Numerical methods for eigenvalues and eigenvectors, MAT 3110 UiO

September 21, 2023

In these notes we present applications of Gershgorin's circle theorem, which is a useful for rough estimates of eigenvalues of a matrix, three iteration methods for computing eigenpairs of matrices, and a perturbation analysis on how sensitive eigenvalues are to perturbations in the matrix A. The topics covered here largely relate to sections 5.3, and 5.7-10 in Suli and Mayers, with some topics treated exclusively in these notes, such as power iteration.
The fundamental question we want to study is: how does one numerically compute eigenvalues and eigenvectors of a matrix $A \in \mathbb{R}^{n\times n}$? A natural idea would be to proceed as follows:

1. For $\lambda \in \mathbb{R}$, compute the characteristic polynomial $p(\lambda) = \det(A - \lambda I)$.
2. Find an eigenvalue of A by solving $p(\lambda) = 0$ using some iteration method (e.g., simple iteration, Newton's method, Secant or bisection).
3. Having obtained a numerical solution $\bar{\lambda} = \lambda_K$, compute eigenvector $\bar{x} \in \mathbb{R}^n_*$ (if you also seek eigenvector) by solving $(A - \bar{\lambda} I)\bar{x} = 0$.

This approach turns out to be bad idea for two reasons. First, every step in your iteration method, say, e.g., the Secant method

$$\lambda_{k+1} = \lambda_k - p(\lambda_k)\left(\frac{\lambda_k - \lambda_{k-1}}{p(\lambda_k) - p(\lambda_{k-1})}\right) \qquad k = 1, 2, \ldots$$

requires that you compute the determinant $p(\lambda_k) = \det(A - \lambda_k I)$. This costs $\mathcal{O}(n^3)$ operations per iteration (by the procedure we presented in Oblig 1, exercise 3), which is very expensive when n is large. Second, if A is not a symmetric matrix, it may be that some of the solutions to $p(\lambda) = 0$ are complex-valued, so then we rather have to solve the more technical eigenvalue problem $p : \mathbb{C} \to \mathbb{C}$ with an iteration method, essentially on $\mathbb{R}^2$. This is more complicated than when eigenvalues are real-valued, but often possible. Having said that, we will largely shy away for complications related to complex-valued in these notes by assuming that A is a symmetric matrix (which ensures that all its eigenvalues are real-valued).
Before looking into more efficient algorithms for computing eigenvalues, we first consider the more fundamental question of obtaining coarse estimates of the eigenvalues of A. This is relevant information for most iteration methods, as they often require good start values to achieve convergence.

5.1 Gershgorin theorems

Notation: For an $n \times n$ matrix A, let $\sigma(A) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ denote its set of eigenvalues.
The following result is useful for estimating the values in the set $\sigma(A)$. In the Gershgorin results that follow, the eigenvalues λ_i are not ordered according to magnitude:

Theorem 5.1 (Gershgorin's circle theorem) Consider a matrix $A = (a_{ij}) \in \mathbb{R}^{n\times n}$ and associate its i-th row to the off-diagonal radius

$$r_i = \sum_{j\neq i} |a_{ij}|, \quad \text{and the } i\text{-th Gershgorin disc} \quad D_i := \{z \in \mathbb{C} \mid |z - a_{ii}| \leq r_i\}.$$

Then each eigenvalue lies inside some Gershgorin disc, $\lambda \in D_i$ for some $1 \leq i \leq n$, and thus also $\sigma(A) \subset \cup_{i=1}^{n} D_i$.

Proof: Let (λ, v) be an eigenpair of A. Multiply the eigenvector with a scalar so that $\|v\|_\infty = 1$ and $v_i = 1$ for some $i \in \{1, \ldots, n\}$. Then, $|v_j| \leq 1$ for all $j \in \{1, \ldots, n\}$, and we have that

$$(Av)_i = (\lambda v)_i = \lambda \qquad \text{and also} \qquad (Av)_i = a_{ii} + \sum_{j \neq i} a_{ij} v_j.$$

We conclude that

$$|\lambda - a_{ii}| \leq \left| \sum_{j \neq i} a_{ij} v_j \right| \leq \sum_{j \neq i} |a_{ij}| \underbrace{|v_j|}_{\leq 1} \leq \sum_{j \neq i} |a_{ij}| = r_i.$$

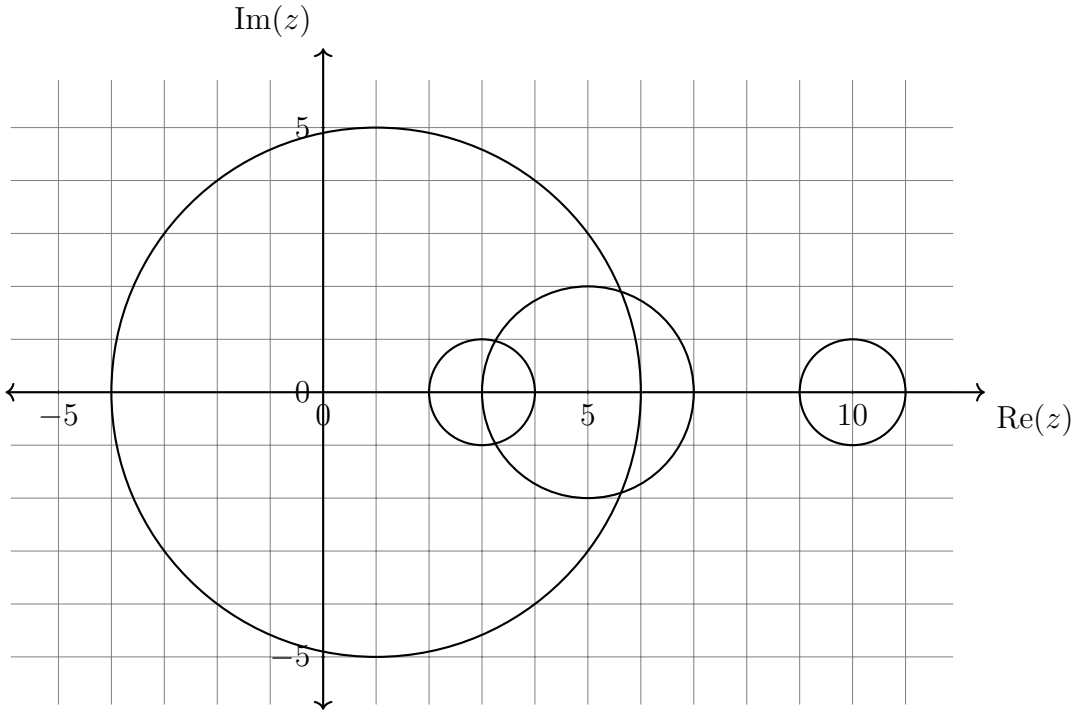
The argument holds for any eigenpair of A. □

Example 5.2

$$A = \begin{bmatrix} 1 & 0 & 5 & 0 \\ 1 & 3 & 0 & 0 \\ 0 & 1 & 5 & 1 \\ 0 & 1 & 0 & 10 \end{bmatrix}$$

with (approximately-valued) eigenvalues $1.80 \pm 0.61i, 5.38, 10.02$

$$D_1 = D(1,5), \quad D_2 = D(3,1), \quad D_3 = D(5,2), \quad D_4 = D(10,1).$$



Remark 5.3 a) **Note:** The theorem does not say that each Gershgorin disc contains an eigenvalue. Some discs may contain many, others none.

b) If all the Gershgorin discs are disjoint, then one can show that each disc D_i must contain one and only one eigenvalue.

The last remark generalizes to the following theorem:

Theorem 5.4 It the Gershgorin discs of a matrix $A \in \mathbb{R}^{n\times n}$ satisfies (for some ordering) that $B_1 = \cup_{i=1}^{k} D_i$ is disjoint from $B_2 = \cup_{i=k+1}^{n} D_i$, meaning $B_1 \cap B_2 = \emptyset$, then k eigenvalues belong to B_1 and $n-k$ eigenvalues belong to B_2.
Furthermore, if all Gershgorin discs are disjoint, then each disc contains one and only one eigenvalue.

Proof: See Suli and Mayers Theorem 5.5 for proof □

Applications of Gershgorin's theorem

A matrix $A \in \mathbb{R}^{n\times n}$ is said to be strictly diagonally dominant if

$$|a_{ii}| > \underbrace{\sum_{j\neq i} |a_{ij}|}_{=r_i} \qquad \forall i \in \{1,\ldots,n\}.$$

Theorem 5.5 (Diagonal dominance) Every strictly diagonally dominant matrix is non-singular.

Proof: Every eigenvalue of A lies inside the union of Gershgorin discs, meaning

$$\sigma(A) \subset \cup_{i=1}^{n} D_i$$

The disc D_i is centered at a_{ii} and has the radius $r_i < |a_{ii}|$. The point $z = 0$ is not inside the disc, since the diagonal dominance of A implies that

$$|a_{ii} - 0| = |a_{ii}| > r_i.$$

This holds for all $i \in \{1,\ldots,n\}$, so $0 \notin \cup_{i=1}^{n} D_i$..
0 is therefore not an eigenvalue of A, and the non-singularity of A follows from

$$\det(A) = \prod_{\lambda\in\sigma(A)} \lambda \neq 0.$$

□

Example 5.6

$$A = \begin{bmatrix} 2 & 1 & -1/2 \\ -1 & 3 & 1 \\ 0 & 1 & -2 \end{bmatrix}$$

is non-singular as

$$|a_{11}| = 2 > 1 + |-1/2|, \qquad |a_{22}| = 3 > |-1| + 1, \quad \text{and} \quad |a_{33}| = |-2| > 1 + 0.$$

If $T \in \mathbb{R}^{n\times n}$ is invertible, then we recall that $T^{-1}AT$ is called a similarity transformation of A.
Similarity transformations preserve the spectrum $\sigma(T^{-1}AT) = \sigma(A)$, since the characteristic polynomial is preserved:

$$p_{T^{-1}AT}(\lambda) = \det(T^{-1}AT - \lambda I) = \det(T^{-1}(A-\lambda I)T) = \underbrace{\det(T^{-1})\det(T)}_{=1}\det(A-\lambda I) = p_A(\lambda).$$

Combining Gershgorin's theorem with similarity transformation can lead to improved estimates of the spectrum:

Example 5.7 The matrix

$$A = \begin{bmatrix} 10 & 2 & 3 \\ -1 & 0 & 2 \\ 1 & -1 & 1 \end{bmatrix}$$

has $\sigma(A) = \{10.226, 0.387 \pm 2.216i\}$. Let us assume that $\sigma(A)$ is unknown and try to estimate it.
By Gershgorin's theorem,

$$D_1 = D(10,5), \quad D_2 = D(0,3), \quad D_3 = D(1,2).$$

Since D_1 does not intersect with $D_2 \cup D_3$ we know that D_1 must contain one eigenvalue, and it must be real-valued one, as complex-valued eigenvalues come in conjugate pairs.

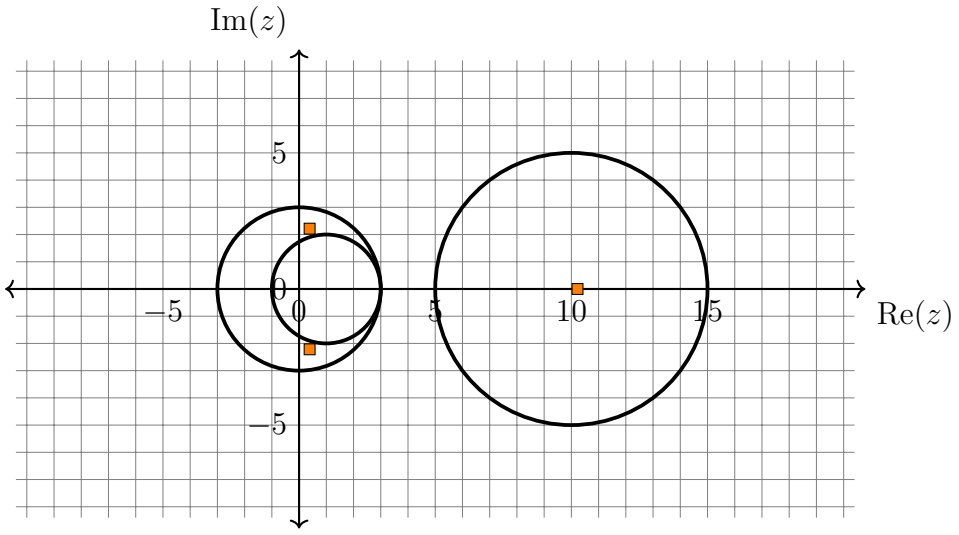


Figure 5.1: Gershgorin circles D_1, D_2, D_3 of A, and eigenvaules in orange squares.

To improve our information of the dominant eigenvalue λ_1, consider the similarity transformation

$$\tilde{A} = T^{-1}AT \quad \text{with} \quad T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix} \implies \tilde{A} = \begin{bmatrix} 10 & 2\alpha & 3\alpha \\ -1/\alpha & 0 & 2 \\ 1/\alpha & -1 & 1 \end{bmatrix}$$

Since $\sigma(\tilde{A}) = \sigma(A)$, we apply Gershgorin's theorem on $\tilde{A}$ to obtain the discs

$$\tilde{D}_1 = B((10,0),5\alpha), \quad \tilde{D}_2 = B((0,0),2+1/\alpha), \quad \tilde{D}_3 = B((1,0),1+1/\alpha).$$

To ensure that $\lambda_1 \in \tilde{D}_1$, we need to choose $\alpha > 0$ so that

$$\tilde{D}_1 \cap (\tilde{D}_2 \cup \tilde{D}_3) = \emptyset \iff \tilde{D}_1 \cap D_2 \iff 10 - 5\alpha > 2 + 1/\alpha.$$

This holds for instance when $\alpha = 1/7$. Hence $\lambda_1 \in \tilde{D}_1(\alpha = 1/7)$ and real-valued: $\lambda_1 \in [10 - 5/7, 10 + 5/7]$.
One could also try to improve the information on λ_2 and λ_3 by varying α, but the considered similarity transformation is not suitable for that purpose.

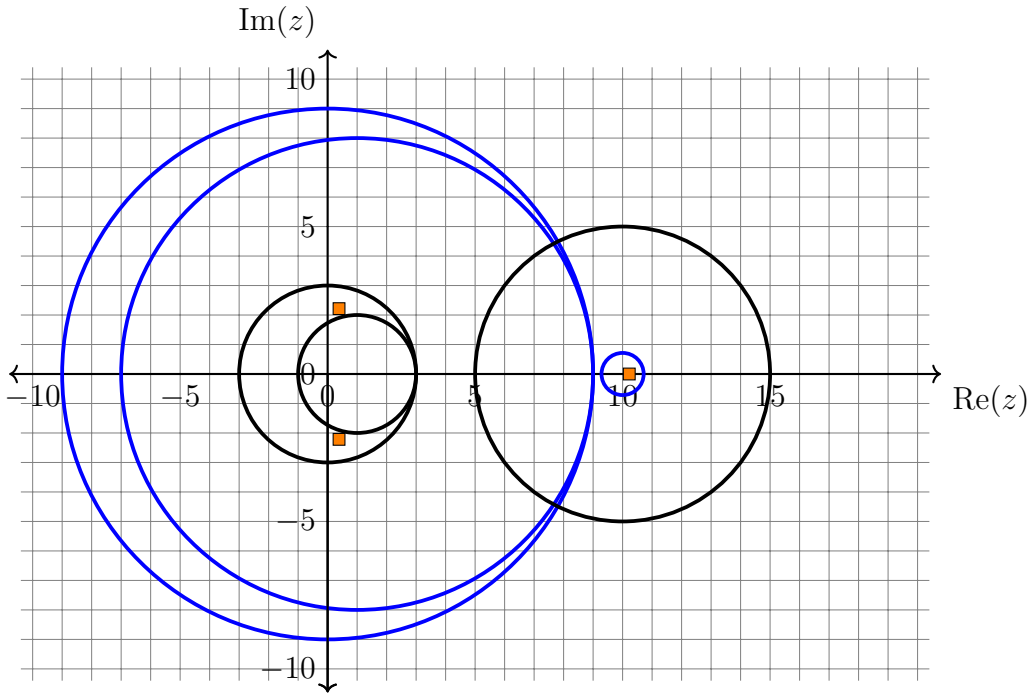


Figure 5.2: Gershgorin discs $\tilde{D}_1, \tilde{D}_2$ and $\tilde{D}_3$ of $\tilde{A}$ for $\alpha = 1/7$ in blue, and black Gershgorin discs for D_1, D_2 and D_3 for $\tilde{A} = A$ with $\alpha = 1$.

5.2 Power iteration

Is an algorithm that computes the dominating (largest in absolute value) eigenvalue of a matrix.

Algorithm 1: Power iteration

Data: $A \in \mathbb{R}^{n\times n}$

Choose a start vector $x^{(0)} = x_0 \in \mathbb{R}^n \setminus \{0\}$.

for $k = 1, 2, \ldots$ **do**

$$x^{(k)} \leftarrow Ax^{(k-1)} \tag{5.1}$$

Compute the normalized vector

$$z^{(k)} \leftarrow \frac{x^{(k)}}{\|x^{(k)}\|_2}$$

and the so-called Rayleigh quotient

$$\lambda^{(k)} \leftarrow (z^{(k)})^T A z^{(k)}.$$

end

Remark 5.8 a) Let λ_1 denote the dominating eigenvalue of A Then under some assumptions,

$$\lim_{k\to\infty} \lambda^{(k)} = \lambda_1$$

and $z^{(k)}$ will asymptotically belong to the eigenspace of λ_1.

b) Normally, one replaces the step (5.1) by

$$z^{(k+1)} = \frac{Az^{(k)}}{\|Az^{(k)}\|_2},$$

to avoid the need for storing the $(x^{(k)})$ sequence.

Example 5.9 Consider

$$A = \begin{bmatrix} 7/2 & 5 \\ 5/2 & 1 \end{bmatrix} \quad \text{with} \quad \sigma(A) = \{6, -3/2\} \quad \text{and } v_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

The start vector

$$x^{(0)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

yields

$$x^{(1)} = Ax^{(0)} = \frac{1}{2}\begin{bmatrix} 7 \\ 5 \end{bmatrix}, \qquad x^{(2)} = Ax^{(1)} = \frac{1}{4}\begin{bmatrix} 99 \\ 45 \end{bmatrix}, \qquad x^{(3)} = \frac{1}{8}\begin{bmatrix} 1143 \\ 585 \end{bmatrix} \ldots$$

and the following sequence approximates λ_1:

$$\lambda^{(1)} = (z^{(1)})^T A z^{(1)} = 6.2027, \quad \lambda^{(2)} = (z^{(2)})^T A z^{(2)} = 5.8973, \quad \ldots, \quad \lambda^{(8)} = 6.0001$$

and $\lim_{k\to\infty} z^{(k)} = v_1$. (see Remark 5.11b)). Numerical verification of this convergence:

$$\left\| z^{(1)} - v_1 \right\|_2 = 0.1564, \quad \left\| z^{(2)} - v_1 \right\|_2 = 0.0370, \quad \ldots, \quad \left\| z^{(10)} - v_1 \right\|_2 = 5.7220 \cdot 10^{-7}.$$

Theorem 5.10 (Convergence of the power iteration) Let $A \in \mathbb{R}^{n\times n}$ be symmetric with real-valued eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}$ such that

$$\lambda_1 = \lambda_2 = \ldots = \lambda_r, \qquad \text{and} \qquad |\lambda_r| > |\lambda_{r+1}| > \ldots > |\lambda_n| \qquad \text{for some} \quad r \leq n,$$

and corresponding orthonormal eigenvectors $v_1, \ldots, v_n$. Let the start vector for the power iteration be

$$x^{(0)} = \sum_{j=1}^{n} \alpha_j v_j \qquad \text{with } \sum_{j=1}^{r} |\alpha_j| \neq 0.$$

Then, the normalized power iteration sequence $z^{(k)} := x^{(k)}/\|x^{(k)}\|$ satisfies

$$Az^{(k)} = \lambda_1 z^{(k)} + \mathcal{O}(q^k) \qquad \text{where} \quad q := \frac{|\lambda_{r+1}|}{|\lambda_1|},$$

and

$$\lambda^{(k)} = \left(z^{(k)}\right)^T Az^{(k)} = \lambda_1 + \mathcal{O}(q^{2k}).$$

For the sake of clarity, the notation $y^{(k)} = w + \mathcal{O}(q^k)$ for a sequence of vectors $\{y^{(k)}\}_k$ in $\mathbb{R}^n$ means that there exists a constant $C > 0$ such that

$$\|y^{(k)} - w\| \leq Cq^k \qquad \forall k \geq 0.$$

Proof: By writing

$$x^{(0)} = \underbrace{\sum_{j=1}^{r} \alpha_j v_j}_{=:\tilde{v}_1} + \sum_{j=r+1}^{n} \alpha_j v_j,$$

we obtain that

$$x^{(1)} = Ax^{(0)} = A\tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j Av_j = \lambda_1 \tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j \lambda_j v_j$$

and, similarly,

$$x^{(k)} = A^k x^{(0)} = \lambda_1^k \tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j \lambda_j^k v_j.$$

This implies that,

$$\lambda_1^{-k} x^{(k)} = \tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j \left(\frac{\lambda_j}{\lambda_1}\right)^k v_j = \tilde{v}_1 + \mathcal{O}(q^k),$$

and by Taylor expansion,

$$z^{(k)} = \frac{x^{(k)}}{\|x^{(k)}\|} = \frac{x^{(k)}}{|\lambda_1^k| \|\lambda_1^{-k} x^{(k)}\|} = \frac{(\lambda_1/|\lambda_k|)\tilde{v}_1 + \mathcal{O}(q^k)}{\|\tilde{v}_1\| + \mathcal{O}(q^k)} = \operatorname{sgn}(\lambda_1^k) \frac{\tilde{v}_1}{\|\tilde{v}_1\|} + \mathcal{O}(q^k).$$

We conclude that

$$Az^{(k)} = A \operatorname{sgn}(\lambda_1^k) \frac{\tilde{v}_1}{\|\tilde{v}_1\|} + \mathcal{O}(q^k) = \operatorname{sgn}(\lambda_1^k) \frac{A\tilde{v}_1}{\|\tilde{v}_1\|} + \mathcal{O}(q^k) = \lambda_1 \frac{x^{(k)}}{\|x^{(k)}\|} + \mathcal{O}(q^k),.$$

By the orthogonality of the eigenvectors, note further that

$$(x^{(k)})^T x^{(k)} = \left(\lambda_1^k \tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j \lambda_j^k v_j\right)^T \left(\lambda_1^k \tilde{v}_1 + \sum_{j=r+1}^{n} \alpha_j \lambda_j^k v_j\right) = \lambda_1^{2k} \|\tilde{v}_1\|_2^2 + \sum_{j=r+1}^{n} \alpha_j^2 \lambda_j^{2k}$$

and

$$(x^{(k)})^T A x^{(k)} = \lambda_1^{2k+1} \|\tilde{v}_1\|_2^2 + \sum_{j=r+1}^{n} \alpha_j^2 \lambda_j^{2k+1}.$$

From this we obtain

$$\left(z^{(k)}\right)^T A z^{(k)} = \frac{(x^{(k)})^T A x^{(k)}}{(x^{(k)})^T x^{(k)}} = \frac{\lambda_1 \|\tilde{v}_1\|_2^2 + \sum_{j=r+1}^{n} \alpha_j^2 \lambda_j \left(\frac{\lambda_j}{\lambda_1}\right)^{2k}}{\|\tilde{v}_1\|_2^2 + \sum_{j=r+1}^{n} \alpha_j^2 \left(\frac{\lambda_j}{\lambda_1}\right)^{2k}} = \lambda_1 + \mathcal{O}(q^{2k})$$

□

Remark 5.11 a) The assumption that $\sum_{j=1}^{r} |\alpha_j| \neq 0$ for $x^{(0)}$ is often difficult to verify, as one typically knows little about the eigenvectors of A. For instance if the starting vector is drawn randomly, one tends to meet this assumption, cf. Example 5.12.

b) The normalized vector

$$z^{(k)} = \operatorname{sgn}(\lambda_1^k) \frac{\tilde{v}_1}{\|\tilde{v}_1\|} + \mathcal{O}(q^k),$$

will converge as $k \to \infty$ iff $\lambda_1 \geq 0$. But regardless of this convergence, $z^{(k)}$ will asymptotically belong to the span of $\tilde{v}_1$, which belongs to the eigenspace of the dominating eigenvalue.

c) The smaller the ratio between the sub-dominating and the dominating eigenvalue

$$q = \left|\frac{\lambda_{r+1}}{\lambda_1}\right|$$

the faster the convergence is.

d) Power iteration also applies to diagonalizable and even to non-diagonalizable square matrices, but proving particularly the latter result is more technical.

Example 5.12 (Sensitivity with respect to the start vector) Consider the matrix in the previous example. How sensitive is the power iteration to the start vector $x^{(0)}$?

Experiment: draw the components in $x^{(0)}$ as independent $U[0,1]$ random variables, and compute

$$z^{(10)} = x^{(10)} / \|x^{(10)}\|_2$$

We repeat the experiment 5 times. Matlab code:

```
x0 = rand(2,5) %5 columns with x0 vectors
x10 = A^(10) * x0;
z =zeros(2,5);
for i = 1:5
     z(:,i) = x10(:,i)/norm(x10(:,i));
end
z % output
```

This yields the output

```
x0 =

    0.7513    0.5060    0.8909    0.5472    0.1493
    0.2551    0.6991    0.9593    0.1386    0.2575


z =

    0.8944    0.8944    0.8944    0.8944    0.8944
    0.4472    0.4472    0.4472    0.4472    0.4472
```

Definition 5.13 (Rayleigh quotient) For a symmetric $A \in \mathbb{R}^{n\times n}$, the Rayleigh quotient for a nonzero vector $x \in \mathbb{R}^n$ is defined by

$$R(x) := \frac{x^T Ax}{x^T x}$$

(The Rayleigh quotient is normally defined only for symmetric matrices A, but we used a similar quotient mapping for more general matrices in the power iteration algorithm.)

Theorem 5.14 Let $A \in \mathbb{R}^{n\times n}_{sym}$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$. Then it holds that

$$\lambda_1 = \sup_{x\in\mathbb{R}^n_*} R(x) \qquad \lambda_n = \inf_{x\in\mathbb{R}^n_*} R(x)$$

Proof: Let $\{(\lambda_i, v_i)\}_{i=1}^n$ denote the eigenpairs of A. Since A is symmetric we may assume the eigenvectors are orthonormal (as any symmetric matrix is orthogonally diagonalizable). Any $x \in \mathbb{R}^n$ can thus be written

$$x = \sum_{j=1}^{n} \alpha_j v_j$$

and

$$R(x) = \frac{x^T Ax}{x^T x} = \frac{\sum_{j,k} \alpha_j \alpha_k v_k^T A v_j}{\sum_{j,k} \alpha_j \alpha_k v_k^T v_j} = \frac{\sum_{j=1}^n \alpha_j^2 \lambda_j}{\sum_{j,k} \alpha_j^2} \leq \frac{\sum_{j=1}^n \alpha_j^2 \lambda_1}{\sum_j \alpha_j^2} = \lambda_1.$$

And by $x = v_1$, we obtain $R(x) = \lambda_1$. The lower bound $R(x) \geq \lambda_n$ and $R(v_n) = \lambda_n$ is proved similarly. □

Remark 5.15 a) For any eigenvector v_j, it holds that

$$R(v_j) = \lambda_j.$$

b) For the approximation of an eigenvector $\tilde{v} = v_j + \Delta v$ where $\Delta v = \sum_{i=1}^{n} \varepsilon_i v_i$, it holds that (exercise)

$$|R(\tilde{v}) - \lambda_j| \leq 2(n-1)\|A\|_2 \|\Delta v\|_2^2.$$

5.3 Inverse iteration/inverse power method

If A has eigenvalues $\{\lambda_i\}_{i=1}^n$ that can be ordered

$$|\lambda_n| < |\lambda_{n-1}| \leq \ldots \leq \lambda_1,$$

then A^{-1} has eigenvalues $\{\lambda_i^{-1}\}_{i=1}^n$ with

$$|\lambda_n^{-1}| > |\lambda_{n-1}^{-1}| > \ldots$$

If we apply the inverse power iteration

$$Ax^{(k+1)} = x^{(k)} \qquad k = 0, 1, \ldots$$

and if $x^{(0)} = \sum_{j=1}^{n} \alpha_j v_j$ with $\alpha_n \neq 0$, then $x^{(k)}$ is asymptotically eigenvector to λ_n^{-1} of A^{-1}, and also to λ_n of A, since

$$A^{-1}x = \lambda_n^{-1}x \implies Ax = \lambda_n x.$$

And

$$\lambda^{(k)} = R(x^{(k)}) \to \lambda_n \qquad \text{as } k \to \infty.$$

Example 5.16 Consider again

$$A = \begin{bmatrix} 7/2 & 5 \\ 5/2 & 1 \end{bmatrix} \quad \text{with} \quad \sigma(A) = \{6, -3/2\} \quad \text{and } v_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Inverse iterations applied to the start vector

$$x^{(0)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

yields in Matlab

```
x = [1; 0]; % startvector
z = zeros(2,7);
for i = 1:7
    x = A\x;
    z(:,i) = x/norm(x);
end
z % i-th column of z equals z^(i)
%%% OUTPUT %%%
z =
   -0.3714    0.7682   -0.6902    0.7112   -0.7061    0.7074   -0.7070
    0.9285   -0.6402    0.7236   -0.7030    0.7081   -0.7068    0.7072
```

5.3.1 Shift

Inverse iteration may also compute the eigenvalue of A closest to a $\mu \in \mathbb{R}$ through the following steps:

1. Apply inverse iterations to the shifted matrix $(A-\mu I)$:

$$(A-\mu I)x^{(k+1)} = x^{(k)} \qquad \text{for } k = 0, 1, \ldots$$

2. The dominant eigenvalue of $(A-\mu I)^{-1}$ equals

$$\hat{\lambda}^{-1} = (\lambda_i - \mu)^{-1},$$

   where $\lambda_i = \arg\min_{\lambda \in \sigma(A)} |\lambda - \mu| = \lambda_{\text{closest to } \mu}$.

3. If $x^{(0)} = \sum_{j=1}^{n} \alpha_j v_j$ with $\alpha_i \neq 0$, then $x^{(k)}$ is asymptotically eigenvector to $(\lambda_i - \mu)^{-1}$ of $(A-\mu I)^{-1}$, and also to λ_i of A, since

$$(A-\mu I)^{-1}x = (\lambda_i - \mu)^{-1}x \implies (A-\mu I)x = (\lambda_i - \mu)x \implies Ax = \lambda_i x$$

   And

$$\lambda^{(k)} = R(x^{(k)}) \to \lambda_i \qquad \text{as } k \to \infty.$$

Summary

- Gershgorin's circle theorem may be used in combination with similarity transformations to improve eigenvalue estimates.
- Power iteration and inverse iteration are methods for computing eigenpairs of matrices.

5.4 QR iteration

QR iteration can be viewed as an extension of the power iteration method that simultaneously computes all eigenvalues of a matrix.
We recall that for $A \in \mathbb{R}^{n \times n}_{sym}$, the power iteration

$$x^{(m)} = Ax^{(m-1)} \tag{5.2}$$

$$z^{(m)} = \frac{x^{(m)}}{\|x^{(m)}\|_2} \tag{5.3}$$

$$\lambda^{(m)} = (z^{(m)})^T A z^{(m)} \tag{5.4}$$

$$\tag{5.5}$$

computes the dominant eigenvalue of A, and an eigenvector in the corresponding eigenspace.
QR iterations computes (under some assumptions) all eigenpairs of A:

Algorithm 2: QR iteration

Data: $A \in \mathbb{R}^{n\times n}$
Set $A_0 = A$.
for $m = 0, 1, 2, \ldots$ **do**
Compute a QR factorization

$$Q_m R_m = A_m$$

for an orthogonal $Q_m \in \mathbb{R}^{n\times n}$ and an upper triangular $R_m \in \mathbb{R}^{n\times n}$.
Assign value

$$A_{m+1} \leftarrow R_m Q_m.$$

end

Remark 5.17 a) Under some assumptions, the sequence of matrices $\{A_m\}$ converges to an upper triangular matrix with the eigenvalues of A on its diagonal as $m \to \infty$.

We will show that QR iteration is a sequence of orthogonal similarity transforms

$$A_{m+1} = (Q_0 Q_1 \ldots Q_m)^T A (Q_0 Q_1 \ldots Q_m).$$

The diagonal components of A_m may thus be viewed as an extension of Rayleigh quotient iteration

$$\lambda^{(m)} = (z^{(m)})^T A z^{(m)}.$$

b) The set of orthogonal $n \times n$ matrices equipped with the matrix multiplication operation form a group. The closure property is most important for us:

$$A, B \in \mathbb{R}^{n\times n} \text{ orthogonal } \implies C = AB \quad \text{ is orthogonal.} \tag{5.6}$$

Example 5.18 (Application of QR iteration) Consider

$$A = \begin{bmatrix} 0.7491 & 1.5494 & 0.7901 \\ 1.5494 & 0.3120 & 1.0222 \\ 0.7901 & 1.0222 & 1.2022 \end{bmatrix}$$

```
%%Matlab implementation of QR iteration
Qm = eye(length(A));
for m=0:100
    [Q,R] = qr(A);
    A = R*Q;
    Qm = Qm*Q; % for eigenvectors Q^{(m)}
end
```

Results:

$$A_5 = \begin{bmatrix} 2.9973 & 0.0087 & 0.0000 \\ 0.0087 & -1.0705 & 0.0002 \\ 0.0000 & 0.0002 & 0.3366 \end{bmatrix}, \quad A_{10} = \begin{bmatrix} 2.9973 & -0.0001 & -0.0000 \\ -0.0001 & -1.0705 & 0.0000 \\ -0.0000 & 0.0000 & 0.3366 \end{bmatrix}$$

and

$$Q^{(5)} = \begin{bmatrix} 0.5919 & -0.6042 & -0.5335 \\ 0.5598 & 0.7844 & -0.2672 \\ 0.5799 & -0.1405 & 0.8025 \end{bmatrix}, \quad Q^{(10)} = \begin{bmatrix} -0.5906 & 0.6053 & -0.5336 \\ -0.5614 & -0.7832 & -0.2671 \\ -0.5796 & 0.1418 & 0.8024 \end{bmatrix}$$

Compare to reference eigenvalues of A:

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} 2.9973 \\ -1.0705 \\ 0.3366 \end{bmatrix}$$

and eigenvectors

$$[v_1\, v_2\, v_3] = \begin{bmatrix} 0.5906 & 0.6053 & 0.5336 \\ 0.5614 & -0.7832 & 0.2671 \\ 0.5796 & 0.1418 & -0.8024 \end{bmatrix}$$

Example 5.19 (Application of the QR iteration method)

```
%%Matlab implementation
%A_0 = A
for m=0:10
    [Q,R] = qr(A);  % Q_{m}*R_{m} = A_m
    A = R*Q;        % A_{m+1} = R_m*Q_m
end
```

QR iteration applies under some conditions not only to symmetric but also to diagonalizable matrices (for definition see last subsection of notes), as for example the matrix

$$A = \begin{bmatrix} 1.271 & -6.409 & 9.208 \\ -2.875 & -25.668 & 38.705 \\ -2.120 & -20.259 & 30.397 \end{bmatrix}$$

This matrix is diagonalizable as

$$A = TDT^{-1}, \quad \text{with} \quad T = \begin{bmatrix} 0.298 & 0.938 & 0.055 \\ 0.756 & 0.245 & 0.820 \\ 0.582 & 0.244 & 0.569 \end{bmatrix} \quad \text{and} \quad D = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

and QR iterations yield:

$$A_0 = A = \begin{bmatrix} 1.271 & -6.409 & 9.208 \\ -2.875 & -25.668 & 38.705 \\ -2.120 & -20.259 & 30.397 \end{bmatrix}$$

$$A_1 = \begin{bmatrix} 3.340 & 0.175 & -58.656 \\ -0.444 & 1.915 & 13.242 \\ 0.010 & -0.002 & 0.745 \end{bmatrix}$$

$$A_2 = \begin{bmatrix} 3.175 & 0.432 & 59.897 \\ -0.237 & 1.898 & -5.395 \\ -0.003 & 0.001 & 0.927 \end{bmatrix}$$

$$\vdots$$

$$A_{10} = \begin{bmatrix} 3.005 & 0.756 & 59.787 \\ -0.007 & 1.995 & 6.519 \\ -0.000 & 0.000 & 1.000 \end{bmatrix}$$

5.5 Theoretical results for QR iteration

Lemma 5.20 (Properties of QR iteration) For the iterative method

$$\begin{aligned} A_0 &= A \\ Q_m R_m &= A_m \\ A_{m+1} &= R_m Q_m \end{aligned}$$

it holds that

i) $A_{m+1} = Q_m^T A_m Q_m$

ii) $A_m = (Q^{(m)})^T A Q^{(m)}$ where $Q^{(m)} = Q_0 Q_1 \dots Q_{m-1}$ is orthogonal (cf. (5.6)).

iii) For the matrix power, it holds that $A^m = Q^{(m)} R^{(m)}$ for any integer $m \geq 1$, where $R^{(m)} = R_{m-1} \dots R_0$ is upper triangular (cf. (**??**)).

Proof:

i):

$$A_m = Q_m R_m \implies R_m = Q_m^T A_m$$

and thereby

$$A_{m+1} = P R_m Q_m = Q_m^T A_m Q_m.$$

ii): By iterative use of property i),

$$\begin{aligned} A_m &= Q_{m-1}^T \, A_{m-1} \, Q_{m-1} \\ &= Q_{m-1}^T \, Q_{m-2}^T A_{m-2} \, Q_{m-2} Q_{m-1} \\ &= \dots = \underbrace{Q_{m-1}^T \dots Q_0^T}_{(Q^{(m)})^T} \underbrace{A_0}_{A} \underbrace{Q_0 \dots Q_{m-1}}_{Q^{(m)}}. \end{aligned}$$

iii): We prove this property by induction. The property holds for $m = 1$ as by definition, $Q^{(1)} = Q_0$, $R^{(1)} = R_0$ and

$$A^1 = A = Q_0 R_0 = Q^{(1)} R^{(1)}.$$

Assume that $A^m = Q^{(m)} R^{(m)}$ for some $m \geq 1$, and observe that that by ii) that $A = Q^{(m)} A_m (Q^{(m)})^T$ and that by the QR decomposition $Q_m R_m = A_m$. Consequently,

$$\begin{aligned} A^{m+1} &= A A^m \\ &= Q^{(m)} A_m (Q^{(m)})^T Q^{(m)} R^{(m)} \\ &= Q^{(m)} A_m R^{(m)} \\ &= Q^{(m)} Q_m R_m R^{(m)} \\ &= Q^{(m+1)} R^{(m+1)}. \end{aligned}$$

□

Remark 5.21 A hand-waving idea of why the method works goes as follows:

a) Considering the power iteration $x^{(m)} = A^m e_1$ with the standard basis vector e_1. Then, if e_1 contains a non-zero contribution from the eigenspace of the dominating eigenvalue, we know that $x^{(m)}$ asymptotically is an eigenvector of $\lambda_{\max}$.

Moreover

$$x^{(m)} = A^m e_1 \overset{iii)}{=} Q^{(m)} R^{(m)} e_1 = Q^{(m)} \begin{bmatrix} R_{11}^{(m)} \\ 0 \\ \vdots \\ 0 \end{bmatrix} = R_{11}^{(m)} q_1^{(m)}$$

where $q_1^{(m)} \in \mathbb{R}^n$ denotes the first column of $Q^{(m)}$. Consequently, $q_1^{(m)}$ is asymptotically an eigenvector to $\lambda_{\max}$, and, to leading order,

$$A_m e_1 \overset{ii)}{=} (Q^{(m)})^T A Q^{(m)} e_1 = (Q^{(m)})^T A q_1^{(m)} = (Q^{(m)})^T \lambda_{\max} q_1^{(m)} = \lambda_{\max} e_1.$$

Conclusion: $A_m e_1$ converges towards $\lambda_{\max} e_1$ as $m \to \infty$.

b) With a similar argument applied to inverse iteration of a non-singular A, considering the iteration $x^{(m)} = e_n^T A^{-m}$, one can verify that the last row of A_m equals $(0, \ldots, 0, \lambda_n)$.

Theorem 5.22 (Convergence of QR iteration) Let $A \in \mathbb{R}^{n \times n}_{sym}$ with eigenvalue decomposition

$$A = Q \Lambda Q^T, \qquad \text{with} \quad \Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n),$$

where Q is orthogonal and eigenvalues are non-repeating and satisfying

$$|\lambda_1| > |\lambda_2| > \ldots > |\lambda_n| > 0.$$

Then the QR iteration sequence $A_m = R_m Q_m = (Q^{(m)})^T A Q^{(m)}$ satisfies

$$\lim_{m \to \infty} A_m = \Lambda \quad \text{and} \quad Q^{(m)} \approx [\pm v_1, \pm v_2, \ldots, \pm v_n] \quad \text{for} \quad m \gg 1.$$

Proof of Theorem 5.22 (not curriculum)

For those interested, we include a proof of QR iteration. Note however that this proof and the rest of section 5.5 is not part of curriculum.
The following result will be useful for proving the theorem:

Lemma 5.23 If $U \in \mathbb{R}^{n \times n}$ is upper triangular and non-singular, then U^{-1} is also upper triangular.

(See MAT3110 course Exercise 1 for September 27.)
Proof of Theorem 5.22: Let $Q^T = LU$ be an LU factorization of Q^T where we recall that this means $U \in \mathbb{R}^{n\times n}$ is upper triangular and $L \in \mathbb{R}^{n\times n}$ is lower triangular. (NB! sometimes a pivot is also needed in the LU factorization, we assume not here, see Remark 5.25 for extension to that setting.)
The eigendecomposition of A combined with LU factorization of Q give the relationship

$$A^m = (Q\Lambda Q^T)^m = Q\Lambda^m Q^T = Q\Lambda^m LU,$$

and by Lemma 5.20 iii) we also have that

$$A^m = Q^{(m)}R^{(m)} = \underbrace{(Q_0 \dots Q_{m-1})}_{\text{orthogonal}}\underbrace{(R_{m-1}\dots R_0)}_{\text{upper triangular}}$$

Consequently,

$$Q\Lambda^m L\Lambda^{-m} = Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m} \tag{5.7}$$

and $R^{(m)}U^{-1}\Lambda^{-m}$ is upper triangular.
Since L is unit lower triangular,

$$(\Lambda^m L\Lambda^{-m})_{ij} = L_{ij}\left(\frac{\lambda_i}{\lambda_j}\right)^m = \begin{cases} L_{ij}\left(\frac{\lambda_i}{\lambda_j}\right)^m & j < i \\ 1 & i = j \\ 0 & \text{otherwise.} \end{cases}$$

We conclude that for $p := \max_{i=1,\dots,n} |\lambda_{i+1}/\lambda_i|$,

$$\Lambda^m L\Lambda^{-m} = I + \mathcal{O}(p^m)$$
$$Q\Lambda^m L\Lambda^{-m} = Q(I + \mathcal{O}(p^m)) = Q + \mathcal{O}(p^m)$$

and by (5.7) also that

$$Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m} = Q\Lambda^m L\Lambda^{-m} = Q + \mathcal{O}(p^m) \tag{5.8}$$

(**Remark:** we seek to prove that

$$A_m = (Q^{(m)})^T AQ^{(m)} \to \Lambda = Q^T AQ,$$

and our path will be to study in what sense $Q^{(m)}$ asymptotically approximates Q. We know now that $Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m} \to Q$, so by next studying the asymptotic behavior of the sequence $\{R^{(m)}U^{-1}\Lambda^{-m}\}$, we will also gain knowledge on how $Q^{(m)}$ relates to Q.)
Decomposing the upper diagonal matrix

$$R^{(m)}U^{-1}\Lambda^{-m} =: D^{(m)} + N^{(m)}$$

where $D^{(m)}$ denotes the diagonal part of the matrix and $N^{(m)}$ denotes the strictly upper triangular part, we obtain

$$\begin{aligned}(R^{(m)}U^{-1}\Lambda^{-m})^T(R^{(m)}U^{-1}\Lambda^{-m}) &= (D^{(m)} + N^{(m)})^T(D^{(m)} + N^{(m)}) \\ &= (D^{(m)})^2 + \underbrace{D^{(m)}N^{(m)} + (N^{(m)})^T D^{(m)} + \underbrace{(N^{(m)})^T N^{(m)}}_{=0}}_{\text{strictly non-diagonal}}\end{aligned}$$

But using (5.8) we also have that

$$\begin{aligned}(R^{(m)}U^{-1}\Lambda^{-m})^T(R^{(m)}U^{-1}\Lambda^{-m}) \\ &= \left(Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m}\right)^T\left(Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m}\right) \\ &= I+\mathcal{O}(p^m).\end{aligned}$$

Conclusion:

$$(D^{(m)})^2 = I+\mathcal{O}(p^m) \quad \text{and} \quad N^{(m)} = \mathcal{O}(p^m).$$

This means $(D_{ii}^{(m)})^2 = 1+\mathcal{O}(p^m)$ for $i = 1,\ldots,n$, i.e.,

$$\text{either } D_{ii}^{(m)} = -1+\mathcal{O}(p^m) \text{ or } D_{ii}^{(m)} = 1+\mathcal{O}(p^m).$$

So if we take the sequence of diagonal matrices $\{S^{(m)}\}$ with $S_{ii}^{(m)} = \operatorname{sgn}(D_{ii}^{(m)})$, then

$$S^{(m)} = D^{(m)}+\mathcal{O}(p^m)$$

and

$$R^{(m)}U^{-1}\Lambda^{-m} = D^{(m)}+N^{(m)} = S^{(m)}+\mathcal{O}(p^m).$$

Hence,

$$Q^{(m)}R^{(m)}U^{-1}\Lambda^{-m} = Q^{(m)}S^{(m)}+\mathcal{O}(p^m).$$

And by (5.8) and using that $S^{(m)}$ is symmetric and orthogonal, we obtain (by right multiplication of $S^{(m)}$ in first equality)

$$Q^{(m)}S^{(m)} = Q+\mathcal{O}(p^m) \implies Q^{(m)} = QS^{(m)}+\mathcal{O}(p^m)$$

We have finally reached the end of the proof:

$$A_m = (Q^{(m)})^TAQ^{(m)} = (S^{(m)})Q^TAQ(S^{(m)})^T+\mathcal{O}(p^m) = S^{(m)}\Lambda S^{(m)}+\mathcal{O}(p^m) = \Lambda+\mathcal{O}(p^m).$$

□

Example 5.24 (What happens when A has complex-valued eigenvalues?) When there is a complex-valued pair of eigenvalues

$$\lambda_j = \overline{\lambda}_{j+1},$$

then $|\lambda_j| = |\lambda_{j+1}|$. This setting does not fulfill the separation-of-eigenvalues assumption in Theorem 5.22, and it turns out that A_m then will converge towards a **block upper triangular** matrix, as the diagonal of A_m will contain a 2×2 block matrix whose matrix has eigenvalues λ_j ad λ_{j+1} (A_m converges to the real Schur form of A). For example, consider

$$A = \begin{bmatrix}30 & -18 & 5\\ 15 & 9 & -5\\ 9 & -27 & 24\end{bmatrix} \qquad \text{with} \quad \sigma(A) = \{27+9i, 27-9i, 9\}.$$

QR iteration with start matrix $A_0 = A$ yields

$$A_1 = \begin{bmatrix} 24.112 & -20.311 & 25.109 \\ 6.315 & 34.734 & -6.260 \\ -1.941 & 5.921 & 4.154 \end{bmatrix}, \qquad A_5 = \begin{bmatrix} 35.799 & -14.881 & -19.641 \\ 10.604 & 18.236 & -23.492 \\ -0.016 & 0.053 & 8.965 \end{bmatrix}$$

and

$$A_{10} = \begin{bmatrix} 22.957 & -20.934 & 30.563 \\ 4.650 & 31.043 & -0.604 \\ 0.000 & -0.000 & 9.000 \end{bmatrix}$$

where

$$\sigma\left(\begin{bmatrix} 22.957 & -20.934 \\ 4.650 & 31.043 \end{bmatrix}\right) = \{26.999 + 9.000i, 26.999 - 9.000i\}$$

Remark 5.25 a) Theorem 5.22 extends to any diagonalizable $A \in \mathbb{R}^{n\times n}$ with real-valued non-repeating eigenvalues. Then A_m converges to an upper triangular matrix with diagonal $(\lambda_1, \ldots, \lambda_n)$.

b) We assumed in the proof that for $A = Q\Lambda Q^T$, there exists an LU factorization of $Q^T = LU$. In general, one may need to partial pivoting as well to achieve this: $PQ^T = LU$, where P is a permutation matrix. Observing that $P^TP = I$ and

$$A = Q\Lambda Q^T = (QP^T)P\Lambda P^T(PQ^T)$$

with $P\Lambda P^T$ a reordered diagonal matrix, the result extends with

$$A_m \to P\Lambda P^T.$$

5.6 Tridiagonalization of A

Every QR iteration step of a full matrix A_m costs $\mathcal{O}(n^3)$ operations. "Preconditioning" your start matrix through similarity transforms may improve the efficiency considerably. That is, instead of using $A_0 = A$, set $A_0 = QAQ^T$, where Q is an orthogonal matrix being a product of Householder transformations (see Suli and Mayers, Chp 5.5 if interested). The upper Hessenberg matrix approach (requiring three Householder transformations):

$$A = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{QAQ^T}{\longmapsto} \underbrace{\begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ & * & * & * & * \\ & & * & * & * \\ & & & * & * \end{bmatrix}}_{\text{upper Hessenberg}}$$

which becomes tridiagonal for symmetric matrices:

$$A = A^T = \begin{bmatrix} * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \\ * & * & * & * & * \end{bmatrix} \overset{QAQ^T}{\longmapsto} \begin{bmatrix} * & * & & & \\ * & * & * & & \\ & * & * & * & \\ & & * & * & * \\ & & & * & * \end{bmatrix}$$

Reason for efficiency gain: the upper Hessenberg form is preserved over QR iterations, and (efficiently) computing the QR decomposition of a full matrix A_m requires $\mathcal{O}(n^3)$ operations. This is cost reduced to $\mathcal{O}(n^2)$ for upper Hessenberg matrices and $\mathcal{O}(n)$ for tridiagonal ones. If interested, see e.g., Dahmen and Reusken "Numerik für Ingenieure und Naturwissenschaftler", chp 7.7.3.

Householder transformations

We next provide a practical example on how to use Householder transformations for triangularization of symmetric matrices $A \in \mathbb{R}^{5\times 5}$. The practical example carries right over to the general setting of how to proceed for $A \in \mathbb{R}^{n\times n}_{sym}$, but for more details on the theory of tridiagonalization, see Suli and Mayers Chp 5.5.
A matrix $H \in \mathbb{R}^{n\times n}$ on the form

$$H = I - \frac{2}{v^T v} v v^T, \qquad \text{with} \quad c \in \mathbb{R} \text{ and } v \in \mathbb{R}^n$$

is called a Householder matrix/transformation.

Properties:

- Orthogonality: $H^T H = I$
- And for any vector $x \in \mathbb{R}^n_*$, one can find a vector $v \in \mathbb{R}^n$ s.t.

$$Hx = \begin{bmatrix} \neq 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \quad \text{(first element is non-zero, others set to zero)}$$

The following choice is for instance one option (that we will stick to here):

$$v = x + ce_1 \quad \text{with} \quad c = \begin{cases} \|x\|_2 & \text{if} \quad x_1 \geq 0 \\ -\|x\|_2 & \text{if} \quad x_1 < 0, \end{cases} \implies Hx = -ce_1. \tag{5.9}$$

(see e.g., Suli and Mayers Lemma 5.4)
We next show how to tridiagonalize the following symmetric 5×5 matrix using a sequence of Householder transformations:

$$\mathbf{A} = \begin{bmatrix} 4 & 1 & 2 & 1 & 3 \\ 1 & 5 & 0 & 2 & 2 \\ 2 & 0 & 3 & 1 & 1 \\ 1 & 2 & 1 & 6 & 0 \\ 3 & 2 & 1 & 0 & 7 \end{bmatrix}$$

Step 1: Find $H \in \mathbb{R}^{4\times 4}$ such that last three elements of first row is removed, mean for

$$x = \begin{bmatrix} a_{21} \\ a31 \\ a_{41} \\ a_{51} \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 1 \\ 3 \end{bmatrix} \quad \text{we seek } H \text{ s.t.} \quad Hx = \begin{bmatrix} \neq 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} =$$

Pick $v = x + \|x\|_2 e_1 = (1+\sqrt{15}, 2, 1, 3)^T$ and set

$$H = I_4 - \frac{2}{v^T v} v v^T = \begin{bmatrix} -0.2582 & -0.5164 & -0.2582 & -0.7746 \\ -0.5164 & 0.7881 & -0.1060 & -0.3179 \\ -0.2582 & -0.1060 & 0.9470 & -0.1590 \\ -0.7746 & -0.3179 & -0.1590 & 0.5231 \end{bmatrix}$$

Then, by (5.9)

$$Hx = -\|x\|_2 e_1 = -\sqrt{15} e_1$$

And for

$$H_{(5,4)} := \begin{bmatrix} 1 & 0^T \\ 0 & H \end{bmatrix} \in \mathbb{R}^{5\times 5}, \qquad 0 \in \mathbb{R}^{4\times 1}$$

We obtain

$$H_{(5,4)} A H_{(5,4)}^T = \begin{bmatrix} 4.0000 & -3.8730 & 0 & -0.0000 & 0 \\ -3.8730 & 7.8667 & 2.0243 & -0.2788 & 0.4545 \\ 0 & 2.0243 & 4.1788 & 0.2387 & 0.8876 \\ -0.0000 & -0.2788 & 0.2387 & 4.9440 & -2.0823 \\ 0 & 0.4545 & 0.8876 & -2.0823 & 4.0106 \end{bmatrix}$$

Motivation for above structure:

- Multiplying with $H_{(5,4)}$ from left preserves/leaves elements in first row unchanged.
- Thereafter by $H_{(5,4)}^T$ from right preserves elements in first column (and zeros tail elements in first row by same reason $H_{(5,4)}$ zeroed tail elements in first column).

Step 2: Find $H \in \mathbb{R}^{3\times 3}$ that zeros last two terms in column 2 of matrix $H_{(5,4)} A H_{(5,4)}^T$, i.e. of vector

$$x = \begin{bmatrix} 2.0243 \\ -0.2788 \\ 0.4545 \end{bmatrix}$$

Choose

$$v = x + \|x\|_2 e_1 \quad \text{and} \quad H = I - \frac{2}{v^T v} v v^T.$$

Set

$$H_{(4,3)} = \begin{bmatrix} I_2 & 0^T \\ 0 & H \end{bmatrix} \in \mathbb{R}^{5\times 5}, \qquad 0 \in \mathbb{R}^{3\times 2}$$

and obtain

$$H_{(4,3)} H_{(5,4)} A H_{(5,4)}^T H_{(4,3)}^T = \begin{bmatrix} 4.0000 & -3.8730 & -0.0000 & -0.0000 & -0.0000 \\ -3.8730 & 7.8667 & -2.0934 & 0.0000 & -0.0000 \\ -0.0000 & -2.0934 & 4.6161 & 0.2827 & -1.0331 \\ -0.0000 & 0.0000 & 0.2827 & 4.9360 & -1.9441 \\ -0.0000 & 0.0000 & -1.0331 & -1.9441 & 3.5812 \end{bmatrix}$$

After another such step, finding $H_{(3,2)}$ that zeros last element in third column of latest matrix and leaves first three rows unchanged, we have a tridiagonal symmetric matrix

$$A_0 = \underbrace{H_{(3,2)}H_{(4,3)}H_{(5,4)}}_{Q} A \underbrace{H_{(5,4)}^T H_{(4,3)}^T H_{(3,2)}^T}_{Q^T}$$
$$= \begin{bmatrix} 4.0000 & -3.8730 & -0.0000 & 0.0000 & -0.0000 \\ -3.8730 & 7.8667 & -2.0934 & -0.0000 & -0.0000 \\ -0.0000 & -2.0934 & 4.6161 & -1.0711 & 0.0000 \\ 0.0000 & 0.0000 & -1.0711 & 4.6654 & -2.0181 \\ -0.0000 & 0.0000 & 0 & -2.0181 & 3.8519 \end{bmatrix}$$

5.7 Perturbation analysis

Definition 5.26 A matrix $A \in \mathbb{R}^{n\times n}$ is diagonalizable if and only if there exists an invertible matrix $T \in \mathbb{R}^{n\times n}$, s.t.

$$D = T^{-1}AT,$$

where D is a diagonal matrix.

A sufficient condition for A being diagonalizable is that the matrix has n distinct eigenvalues (as then the eigenvectors are linearly independent and the matrix $T = [v_1\ v_2\ \dots v_n]$ will diagonalize A).

Theorem 5.27 (Bauer–Fike) Consider a diagonalizable matrix $A = T\Lambda T^{-1} \in \mathbb{R}^{n\times n}$ with $\Lambda = \mathrm{diag}(\lambda_1, \dots, \lambda_n)$, and a perturbation $\Delta A \in \mathbb{R}^{n\times n}$. Then for any eigenvalue of the perturbed matrix $\mu \in \sigma(A + \Delta A)$, it holds that

$$\min_{\lambda\in\sigma(A)} |\mu - \lambda| \le \underbrace{\|T\|_2\|T^{-1}\|_2}_{=:\kappa_2(T)} \|\Delta A\|_2, \tag{5.10}$$

Definition 5.28 (Absolute condition number) For the setting in Theorem 5.27 and for the sake of interpreting our perturbation result, we think of/define

$$\frac{\min_{\lambda\in\sigma(A)} |\mu - \lambda|}{\|\Delta A\|_2} \qquad \left(= \frac{\text{error output}}{\text{error input}}\right)$$

as the absolute condition number of $\mu = \lambda(A + \Delta A)$ (for comparision with course literature, see (2.42) in Suli and Mayers). In other words, the inequality (5.10) becomes

$$\frac{\text{error output}}{\text{error input}} = \min_{\lambda\in\sigma(A)} \frac{|\mu - \lambda|}{\|\Delta A\|_2} \le \kappa_2(T).$$

We refer to the eigenvalue problem as well-conditioned when $\kappa_2(T)$ is "small".

For proving the Theorem 5.27, we will use the fact that for any diagonal matrix $D = \mathrm{diag}(d_1, \dots, d_n)$

$$\|D\|_2 = \max_{i\in\{1,\dots,n\}} |d_i| \tag{5.11}$$

Proof of Theorem 5.27 : Since $A-\mu I = T(\Lambda-\mu I)T^{-1}$, it holds that

$$\|(A-\mu I)^{-1}\|_2 = \|T(\Lambda-\mu I)^{-1}T^{-1}\|_2 \le \underbrace{\|T\|_2\|T^{-1}\|_2}_{=\kappa_2(T)}\|(\Lambda-\mu I)^{-1}\|_2,$$

Since

$$(\Lambda-\mu I)^{-1} = \operatorname{diag}\Big((\lambda_1-\mu)^{-1},\dots,(\lambda_n-\mu)^{-1}\Big),$$

the property 5.11 implies that

$$\|(\Lambda-\mu I)^{-1}\|_2 = \max_{i\in\{1,\dots,n\}}|(\lambda_i-\mu)^{-1}| = \frac{1}{\min_{i\in\{1,\dots,n\}}|\lambda_i-\mu|}.$$

Consequently,

$$\|(A-\mu I)^{-1}\|_2 \le \kappa_2(T)\frac{1}{\min_{i\in\{1,\dots,n\}}|\lambda_i-\mu|}$$

so that

$$\min_{i\in\{1,\dots,n\}}|\lambda_i-\mu| \le \kappa_2(T)\frac{1}{\|(A-\mu I)^{-1}\|_2}.$$

Let v be an eigenvector satisfying

$$(A+\Delta A)v = \mu v, \qquad \text{then} \quad (A-\mu I)v = -\Delta A v$$

and

$$\|v\|_2 = \|(A-\mu I)^{-1}\Delta A v\|_2 \le \|(A-\mu I)^{-1}\|_2\|\Delta A\|_2\|v\|_2 \implies \frac{1}{\|(A-\mu I)^{-1}\|_2} \le \|\Delta A\|_2.$$

□

Remark 5.29 a) The upper bound for absolute condition number of the eigenvalue problem, $\kappa_2(T)$, only depends on T, and, perhaps surprisingly, not explicitly on the eigenvalues of A.

b) For symmetric A, we can find an orthogonal T. This implies that $\kappa_2(T) = 1$. (Eigenvalue perturbation is therefore a well-conditioned problem for such matrices.)

c) In general, when eigenvalues are repeating, or clustered very closely together, then they can be very sensitive to small perturbations in the matrix. Consider for example the non-diagonalizable matrix (not covered by the Bauer–Fike theorem):

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}$$

with repeated eigenvalue $\lambda = 1$. For

$$A+\Delta A = \begin{bmatrix} 1 & \varepsilon \\ 1 & 1 \end{bmatrix}$$

with eigenvalues $1 \pm \sqrt{\varepsilon}$.

$$\text{Input/perturbation error } \|\Delta A\|_2 = \varepsilon \ll \sqrt{\varepsilon} = \text{output error}.$$