{|\Phi'_{z+h}(0)|}$ must also be guaranteed. Proceeding in this way, *Condition C* becomes highly reliable because it is practically impossible to have the situation where both derivatives $\Phi'_z(0)$ and $\Phi'_{z+h}(0)$ vanish since each of the two events is very rare (Φ'_z and Φ'_{z+h} are polynomials and, as such, have finite numbers of zeros). In all our experiments, we never encountered an example in which the condition failed.

When *Condition C* is violated, we insert M uniformly spaced points between z and $z+h$ where

$$M = \min\left(\lceil |h|\,|\Phi'_z(0)| \rceil, M_{\max}\right), \tag{4.3}$$

with $M_{\max}$ being some user defined parameter. When *Condition B'* is violated and *Condition C* is satisfied, we insert the point $z+h/2$ in the list. The following example illustrates the effect of this step size control.

EXAMPLE 4.1. Let A be the random matrix :

$$A = \begin{bmatrix} -0.63 & 0.80 & 0.68 & 0.71 & -0.31 \\ -0.81 & 0.44 & -0.94 & 0.16 & 0.93 \\ 0.75 & -0.09 & -0.91 & -0.83 & -0.70 \\ -0.83 & -0.92 & 0.03 & -0.58 & -0.87 \\ -0.26 & -0.93 & -0.60 & -0.92 & -0.36 \end{bmatrix}.$$

The polygonal line Γ is determined by 10 points regularly spaced on the circle of center 0 and radius 1.3. In Figure 4.1, are displayed the eigenvalues of A, the line Γ and the points that are automatically inserted by the procedure. The figure illustrates that, when the line gets closer to some eigenvalue, the segment length becomes smaller.

4.4. Global algorithm. The algorithm is sketched in Algorithm 4.1[1]. From a first list Z of points, it extends the list Z in order to determine a safe split of the integral (2.1).

[1] A Maltab code is available from the authors at
http://www.irisa.fr/sage/bernard/EIGENTOOL/EIGENCNT/

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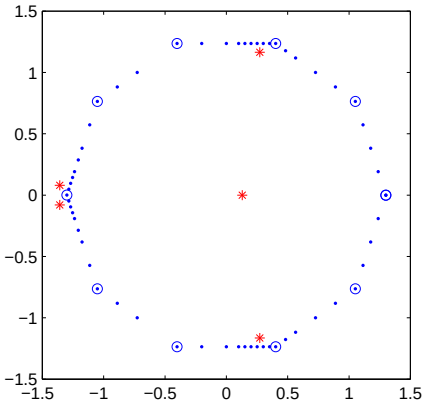

FIG. 4.1. *Example 4.1. The eigenvalues are indicated by the stars. The polygonal line is defined by the 10 points with circles; the other points of the line are automatically introduced to insure the conditions as specified in Section 4.3 ($M_{\max} = 1$ in (4.3)).*

ALGORITHM 4.1 (`EIGENCNT`).

Require:
Z={edges of Γ} ;
$M_{\rm pts}$ = maximum number of allowed points;
$M_{\max}$ = maximum number of points to insert simultaneously ;
Ensure:
`neg` = number of eigenvalues surrounded by Γ ;
Status(Z)=-1 ;
while Status(Z)$\neq$ 0 & length(Z) $< M_{\rm pts}$, **do**
  for $z \in Z$ such that Status(z)$== -1$, **do**
    Compute $\det(zI - A)$ and $\Phi'_z(0)$;
    Status(z) = 1 ;
  end for
  for $z \in Z$ such that Status(z)=1, **do**
    if *Condition C* not satisfied at z, **then**
      Generate M points $\tilde{Z}$ as in (4.3);
      Z=$Z \cup \tilde{Z}$; Status($\tilde{Z}$)=-1;
    else if *Condition B'* not satisfied at $z + h$; **then**
      Z=$Z \cup \{z + h/2\}$; Status($z + h/2$)=-1;
    else
      Status(z)=0 ;
    end if
  end for
  if no new points were inserted in Z, **then**
    for $z \in Z$, **do**
      if *Condition C* is backwardly violated, **then**
        Z=$Z \cup \{z - h/2\}$; Status($z - h/2$)=-1;
      end if
    end for
  end if
end while
Integral = $\sum_{z \in Z} \mathrm{Arg}(\Phi'_z(0))$; `neg` = round(Integral/ 2π) ;

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The complexity of the algorithm is based on the number of computed determinants. For each $z \in Z$, the complex numbers $\det(zI - A)$ and $\Phi'_z(0)$ are computed; they involve two evaluations of the determinant. Therefore, for N final points in Z, the complexity can be expressed by:

$$\mathcal{C} = 2\mathcal{L}_{LU}N,$$

where $\mathcal{L}_{LU}$ is the number of operations involved in the complex LU factorization of $zI - A$.

When the matrix A is real and, assuming that the polygonal line Γ is symmetric with respect to the real axis and intersects it only in two points, half of the computation can be saved since

$$N_\Gamma = \frac{1}{\pi}\,\mathcal{I}\left(\int_{\Gamma_+} \frac{f'(z)}{f(z)}dz\right),$$

where (Γ_+) is the upper part of Γ when split by the real axis, and $\mathcal{I}(Z)$ denotes the imaginary part of Z.

5. Numerical tests. The tests are run on a desktop, equipped with two processors, each with 6 cores Intel(R) Xeon(R) ; clock : 3.47GHz; RAM: 48GB. The program `EIGENCNT` is coded in `C` and uses `LAPACK` [3] and `UMFPACK` [11] to perform the LU factorizations.

5.1. First experiments. In the following tests, we describe the performance of the algorithm using three real matrices chosen from the set Matrix Market [1]. The maximum inserted points in an interval is $M_{\max} = 10$. When Γ is symmetric with respect to the real axis, only half of the integration is performed. The storage of the matrices is kept sparse (except when computing the spectra of the matrices of the two first examples).

EXAMPLE 5.1 (Matrix ODEP400A). This matrix is a model eigenvalue problem of small order coming from an ODE with the following characteristics: order: $n = 400$; 1-norm: $\|A\|_1 = 7$; spectral radius: $r = 4.00$; spectrum included in the rectangle: $[-4, 4.38 \times 10^{-4}] \times [-0.01i, 0.01i]$. Its spectrum is displayed in Figure 5.1.

The first experiment consists of focusing on the right part of the spectrum by defining a regular polygon of 10 vertices; the polygon is centered at the origin, symmetric with respect to the real axis as shown in Figure 5.2 (only its upper part is drawn), with radius $R = 10^{-3}$. Five eigenvalues were correctly found as surrounded by the polygon. Some statistics are displayed in the first line of Table 5.1.

TABLE 5.1
Statistics for Example 5.1.

	Nr. of eigenvalues in Γ	Nr. of intervals	Elapsed time
Experiment 1	5	25	0.02 s
Experiment 2	89	1519	1.5 s

The second experiment focuses on the bifurcation between real and complex eigenvalues in the neighborhood of -3.5. In the box $[-4, -3.4] \times [-10^{-3}i, 10^{-3}i]$, 89 eigenvalues are counted (see the statistics in the second line of Table 5.1). The aspect ratio of the box is large. The refining process proceeds in 16 steps to produce 1519 intervals from the initial four. If the integral is computed by the relation (3.5) at each step (hence even if the necessary conditions for correctness are not satisfied), it would only have been correct at the fifth step and after; this corresponds to 825 intervals. This illustrates the loss in efficiency which is imposed by the constraint for a safe computation.

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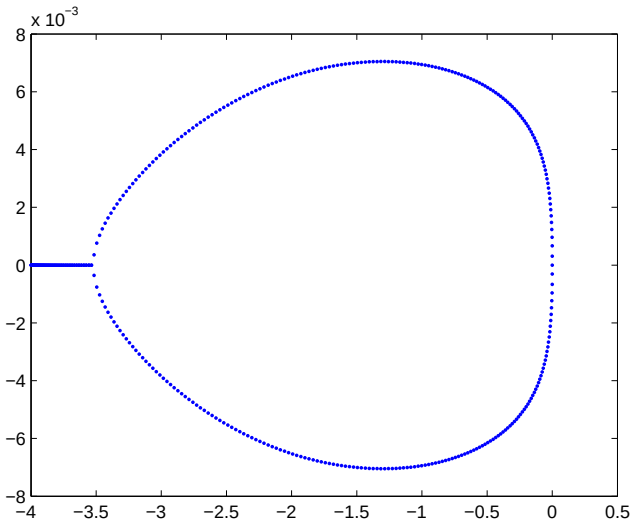

FIG. 5.1. *Spectrum of the matrix of Example 5.1.*

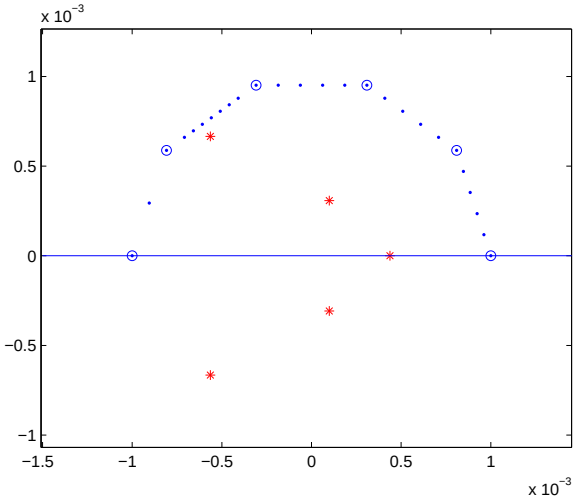

FIG. 5.2. *Example 5.1: First experiment on the right end of the spectrum.*

EXAMPLE 5.2 (Matrix TOLS2000). This matrix comes from a stability analysis of a model of an airplane in flight with the following characteristics: order: $n = 2000$; 1-norm: $\|A\|_1 = 5.96 \times 10^6$; spectral radius: $r = 2.44 \times 10^3$; spectrum included in the rectangle: $[-750, 0] \times [-r\,i, +r\,i]$. In Figure 5.3, the spectrum and two zooms on it are displayed.

Two experiments consider the right part of the spectrum. A first box $[-20, 0] \times [75i, 125i]$ is not symmetric with respect to the real axis. Therefore, the integration is not reduced. Eight eigenvalues are found. The second box $[-20, 0] \times [-500i, 500i]$ is symmetric with respect to the real axis but it includes 542 eigenvalues. The statistics are reported in Table 5.2.

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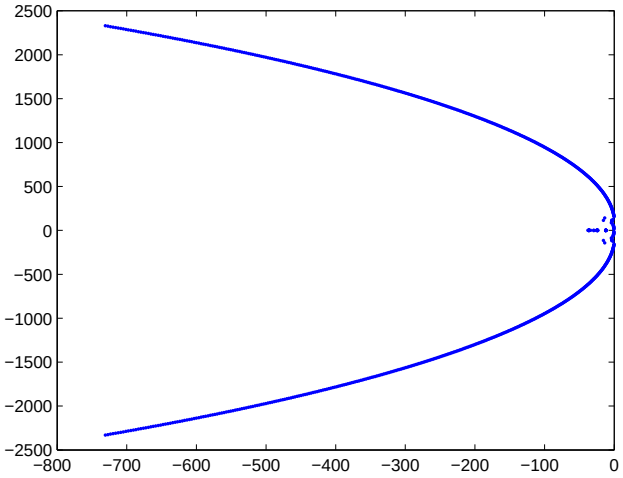
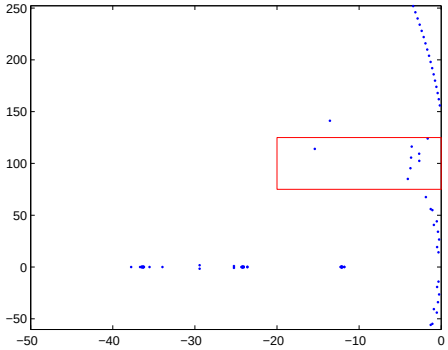
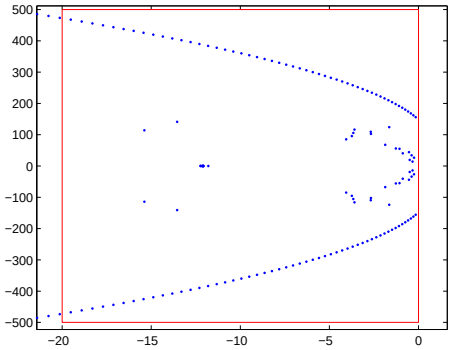


Entire spectrum of the matrix TOLS2000





Experiment 1: Box=$[-20, 0] \times [75i, 125i]$ Experiment 2: Box=$[-20, 0] \times [-500i, 500i]$

FIG. 5.3. *Example 5.2: Spectrum of the matrix (up) and zooms on the two regions of experiments.*

TABLE 5.2
Statistics for Example 5.2.

	Nr. of eigenvalues in Γ	Nr. of intervals	Elapsed time
Experiment 1	8	2611	8.45 s
Experiment 2	542	15669	50.6 s

EXAMPLE 5.3 (Matrix E40R5000). This sparse matrix comes from modeling 2D fluid flow in a driven cavity, discretized on a 40×40 grid and with a Reynolds number is $Re = 5000$, with the following characteristics: order: $n = 17,281$; 1-norm: $\|A\|_1 = 1.21 \times 10^2$; spectral radius: $r = 65.5$ (estimated by the Matlab procedure `eigs`); spectrum included in the rectangle: $[-750, 0] \times [-r\ i, +r\ i]$.

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This example shows the reliability of the proposed procedure. Computing the 6 eigenvalues with the largest real part using the Matlab procedure `eigs` (which implements the ARPACK code) returns six eigenvalues: $\{8.371 \pm 64.65i, 8.803 \pm 64.88i, 16.20, 20.17\}$. By increasing the number p of requested eigenvalues, only a few of them are found: for example when $p = 20$, only the two rightmost were found. Increasing even further up say, $p = 100$, only 14 eigenvalues were returned, among which the already computed two rightmost and 12 additional ones with real parts belonging to the interval [12.2,12.9]. In such a case, the user would like to have the exact count in this region. Defining the rectangle $\Gamma = \Gamma_+ \cap \Gamma_-$ where $\Gamma_+ = (14, 14 + 2i, 12 + 2i, 12)$ and where Γ_- is the symmetric of Γ_+ with respect to the real axis, the procedure `EIGENCNT` returns

TABLE 5.3
Statistics for Example 5.3.

Number of eigenvalues in Γ	Number of intervals	Elapsed time
116	7986	4241 s

Actually, the right number of eigenvalues was already given before the last refining step with 3994 intervals. Taking into account the result of the experiment, after several tries of shifts with the MATLAB procedure `eigs`, all the 116 eigenvalues surrounded by Γ were obtained by requesting $p = 200$ eigenvalues in the neighborhood of the shift $\lambda = 13.5$ (elapsed time: 10.2s).

5.2. Additional experiments. In this section, additional tests illustrate the behavior of the code `EIGENCNT` on the matrices which are listed in increasing order of size in Table 5.4. The first matrix is complex symmetric, all other are real non-symmetric. The matrices belong to the Matrix Market set of tests matrices [1] except the last two which are obtained as iteration matrices when solving a BDF step in two discretizations of a transport diffusion process. The real part of the eigenvalues of these two last matrices are included in the interval $(0, 1)$ with a spectral radius smaller than 1.

TABLE 5.4
Characteristics of the test matrices (`Name`: Matrix Market name ; n : order of the matrix ; `Origin`: physical or mathematical origin.)

`Name`	n	`Origin`	`Type`	2-norm
YOUNG1	841	Acoustic scattering	Complex Symmetric	7×10^2
UTM3060	3,060	Tokamac	Real non-symmetric	3×10^0
CRY10000	10,000	Crystal growth	Real non-symmetric	4×10^4
AF23560	23,560	Navier Stokes	Real non-symmetric	6×10^2
ITER1	48,000	Iteration matrix	Real non-symmetric	2×10^2
ITER2	300,000	Iteration matrix	Real non-symmetric	3×10^2

Several polygonal lines are considered for each matrix. For all the tests on real matrices, symmetry of the spectrum with respect to the real axis is used to halve the computation. The results are given in Table 5.5.

6. Conclusion. In this paper, we have developed a reliable method for counting the eigenvalues in a region surrounded by a user-defined polygonal line. The main difficulty to tackle lies in the step control which must be used during the complex integration along the line. The method is reliable and robust but computationally expensive. Some questions may be raised about the benefit of such a procedure; our answer is that one has to pay the price for

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TABLE 5.5
Tests (`Name`: matrix name as given in Table 5.4; n : order of the matrix; Γ : definition of the polygonal line (vertices are regularly distributed on a circle C[center,radius], or on an ellipse E[center,horizontal semi-axis,vertical semi-axis], or defined by a rectangle); `Neig` : number of surrounded eigenvalues; `Time`: elapsed time (s); `Nintv`: number of intervals.)

`Name`	n	Γ	`Neig`	`Time`	`Nintv`
YOUNG1	841	C[(0,0),10^{-2}], 100 vertices	269	23.2	3649
UTM3060	3,060	[-1.8;-1.2]×[-0.4i;0.4i]	410	506	6566
CRY10000	10,000	C[(0,0),10^{-6}], 10 vertices	1	2.3	20
CRY10000	-	C[(0,0),10^{-3}], 100 vertices	169	78	741
CRY10000	-	C[(0,0),1], 100 vertices	1749	655	6246
AF23560	23,560	C[(-0.1,0),0.1], 10 vertices	0	1243	252
AF23560	-	E[(-1/3,0),1/3,1], 10 vertices	14	5412	2248
AF23560	-	[-6;-4]×[-0.5i;0.5i]	67	7933	2105
ITER1	48,000	E[(1,0),10^{-3},10^{-2}], 10 vertices	7	4335	1398
ITER2	300,000	E[(1,0),10^{-4},5×10^{-4}], 10 vertices	14	6734	126

reliability and robustness. If for dense matrices, the whole spectrum can be computed with a high precision by the QR algorithm, it is not the same for sparse matrices. We have illustrated in Example 5.3 that the classical algorithm ARPACK used with a shift-and-invert technique may easily miss some eigenvalues in an a priori given neighborhood. Therefore, the procedure `EIGENCNT` should be seen as a robust and reliable tool for eigenvalue localization. It can be combined with the pseudospectrum determination; since the latter needs the computation of the smallest singular value of the matrix $(zI - A)$, this value and the determinant can be obtained simultaneously from the LU factorization of this matrix. In most of the cases, the determination of the number of eigenvalues inclosed in the pseudospectrum can be freely determined once the pseudospectrum is obtained.

The code `EIGENCNT` involves a high potential for parallelism since most of the determinant computations are independent. In forthcoming work, a parallel version of the method will be developed and implemented. The first results which were obtained with a straight parallelization are encouraging: see Figure 6.1, where speedups for Example 5.2 (Experiment 2) and Example 5.3 are reported. A second level of parallelism is also investigated within the computation of a determinant for matrices arising in domain decompositions [17].

7. Acknowledgement. The authors are indebted to Louis Bernard Nguenang for having programmed in C the code they first developed in MATLAB, and for running the first parallel versions. They also thank Andreas Stathopoulos for having suggested the reference [12] for computing the diagonal of the inverse of a sparse matrix and the reviewers for their remarks which help to improve the quality of the paper.

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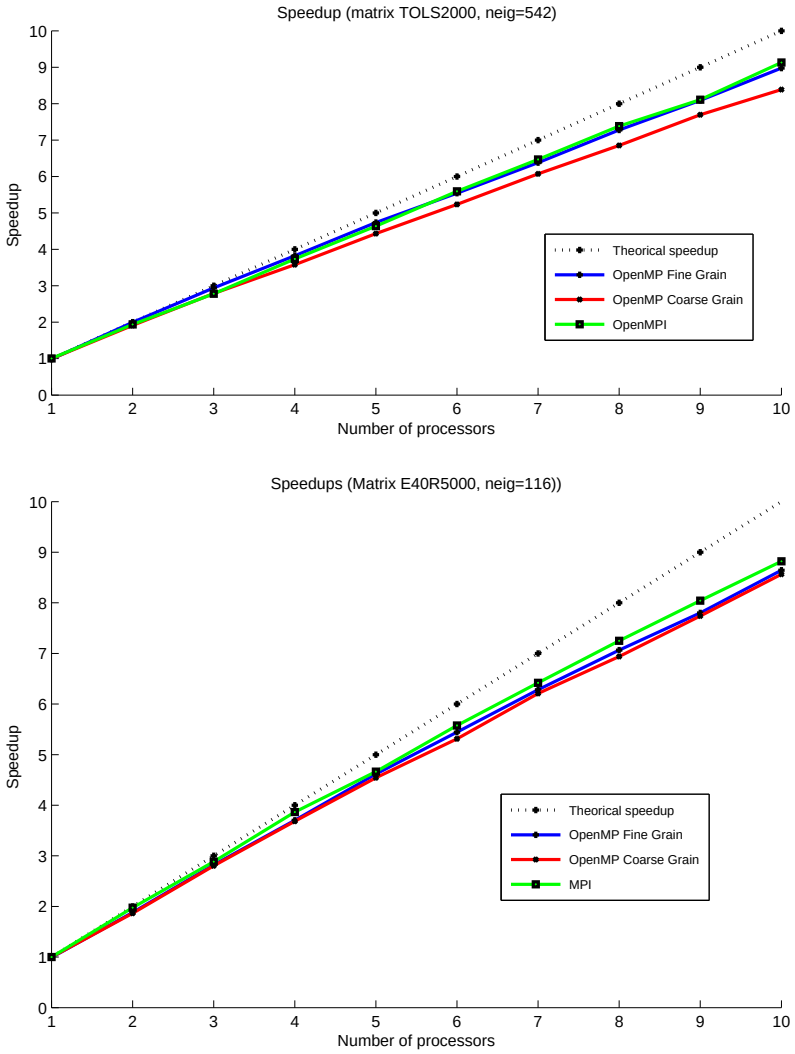

FIG. 6.1. *Parallel* `EIGENCNT` *: measured speedups on two experiments.*

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