

Some Algorithms Providing Rigorous Bounds for the Eigenvalues of a Matrix

Raymond Pavéc
 LIM, Université de Bretagne Occidentale
 Brest, France
 pavec@univ-brest.fr

Abstract: Three algorithms providing rigorous bounds for the eigenvalues of a real matrix are presented. The first is an implementation of the bisection algorithm for a symmetric tridiagonal matrix using IEEE floating-point arithmetic. The two others use interval arithmetic with directed rounding and are deduced from the Jacobi method for a symmetric matrix and the Jacobi-like method of Eberlein for an unsymmetric matrix.

1 Bisection Algorithm for a Symmetric Tridiagonal Matrix

Let A be a symmetric tridiagonal matrix of order n :

$$A = A_n = \begin{pmatrix} a_1 & b_2 & & \\ b_2 & a_2 & \ddots & \\ & \ddots & \ddots & b_n \\ & & b_n & a_n \end{pmatrix}$$

Set $b_1 = 0$, and suppose $b_k \neq 0, k = 2, \dots, n$. The bisection method is based on the fact that the sequence $d_k(x)$ of principal minors of $A - xI$ is a Sturm sequence:

$$d_k(x) = \det(A_k - xI_k), k = 1, \dots, n, \quad d_0 = 1$$

In floating point arithmetic, as pointed out in [Barth, Martin, Wilkinson 1971], the direct use of this sequence is quite impossible: even for small n underflow and overflow are unavoidable. So they consider (the hypothesis $b_k \neq 0, k = 2, \dots, n$ can then be removed):

$$p_k = \frac{d_k}{d_{k-1}}, k = 1, \dots, n$$

This new sequence satisfies the recurrence relations:

$$(\mathcal{S}_x) \quad p_k := \begin{cases} a_k - x & \text{if } b_k = 0 \text{ or } p_{k-1} = -\infty \\ -\infty & \text{if } p_{k-1} = 0 \\ a_k - x - \frac{b_k^2}{p_{k-1}} & \text{otherwise} \end{cases} \quad \text{for } k = 1, \dots, n$$

From the Sturm property and the choice of $p_k = -\infty$ when $p_{k-1} = 0$, it comes that the number of negative terms in (\mathcal{S}_x) is equal to the number of eigenvalues of A smaller than x .

Beginning with an interval containing all the eigenvalues of A , the method of bisection provides intervals as small as desired, containing the eigenvalues of A .

1.1 Setting it to work in floating point arithmetic

In floating point arithmetic there are two problems:

- to perform the calculations *without overflow*,
- to give *bounds for the error*.

[Barth, Martin, Wilkinson 1971] give bounds for all the eigenvalues. Godunov [Godunov et al. 1993], page 315, gives a similar result but uses a different sequence and guarantees no overflow.

The method presented here (using the sequence (\mathcal{S}_x)) guarantees the absence of overflow and provides bounds separately *for each eigenvalue*.

The set of machine-numbers (IEEE standard, available on Macintosh [Apple 1988] or PC compatible [Crawford, Gelsinger 1988]), provides representations for:

$$\begin{cases} 0, -\infty, +\infty \\ \pm 1, a_2 \dots a_t 2^e, a_i = 0 \text{ or } 1, -min \leq e \leq max, \text{ (normalized numbers)} \\ \pm 0, a_2 \dots a_t 2^{-min}, \text{ (denormalized numbers)} \end{cases}$$

t is the number of significative digits used. We suppose $min \leq max$.

The positive normalized numbers lie in the interval $[\epsilon_0, M]$:

$$\epsilon_0 = 2^{-min}, \quad M = 1.1 \dots 1 \times 2^{max} \approx 2 \times 2^{max}$$

Notice that $min \leq max \Rightarrow 1/\epsilon_0 \leq 2^{max} \approx M/2$.

With *rounding to nearest* the relative error in usual operations is less than $eps = 2^{-t}$, (machine precision). For the machine-operations $\hat{\top}$ ($\top \rightarrow +, -, \times, /$) we have:

$$x \hat{\top} y = (x \top y) (1 + \epsilon), \quad |\epsilon| \leq eps$$

for normalized numbers x, y , and $x \top y$. Notice that the presence of denormalized numbers insures that an addition or subtraction that gives 0 is exact.

1.1.1 Calculation without overflow

In the calculation of (\mathcal{S}_x) the critical term is b_k^2/p_{k-1} . To avoid overflow:

- A scaling of the matrix is performed by multiplying it by 2^p , p being chosen so that all elements become less than 1.
- The denormalized numbers occuring during the calculation of (\mathcal{S}_x) are replaced by 0. This induces an absolute error $\leq \epsilon_0$.

Thus, the *operations used* ($\hat{\top}$) are:

$$x \hat{\top} y = \begin{cases} 0 & \text{if } x \tilde{\top} y \text{ is denormalized} \\ x \tilde{\top} y & \text{otherwise} \end{cases}$$

and the calculated sequence is (remember that $b_1 = 0$):

$$(\hat{\mathcal{S}}_x) \hat{p}_k := \begin{cases} a_k \hat{x} & \text{if } b_k = 0 \text{ or } \hat{p}_{k-1} = -\infty \\ -\infty & \text{if } \hat{p}_{k-1} = 0 \\ a_k \hat{x} \hat{b}_k \hat{p}_{k-1} & \text{otherwise} \end{cases} \quad \text{for } k = 1, \dots, n$$

The eigenvalues of A are therefore in $[-3, 3]$, and x also.

If \hat{p}_{k-1} is 0 or infinite there is no problem.

Otherwise $|\hat{p}_{k-1}|$ is a normalized number $\geq \epsilon_0$:

$$|a_k - x - b_k \times b_k / \hat{p}_{k-1}| \leq |a_k| + |x| + 1/\epsilon_0 \leq 4 + 2^{min} < M$$

and this is also true for machine operations.

1.1.2 Error estimation

The scaling of the matrix does not cause any error, except for the elements that become less than ϵ_0 in absolute value and are replaced by 0. The elements b_k^2 that become less than ϵ_0 are also replaced by 0. Thus the matrix becomes $2^p A + E'$. E' is a tridiagonal symmetric matrix which elements are equal to 0 or bounded by ϵ_0 or $\sqrt{\epsilon_0}$.

A is now the scaled matrix. The classical error analysis ($\tilde{\tau}$ operations) shows that the calculation of $(\hat{\mathcal{S}}_x)$ is identical to the calculation of the sequence (\mathcal{S}_x) associated with a matrix $A + E''$. This remains true for the $\hat{\tau}$ operations. A symmetric tridiagonal matrix E :

$$E = \begin{pmatrix} e_1 & f_2 & & \\ f_2 & e_2 & \ddots & \\ & \ddots & \ddots & f_n \\ & & f_n & e_n \end{pmatrix}$$

such that $|E''| \leq E$ will be calculated.

It will be shown that there exist small integers $na, da, nb \leq 3$, depending on k such that:

$$e_k = |a_k - x| ((1 + eps)^{na} - 1) + da \times \epsilon_0$$

$$f_k = |b_k| \left((1 + eps)^{\frac{nb}{2}} - 1 \right)$$

The term $da \times \epsilon_0$ comes from the operations that give 0 or a denormalized result. Let us examine the different cases that occur in the calculation of \hat{p}_k and determine the values of the integers na, da and nb :

- **Case A:** $b_k = 0$ or $\hat{p}_{k-1} = -\infty$.

Then $\hat{p}_k = a_k \hat{x}$. Let $y = a_k \hat{x}$. If y is a normalized number we may write:

$$y = (a_k - x)(1 + \epsilon_1) = a_k + (a_k - x)\epsilon_1 - x, |\epsilon_1| \leq eps$$

So we have: $\hat{p}_k = y, e_k = |a_k - x| eps, f_k = 0$. ($na = 1, da = 0, nb = 0$).

If y is a denormalized number then $|a_k - x| \leq \epsilon_0$ and:

$$\hat{p}_k = 0 = a_k - (a_k - x) - x$$

Thus $e_k = \epsilon_0, f_k = 0$. ($na = 0, da = 1, nb = 0$).

Lastly if $y = 0$, there is no error and $\hat{p}_k = 0, e_k = f_k = 0$. ($na = da = nb = 0$).

• **Case B:** $\hat{p}_{k-1} = 0$.

Then $\hat{p}_k = -\infty$, and $e_k = f_k = 0$. ($na = da = nb = 0$).

• **Case C:** \hat{p}_{k-1} is a normalized number.

For each operation three cases (at the most) are to be considered according to the result: 0, denormalized (replaced by 0), normalized.

◦ *Usual case C0:* In the usual case all operations give a normalized result and we get:

$$\hat{p}_k = \left((a_k - x)(1 + \epsilon_1) - \frac{b_k^2(1 + \epsilon_2)}{\hat{p}_{k-1}}(1 + \epsilon_3) \right) (1 + \epsilon_4), |\epsilon_i| \leq eps$$

The ϵ_i are the relative errors occurring in the operations. Thus:

$$\hat{p}_k = a_k + (a_k - x)(\epsilon_1 + \epsilon_4 + \epsilon_1\epsilon_4) - x - \frac{b_k^2(1 + \epsilon_2)(1 + \epsilon_3)(1 + \epsilon_4)}{\hat{p}_{k-1}}$$

This is the exact result corresponding to:

$$a_k + (a_k - x)(\epsilon_1 + \epsilon_4 + \epsilon_1\epsilon_4) \quad \text{and} \quad b_k^2(1 + \epsilon_2)(1 + \epsilon_3)(1 + \epsilon_4)$$

Thus in this case:

$$e_k = |a_k - x|(2eps + eps^2), (na = 2, da = 0)$$

$$f_k = |b_k| \left(\sqrt{(1 + eps)^3} - 1 \right), (nb = 3)$$

◦ *Case C1:* $b_k \tilde{\times} b_k / \hat{p}_{k-1}$ gives 0 or a denormalized result (and thus replaced by 0). In this case:

$$\hat{p}_k = a_k \hat{-} x$$

So we may write:

$$\hat{p}_k = a_k \hat{-} x + \left[\frac{b_k \tilde{\times} b_k}{\hat{p}_{k-1}} \right] - \frac{b_k^2(1 + \epsilon_2)}{\hat{p}_{k-1}}$$

and in this case we have to add ϵ_0 to the e_k obtained in case **A** (add 1 to da) and $nb = 1$.

◦ *Case C2:* $a_k - x = 0$. Excluding case *C1* we have:

$$\hat{p}_k = - \frac{b_k^2(1 + \epsilon_2)(1 + \epsilon_3)}{\hat{p}_{k-1}}$$

and thus: $e_k = 0, (na = 0, da = 0), \quad f_k = |b_k|eps, (nb = 2)$.

◦ *Case C3*: $a_k \tilde{x}$ is denormalized. This case is the same as *C2*, except that $e_k = \epsilon_0$, ($na = 0, da = 1, nb = 2$).

◦ *Case C4*: All operations give a normalized result, except the last subtraction. If the result is 0, then consider the usual case and set ϵ_4 to 0. It comes:

$$e_k = |a_k - x|eps, f_k = |b_k|eps, (na = 1, da = 0, nb = 2)$$

If the result is denormalized add ϵ_0 to e_k , ($na = 1, da = 1, nb = 2$).

1.2 Bounds for the eigenvalues

Naming $\lambda_i(X), i = 1, \dots, n$, the eigenvalues of a symmetric matrix X of order n , in increasing order, we have [Wilkinson 1965], page 101:

$$\lambda_i(A) + \lambda_1(E'') \leq \lambda_i(A + E'') \leq \lambda_i(A) + \lambda_n(E'')$$

Let ρ be the spectral radius of E'' . We get:

$$\lambda_i(A) - \rho \leq \lambda_i(A + E'') \leq \lambda_i(A) + \rho$$

and also:

$$\lambda_i(A + E'') - \rho \leq \lambda_i(A) \leq \lambda_i(A + E'') + \rho$$

ρ is bounded by $\|E''\|_\infty$, and by $\|E\|_\infty$.

Let m_x be the number of negative terms in (\hat{S}_x) . We have:

$$\begin{aligned} \lambda_i(A + E'') &< x, i = 1, \dots, m_x \\ \lambda_i(A + E'') &\geq x, i = m_x + 1, \dots, n \end{aligned}$$

Naming δ_x the infinite norm of E , it comes:

$$\begin{aligned} \lambda_i(A) &< x + \delta_x, i = 1, \dots, m_x \\ \lambda_i(A) &\geq x - \delta_x, i = m_x + 1, \dots, n \end{aligned}$$

If the interval $[x, y]$ is such that $k = m_y - m_x > 0$, we may say that:

$$\lambda_i(A) \in [x - \delta_x, y + \delta_y[, i = m_x + 1, \dots, m_y$$

It remains to take into account the scaling of the matrix and the initial rounding errors.

The bisection algorithm gives intervals such that $m_x < m_y$: to determine $\lambda_k(A)$ for a given k first choose $[x, y]$ such that $m_x < k \leq m_y$ and calculate $z = (x + y) / 2$ and m_z :

- if $m_z \geq k$ the new interval will be $[x, z]$,
- if $m_z < k$ the new interval will be $[z, y]$.

1.3 Algorithm and example

The general structure of the algorithm is the same as in [Barth, Martin, Wilkinson 1971], except the final test: for each eigenvalue the bisection process is continued until the interval $[x, y]$ is such that x and y are two consecutive machine-numbers (denormalized numbers excluded), or until a fixed maximum number of steps is reached.

The machine precision used is $eps = 2^{-64} \approx 5,5 \times 10^{-20}$. This precision is available on micro-computers [Apple 1988], [Crawford, Gelsing 1988]. The results have been obtained using the software [Pavec 1994].

Consider the matrix of order $n = 30$ from [Barth, Martin, Wilkinson 1971]:

$$a_i = i^4, b_i = i - 1, \quad i = 1, \dots, 30$$

The eigenvalues lie in the interval $[0.933.., 8.100.. \times 10^5]$. A few results are shown in the table below:

- the bounds for the absolute error ' $\Delta\lambda_i$ ' and relative error ' $\Delta\lambda_i/\lambda_i$ ' take in account the final rounding from base 2 to base 10,
- 'Steps' is the number of bisection steps performed and is less than the fixed maximum (= 100).

i	λ_i	$\Delta\lambda_i$	$\Delta\lambda_i/\lambda_i$	Steps
30	8.10000 00818 73846 690 $\times 10^5$	2.3×10^{-13}	2.9×10^{-19}	64
20	1.60000 00056 28909 621 $\times 10^5$	1.4×10^{-13}	8.8×10^{-19}	62
10	1.00000 02006 27702 490 $\times 10^4$	9.3×10^{-14}	9.3×10^{-18}	64
1	0.93340 70848 65963	8.8×10^{-14}	9.5×10^{-14}	68

2 Symmetric Matrices and Jacobi's Algorithm

Jacobi's method [Rutishauser 1991] applied to a symmetric matrix A constructs a sequence of symmetric matrices A_k , similar to A , and converging to a diagonal matrix:

$$A_{k+1} = R_k^T A_k R_k$$

where R_k is a rotation (angle θ_k) matrix calculated to annihilate a non diagonal element (i, j) of A_k . $t_k = \tan \theta_k$ is obtained from $a_{ii}^{(k)}, a_{ij}^{(k)}, a_{jj}^{(k)}$.

2.1 Setting it to work on matrices of intervals

In order to obtain rigorous bounds for the eigenvalues, we work on *matrices of intervals*.

The elementary operations $(+, -, \times, /, \sqrt{\quad})$ on intervals [Moore 1979] are performed using directed rounding provided by the IEEE standard, without using the extensions developed in [Kulisch, Miranker 1981].

A number or a matrix x represented by an interval is written $[x]$.

Let $[A]$ be the initial symmetric matrix of intervals. Starting with $[A]_1 = [A]$, we generate a sequence of symmetric matrices $[A]_k$ such that all symmetric matrix B belonging to $[A]$ is similar to a symmetric matrix B_k belonging to $[A]_k$. Thus the eigenvalues of B are the eigenvalues of a symmetric matrix B_k belonging to $[A]_k$.

For an interval matrix $[A]_k$, in order to restrict the growth of the intervals, a machine-number t_k is calculated on the *midpoint* of the intervals $[a]_{ii}^{(k)}$, $[a]_{ij}^{(k)}$ and $[a]_{jj}^{(k)}$, using ordinary floating point arithmetic.

The corresponding rotation is:

$$R_k = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \quad c = 1/\sqrt{1+t_k^2}, s = t_k c$$

Using interval arithmetic to evaluate c and s , we get an interval matrix $[R]_k$ containing R_k and we set:

$$[A]_{k+1} = [R]_k^T [A]_k [R]_k$$

If B is a symmetric matrix belonging to $[A]$ then

$$B_k = R_{k-1}^T \dots R_1^T B R_1 \dots R_{k-1}$$

is similar to B and belongs to $[A]_k$.

Notice that the sequence $[A]_k$ does not necessarily contain the sequence generated by Jacobi's method, and that the element $[a]_{ij}^{(k)}$ is not annihilated but replaced by a *small* interval.

These rotations are performed in a cyclic way, among the elements that do not contain 0.

2.2 Bounds for the eigenvalues

Let D_k be the diagonal matrix which diagonal elements are the midpoint of the elements of $[A]_k$, and $[C]_k$ a matrix such that:

$$[A]_k \subseteq D_k + [C]_k$$

The theorem of Gershgorin [Wilkinson 1965] shows that the eigenvalues of a symmetric matrix belonging to $[A]$ are in the union of the closed intervals:

$$[d_i - r_i, d_i + r_i], \quad r_i = \sum_{j=1}^n |[c]_{ij}|$$

where $|[c]_{ij}|$ is:

$$|[c]_{ij}| = \max_{t \in [c]_{ij}} |t|$$

2.3 Examples

- Consider the matrix [Wilkinson, Reinsch, 1991], page 223:

$$A = \begin{pmatrix} 10 & 1 & 2 & 3 & 4 \\ 1 & 9 & -1 & 2 & -3 \\ 2 & -1 & 7 & 3 & -5 \\ 3 & 2 & 3 & 12 & -1 \\ 4 & -3 & -5 & -1 & 15 \end{pmatrix}$$

This matrix is stored as zero-length intervals. After a sweep of the lower triangle the Gershgorin's disks are (radius ≤ 2.1):

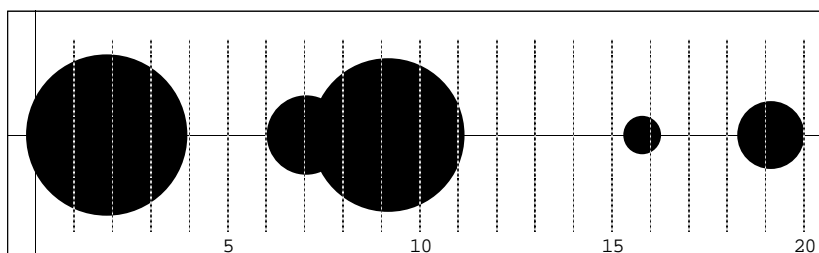


Figure 1: Gershgorin disks after a sweep

Going on with the sweeps until all non-diagonal elements contain 0, the radii of all the disks (*Machine precision*: 2^{-64}) become successively less than:

$$0.073, \quad 1.67 \times 10^{-5}, \quad 2.25 \times 10^{-16}$$

- The matrix $B = 8J - 5J^2 + J^3$ of order 44 [Rutishauser 1991], page 209, where J denotes the tridiagonal matrix with $J_{ii} = 2, J_{i,i+1} = 1$, has eleven eigenvalues in the interval $[4, 4.163]$, the length of which is $1/100$ of the total length of the spectrum.

After 7 sweeps all the eigenvalues are separated, except two that lie in the interval $[4.0032, 4.0065]$.

3 Eberlein's Jacobi-like Method for Unsymmetric Real Matrices

For an unsymmetric real matrix A Eberlein gives a Jacobi-like method [Eberlein 1962]:

$$A_{k+1} = T_k^{-1} A_k T_k$$

A_k generally converges to a block-diagonal matrix, with blocks of order 1 or 2. The blocks of order two have complex conjugate eigenvalues $a \pm ib$:

$$\begin{pmatrix} a & -b \\ b & a \end{pmatrix}$$

T_k is the product of a rotation R_k and of a matrix S_k :

$$S_k = \begin{pmatrix} \cosh y & -\sinh y \\ -\sinh y & \cosh y \end{pmatrix}$$

working in a coordinate plane (i, j) .

3.1 Bounds for the eigenvalues

After some sweeps of Eberlein's method we expect a matrix of the form:

$$\Delta + E$$

where Δ is a block-diagonal matrix, and E a matrix with small elements. The following theorem, that is a particular case of the theorem of Bauer-Fike [Golub, Van Loan 1983], page 342, gives disks of the complex plane containing the eigenvalues of $\Delta + E$:

Theorem. Let $A = \Delta + E$, where Δ is a block-diagonal with blocks of order 1 or 2.

$$\Delta = \text{diag}(\Delta_1, \Delta_2, \dots, \Delta_p)$$

$$\Delta_r = \alpha_r \quad \text{or} \quad \begin{pmatrix} \alpha_r & -\beta_r \\ \beta_r & \alpha_r \end{pmatrix}$$

Δ can be diagonalised with a unitary block-diagonal matrix X which has the same structure as Δ . Let $F = X^{-1}EX$. Then the eigenvalues of A are in the disks of the complex plane, which centers are the eigenvalues of Δ and the radii:

$$r_i = \sum_{j=1}^n |f_{ij}|$$

If the union U of k of these disks is isolated from the others then U contains exactly k eigenvalues of A .

Proof. The blocks of order 1 of X are equal to 1 and the blocks of order 2 to:

$$X_r = \frac{1}{\sqrt{2}} \begin{pmatrix} i & -i \\ 1 & 1 \end{pmatrix}, \quad X_r^{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i & 1 \\ i & 1 \end{pmatrix}$$

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of Δ and

$$\Delta' = X^{-1}\Delta X = \text{diag}(\lambda_1, \dots, \lambda_n)$$

If λ is an eigenvalue of A , then $A - \lambda I$ is singular, and

$$X^{-1}(A - \lambda I)X = \Delta' - \lambda I + F$$

also. There exists a complex vector x , $\|x\|_\infty = 1$, such that:

$$(\Delta' - \lambda I)x = -Fx$$

Thus

$$(\lambda_i - \lambda) x_i = - \sum_{j=1}^n f_{ij} x_j, i = 1, \dots, n$$

Choosing i such that $|x_i| = 1$ we get:

$$|\lambda_i - \lambda| \leq \sum_{j=1}^n |f_{ij}| = r_i$$

r_i is easily expressed in terms of E .

If the union U of k of these disks is isolated from the union V of the others, the disks associated with $A(t) = \Delta + tE$ have the same property for all $t \in [0, 1]$: the centers do not change and the radii are tr_i .

The result comes then from the fact that U contains exactly k eigenvalues of $A(0)$, and V exactly $n - k$. The eigenvalues of $A(t)$ are continuous functions of t , so they cannot jump from U to V .

3.2 Setting it to work on matrices of intervals

A sequence of matrices $[A]_k$ is generated from the initial matrix $[A]$, such that each matrix $B \in [A]$ is similar to $B_k \in [A]_k$.

At each stage of the method $T_k = RS$ is calculated using ordinary floating point arithmetic and the midpoints of the elements of $[A]_k$.

Then

$$[T_k^{-1}] \text{ and } [A]_{k+1} = [T_k^{-1}] [A]_k T_k$$

are calculated using interval arithmetic.

It remains then to decompose $[A]_k$ under the form:

$$[A]_k \subseteq \Delta_k + [C]_k$$

where Δ_k is a block-diagonal matrix and to calculate disks containing the eigenvalues. Bounds for the radii of these disks are deduced from the theorem of the preceding section.

3.3 Examples

- Consider the matrix A [Eberlein, Boothroyd 1971], page 334:

$$A = \begin{pmatrix} 6 & -3 & 4 & 1 \\ 4 & 2 & 4 & 0 \\ 4 & -2 & 3 & 1 \\ 4 & 2 & 3 & 1 \end{pmatrix}$$

A has two double eigenvalues equal to $3 \pm \sqrt{5}$ and is defective.

The three first sweeps give:

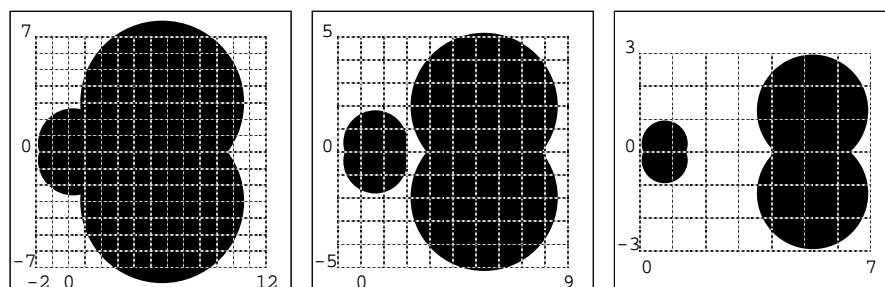


Figure 2: The three first sweeps

After 2 sweeps the disks are included within to disjoint regions.

Finally we get disks which radii bounded by $3,98 \times 10^{-8}$ and $2,2 \times 10^{-8}$.

- For the matrix $B = (b_{ij})$ of order 12 [Eberlein, Boothroyd 1971], page 334, defined by:

$$\begin{cases} b_{ij} = 13 - j, & \text{if } i \leq j \\ b_{i,j} = 12 - j, & \text{if } i = j + 1 \\ b_{ij} = 0, & \text{if } i > j + 1 \end{cases}$$

after 33 sweeps the 12 disks are disjoint and the radii are < 0.001 .

4 Conclusion

These algorithms are implemented in an interactive software [Pavec 1994] working on the Apple Macintosh series of micro-computers. This software is devoted to:

- teaching of mathematics [Pavec 1993]: a very simple Pascal style language lets you create interactively changeable figures containing curves, text, numerical values ...

- and teaching of elementary numerical analysis: interpolation, approximation, ordinary differential equations, numerical integration, systems of equations, eigenvalues.

A commented Pascal version of the algorithm of bisection is available by e-mail (pavec@univ-brest.fr).

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