Chapter 5

Eigenvalue problems

In this chapter, we are interested in the symmetric eigenvalue problem

$$\text{Solve for } (\mu, x) \in \mathbb{R} \times \left(\mathbb{R}^n \setminus \{0\}\right), Ax = \mu x, \tag{5.1}$$

where A is assumed symmetric.

Contrary to the linear solve case, where there is an explicit algorithm to solve the linear problem $Ax_* = b$, for $n \geq 5$, by the Abel-Ruffini theorem, there is no algorithm that computes the eigenvalues of A that stops after a finite number of operations. Otherwise, it would be possible to find the roots of a polynomial of degree n within a finite number of operations. This means that the methods to compute the eigenvalues of a matrix have to be iterative. We start with algorithms which approximate the eigenvalues of a matrix using single vector iterations.

5.1 Single vector iteration methods

5.1.1 Power iteration

Suppose that the eigenvalues $(\mu_i)_{1 \leq i \leq n}$ of the matrix A are ordered such that

$$|\mu_n| > |\mu_{n-1}| \geq \cdots \geq |\mu_1|. \tag{5.2}$$

For a starting vector $x \in \mathbb{R}^n$, consider the sequences $(y^{(k)})$ and $(\lambda^{(k)})$ defined by $y^{(0)} = \frac{x}{\|x\|}$ and $\lambda^{(0)} = \langle y^{(0)}, Ay^{(0)} \rangle$ and for $m \geq 1$

$$\begin{cases} \hat{y}^{(m)} = Ay^{(m-1)} \\ y^{(m)} = \dfrac{\hat{y}^{(m)}}{\|\hat{y}^{(m)}\|} \\ \lambda^{(m)} = \langle y^{(m)}, Ay^{(m)} \rangle. \end{cases} \tag{5.3}$$

By iteration, we see that $y^{(m)} = \frac{A^m x}{\|A^m x\|}$.

Expanding x in the basis of the eigenvectors $(q_i)_{1 \leq i \leq n}$ of A, we have

$$x = \sum_{i=1}^{n} \alpha_i q_i, \quad \alpha_i \in \mathbb{R}, \tag{5.4}$$

thus assuming that $\alpha_n \neq 0$

$$A^m x = \alpha_n \mu_n^m \Big(q_n + \sum_{i=1}^{n-1} \frac{\alpha_i}{\alpha_n} \Big(\frac{\mu_i}{\mu_n}\Big)^m q_i \Big). \tag{5.5}$$

Since $\left|\frac{\mu_i}{\mu_n}\right| < 1$ for $1 \leq i \leq n-1$, $A^m x$ tends to be aligned with the vector q_n *i.e.* the eigenvector associated to the eigenvalue with the largest magnitude.

Algorithm 5.1 Power method

```
function PowerMethod(A, x, ε_tol)
    y^(0) = x / ‖x‖
    λ^(0) = ⟨y^(0), Ay^(0)⟩
    m = 0
    while ‖Ay^(m) − λ^(m) y^(m)‖ > ε_tol do
        m = m + 1
        ŷ^(m) = Ay^(m−1)
        y^(m) = ŷ^(m) / ‖ŷ^(m)‖
        λ^(m) = ⟨y^(m), Ay^(m)⟩
    end while
    return (λ^(m), y^(m))
end function
```

Theorem 5.1 (Convergence of the power method)**.** *Let $A \in \mathbb{R}^{n\times n}$ be a symmetric matrix. Let $(\mu_i)_{1\leq i\leq n}$ be its eigenvalues and $(q_i)_{1\leq i\leq n}$ be the corresponding orthonormal eigenvectors. Suppose that the eigenvalues satisfy Eq. (5.2) and $\mu_n > 0$. Let $x \in \mathbb{R}^n$ such that $\langle x, q_n\rangle > 0$. Then there exists a constant $C > 0$ such that for all $m \geq 1$*

$$\|y^{(m)} - q_n\| \leq C \Big|\frac{\mu_{n-1}}{\mu_n}\Big|^m, \tag{5.6}$$

and

$$|\lambda^{(m)} - \mu_n| \leq C \Big|\frac{\mu_{n-1}}{\mu_n}\Big|^{2m}. \tag{5.7}$$

Proof. From Eq. (5.5), we have

$$\begin{aligned}
\|A^m x\|^2 &= \Big\| \alpha_n \mu_n^m \Big(q_n + \sum_{i=1}^{n-1} \frac{\alpha_i}{\alpha_n} \Big(\frac{\mu_i}{\mu_n}\Big)^m q_i \Big) \Big\|^2 \\
&= |\alpha_n \mu_n^m|^2 \Big(1 + \sum_{i=1}^{n-1} \Big| \frac{\alpha_i}{\alpha_n} \Big(\frac{\mu_i}{\mu_n}\Big)^m \Big|^2 \Big) \\
&= |\alpha_n \mu_n^m|^2 \Big(1 + \mathcal{O}\big(\frac{\mu_{n-1}}{\mu_n}\big)^{2m} \Big).
\end{aligned}$$

Thus we have

$$\begin{aligned}
\|q_n - y^{(m)}\| &= \Big\|q_n - \frac{A^m x}{\|A^m x\|}\Big\| \\
&\le \frac{\|(\|A^m x\| - \alpha_n \mu_n^m) q_n\|}{\|A^m x\|} + \frac{\left\|\sum_{i=1}^{n-1} \alpha_i \mu_i^m q_i\right\|}{\|A^m x\|} \\
&\le C \Big|\frac{\mu_{n-1}}{\mu_n}\Big|^m,
\end{aligned}$$

for some positive constant C independent of m.

For $\lambda^{(m)}$, we first notice that $\|q_n - y^{(m)}\|^2 = 2 - 2\langle q_n, y^{(m)}\rangle$. Thus we have

$$\begin{aligned}
\langle q_n - y^{(m)}, A(q_n - y^{(m)})\rangle &= \langle q_n, Aq_n\rangle - 2\langle y^{(m)}, Aq_n\rangle + \langle y^{(m)}, Ay^{(m)}\rangle \\
&= \mu_n - 2\mu_n\langle y^{(m)}, q_n\rangle + \lambda^{(m)} \\
&= \lambda^{(m)} - \mu_n - 2\mu_n(1 - \langle y^{(m)}, q_n\rangle) \\
&= \lambda^{(m)} - \mu_n - \mu_n\|y^{(m)} - q_n\|^2.
\end{aligned}$$

We deduce the bound

$$|\lambda^{(m)} - \mu_n| \le |\mu_n|\|y^{(m)} - q_n\|^2 + |\langle q_n - y^{(m)}, A(q_n - y^{(m)})\rangle| \le 2|\mu_n|\|y^{(m)} - q_n\|^2 \le C\Big|\frac{\mu_{n-1}}{\mu_n}\Big|^{2m}. \tag{5.8}$$

□

Notice that the eigenvalue converges at a rate which is twice faster than the eigenvector. This is a result which also applies in general.

Remark 5.2. *The power iteration also converges when A is diagonalisable (not necessarily in an orthonormal basis) under the assumption Eq.* (5.2) *on the eigenvalues.*

The convergence of the power iteration is sensitive to an eigenvalue that is close (in magnitude) to the dominant one μ_n. In particular if $\mu_{n-1} = \mu_n(1 - \varepsilon)$ for $\varepsilon > 0$, then

$$\frac{\mu_{n-1}}{\mu_n} = 1 - \varepsilon. \tag{5.9}$$

The convergence rate of the power iteration method in that case can be written

$$\|y^{(m)} - q_n\| \le C(1 - \varepsilon)^m \quad \text{and} \quad |\lambda^{(m)} - \mu_n| \le C(1 - \varepsilon)^{2m}.$$

5.1.2 Inverse power iteration

Assume now that the eigenvalues of A are ordered such that

$$0 < |\mu_1| < |\mu_2| \le \cdots \le |\mu_n|. \tag{5.10}$$

Applying the power method to the matrix A^{-1} gives the following sequence

$$\begin{cases}
\hat{y}^{(m)} = A^{-1} y^{(m-1)} \\
y^{(m)} = \dfrac{\hat{y}^{(m)}}{\|\hat{y}^{(m)}\|} \\
\lambda^{(m)} = \langle y^{(m)}, A^{-1} y^{(m)}\rangle,
\end{cases} \tag{5.11}$$

where $y^{(0)} = \frac{x}{\|x\|}$ and $\lambda^{(0)} = \langle y^{(0)}, A^{-1}y^{(0)}\rangle$.

By Theorem 5.1, $(\lambda^{(m)}, y^{(m)})$ converge to the eigenpair corresponding to the dominant eigenvalue of A^{-1}, thus $(\frac{1}{\mu_1}, q_1)$.

The formulation in Eq. (5.11) is not interesting in practice as it would require the knowledge of the inverse A. However, by introducing the appropriate intermediate variable, it is possible to replace A^{-1} by linear solve at each step.

Algorithm 5.2 Inverse power method

function InversePowerMethod($A, x, \varepsilon_{\mathrm{tol}}$)
  $y^{(0)} = \frac{x}{\|x\|}$
  $x^{(0)}$ solves $Ax^{(0)} = y^{(0)}$
  $\lambda^{(0)} = \langle y^{(0)}, x^{(0)}\rangle$
  $m = 0$
  while $\|y^{(m)} - \lambda^{(m)}Ay^{(m)}\| > \varepsilon_{\mathrm{tol}}$ **do**
    $m = m + 1$
    $y^{(m)} = \frac{x^{(m-1)}}{\|x^{(m-1)}\|}$
    $x^{(m)}$ solves $Ax^{(m)} = y^{(m)}$
    $\lambda^{(m)} = \langle y^{(m)}, x^{(m)}\rangle$
  end while
  return $(\frac{1}{\lambda^{(m)}}, y^{(m)})$
end function

The sequence defined by Algorithm 5.2 is mathematically equivalent to applying the power iteration to A^{-1} but requires only a linear solve per iteration of the while loop. We have by a simple consequence of Theorem 5.1 the following convergence for the inverse power iteration method.

Theorem 5.3. *Let $A \in \mathbb{R}^{n\times n}$ be an Hermitian matrix. Let $(\mu_i)_{1\le i\le n}$ be its eigenvalues and $(q_i)_{1\le i\le n}$ be the corresponding orthonormal eigenvectors. Suppose that the eigenvalues satisfy Eq. (5.10). Let $x \in \mathbb{R}^n$ such that $\langle x, q_1\rangle > 0$. Then there exists a constant $C > 0$ such that for all $m \ge 1$*

$$\|y^{(m)} - q_1\| \le C\left|\frac{\mu_1}{\mu_2}\right|^m, \tag{5.12}$$

and

$$|\lambda^{(m)} - \mu_1| \le C\left|\frac{\mu_1}{\mu_2}\right|^{2m}. \tag{5.13}$$

Again the convergence of the inverse power method is slow if the ratio $\left|\frac{\mu_1}{\mu_2}\right|$ is close to 1.

In this case, if we have a good guess $\tilde{\mu}_1 \ne \mu_1$ to the exact eigenvalue, we can apply the inverse power method to the matrix $A - \tilde{\mu}_1 \,\mathrm{id}_n$ which satisfies

$$|\mu_1 - \tilde{\mu}_1| \ll |\mu_2 - \tilde{\mu}_1| \le \cdots \le |\mu_n - \tilde{\mu}_1|.$$

Hence the inverse power iteration converges much faster for $A - \tilde{\mu}_1$ than for A.

Remark 5.4. *Shifting by $\sigma \in \mathbb{R}$ the matrix A can also be used to target a specific eigenvalue μ_i of A.*

Indeed let σ such that $|\mu_i - \sigma| < |\mu_j - \sigma|$ for all $j \ne i$. Then we have that the inverse power iteration applied to the matrix $A - \sigma\,\mathrm{id}$ converges to the eigenvector q_i of A.

5.2 Krylov methods

We will assume here that A is Hermitian with eigenvalues

$$\mu_1 \leq \cdots \leq \mu_n. \tag{5.14}$$

Inspired by the iterative solver case, we expect a Krylov method for linear solvers to converge faster to the exact eigenvalue than a single vector iteration. In that case, the approximate eigenvector is sought in a Krylov space $\mathcal{K}_{m+1}(A, y)$. If we are interested in the largest eigenvalue μ_n, it is natural to start from the variational characterisation of the eigenvalue (see Proposition 1.12)

$$\mu_n = \max_{\substack{y \in \mathbb{R}^n \\ y \neq 0}} \frac{\langle y, Ay \rangle}{\|y\|^2},$$

and restrict the maximisation problem to the Krylov space $\mathcal{K}_{m+1}(A, y)$

$$\lambda^{(m)} = \max_{\substack{y \in \mathcal{K}_{m+1}(A,y) \\ y \neq 0}} \frac{\langle y, Ay \rangle}{\|y\|^2}.$$

By the restriction, we necessarily have $\mu_n - \lambda^{(m)} \geq 0$.

The Arnoldi/Lanczos algorithm (see Proposition 4.8), as A is symmetric, provides an orthonormal basis $(v_1, \dots, v_{m+1})$ of $\mathcal{K}_{m+1}(A, y)$ such that $V_{m+1}^T A V_{m+1} = T_{m+1}$ where $V_{m+1} = \left[v_1, \dots, v_{m+1}\right] \in \mathbb{R}^{n \times (m+1)}$ and $T_{m+1} \in \mathbb{R}^{(m+1) \times (m+1)}$ is tridiagonal. Using this basis, we can write

$$\lambda^{(m)} = \max_{\substack{y \in \mathcal{K}_{m+1}(A,y) \\ y \neq 0}} \frac{\langle y, Ay \rangle}{\|y\|^2} = \max_{\substack{t \in \mathbb{R}^{m+1} \\ t \neq 0}} \frac{\langle V_{m+1} t, A V_{m+1} t \rangle}{\|V_{m+1} t\|^2} = \max_{\substack{t \in \mathbb{R}^{m+1} \\ t \neq 0}} \frac{\langle t, V_{m+1}^T A V_{m+1} t \rangle}{\|t\|^2} = \max_{\substack{t \in \mathbb{R}^{m+1} \\ t \neq 0}} \frac{\langle t, T_{m+1} t \rangle}{\|t\|^2}.$$

We deduce that $\lambda^{(m)}$ is simply the largest eigenvalue of T_{m+1}. Since T_{m+1} is tridiagonal and smaller than A, it is reasonable to expect efficient eigenvalue solvers for such matrices. Let $t^{(m+1)} \in \mathbb{R}^{m+1}$ a normalised eigenvector associated to $T_{m+1} t^{(m+1)} = \lambda^{(m)} t^{(m+1)}$, then the approximate eigenpair using the Krylov subspace is $(\lambda^{(m)}, V_{m+1} t^{(m+1)})$. The corresponding procedure called the *iterative Arnoldi algorithm* is summarised in the Algorithm 5.3.

Remark 5.5. *In the iterative Arnoldi algorithm 5.3, we can by-pass the estimation of the residual $\|Ay^{(m)} - \lambda^{(m)} y^{(m)}\|$ using that $y^{(m)} = V_m t^{(m)}$ and that*

$$Ay^{(m)} - \lambda^{(m)} y^{(m)} = A V_m t^{(m)} - V_m T_m t^{(m)} = -t_{m+1,m} v_{m+1} e_m^T t^{(m)}.$$

Thus $\|Ay^{(m)} - \lambda^{(m)} y^{(m)}\| = |t_{m+1,m}||t_m^{(m)}|$. To avoid the computation of the largest eigenvalue of T_m, it is also possible to just use the coefficient $t_{m+1,m}$ of the Arnoldi/Lanczos algorithm in order to estimate the residual.

Theorem 5.6. *Let A be a Hermitian matrix with eigenvalues $\mu_1 \leq \cdots \leq \mu_{n-1} < \mu_n$. Let q_n be an eigenvector associated to μ_n. Let $(\lambda^{(m)}, y^{(m)})$ be the result of the iterative Arnoldi algorithm for* `which=largest` *(Algorithm 5.3) starting with the vector y. Assume that $\langle q_n, y \rangle \neq 0$.*

Algorithm 5.3 Iterative Arnoldi algorithm

> **function** IterativeArnoldi($A, y, \varepsilon_{\text{tol}}; \texttt{which} = \{\texttt{largest}, \texttt{smallest}\}$)
> $y^{(0)} = \frac{y}{\|y\|}$
> $\lambda^{(0)} = \langle v^{(0)}, Av^{(0)} \rangle$
> $m = 0$
>   **while** $\|Ay^{(m)} - \lambda^{(m)} y^{(m)}\| > \varepsilon_{\text{tol}}$ **do**
> $m = m + 1$
>   Compute $V_m \in \mathbb{R}^{n \times m}, T_m \in \mathbb{R}^{m \times m}$ of the Hermitian Lanczos algorithm 4.2
>   Compute the `which` eigenvalue $\lambda^{(m)}$ and the eigenvector $t^{(m)}$ of $H_{mm} = V_m^* A V_m$
> $y^{(m)} = V_m t^{(m)}$
>   **end while**
>   **return** $\lambda^{(m)}, y^{(m)}$
> **end function**

Then there exists a constant $C > 0$ independent of m such that the error on the approximated eigenvalue $\lambda^{(m)}$ given after m steps of the iterative Arnoldi algorithm is given by

$$0 \leq \mu_n - \lambda^{(m)} \leq C \frac{\mu_n - \mu_1}{T_m\Big(\frac{2\mu_n - \mu_{n-1} - \mu_1}{\mu_{n-1} - \mu_1}\Big)^2} \leq 4C(\mu_n - \mu_1)\Big(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\Big)^{2m}, \tag{5.15}$$

where T_m is the m-th Chebyshev polynomial of the first kind and $\kappa = \frac{\mu_n - \mu_1}{\mu_n - \mu_{n-1}}$.

Proof. The approximate eigenvalue $\lambda^{(m)}$ is characterised by

$$\lambda^{(m)} = \max_{x \in \mathcal{K}_{m+1}(A,y), x \neq 0} \frac{\langle x, Ax \rangle}{\langle x, x \rangle},$$

hence

$$\mu_n - \lambda^{(m)} = \min_{x \in \mathcal{K}_{m+1}(A,y), x \neq 0} \frac{\langle x, (\mu_n - A)x \rangle}{\langle x, x \rangle}. \tag{5.16}$$

Using that $\mathcal{K}_{m+1}(A, y) = \mathcal{K}_{m+1}(\mu_n - A, y) = \{P(A)y, P \in \mathbb{C}^m[X]\} = \{P(\mu_n - A)y, P \in \mathbb{C}^m[X]\}$, we have that

$$\mu_n - \lambda^{(m)} = \min_{0 \neq P \in \mathbb{C}^m[X]} \frac{\langle P(\mu_n - A)y, (\mu_n - A)P(\mu_n - A)y \rangle}{\langle P(\mu_n - A)y, P(\mu_n - A)y \rangle}. \tag{5.17}$$

Expanding y in the orthonormal eigenvector basis, we have $y = \sum_{i=1}^n \alpha_i q_i$, thus

$$\mu_n - \lambda^{(m)} = \min_{0 \neq P \in \mathbb{C}^m[X]} \frac{\sum\limits_{i=1}^{n-1} |\alpha_i (\mu_n - \mu_i) P(\mu_n - \mu_i)|^2}{\sum\limits_{i=1}^{n} |\alpha_i P(\mu_n - \mu_i)|^2}. \tag{5.18}$$

We thus obtain the upper bound

$$\begin{aligned}
\mu_n - \lambda^{(m)} &\leq (\mu_n - \mu_1) \min_{0 \neq P \in \mathbb{C}^m[X]} \frac{\sum_{i=1}^{n-1} |\alpha_i P(\mu_n - \mu_i)|^2}{\sum_{i=1}^{n} |\alpha_i P(\mu_n - \mu_i)|^2} \\
&\leq (\mu_n - \mu_1) \min_{0 \neq P \in \mathbb{C}^m[X]} \frac{\sum_{i=1}^{n-1} |\alpha_i P(\mu_n - \mu_i)|^2}{|\alpha_n P(0)|^2} \\
&\leq (\mu_n - \mu_1) \frac{\sum_{i=1}^{n-1} |\alpha_i|^2}{|\alpha_n|^2} \min_{0 \neq P \in \mathbb{C}^m[X]} \max_{1 \leq i \leq n-1} \frac{|P(\mu_n - \mu_i)|^2}{|P(0)|^2}.
\end{aligned}$$

We can relax the min-max problem to

$$\min_{0 \neq P \in \mathbb{C}^m[X]} \max_{1 \leq i \leq n-1} \frac{|P(\mu_n - \mu_i)|^2}{|P(0)|^2} \leq \min_{\substack{P \in \mathbb{C}^m[X] \\ P(0)=1}} \max_{\mu_n - \mu_{n-1} \leq \mu \leq \mu_n - \mu_1} |P(\mu)|^2.$$

We recognise the same min-max problem that is solved by a shifted and rescaled Chebyshev polynomial T_k (see Remark 4.18):

$$\min_{\substack{P \in \mathbb{C}^{m-1}[X] \\ P(0)=1}} \max_{\mu_n - \mu_{n-1} \leq \mu \leq \mu_n - \mu_1} |P(\mu)|^2 = \frac{1}{T_{m-1}\left(\frac{2\mu_n - \mu_{n-1} - \mu_1}{\mu_{n-1} - \mu_1}\right)^2} \leq 4\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2m},$$

with $\kappa = \frac{\mu_n - \mu_1}{\mu_n - \mu_{n-1}}$. □

Remark 5.7. *The convergence of the Arnoldi process is also sensitive to μ_{n-1} close to μ_n. However, as in the linear solver case, the situation is better for the Krylov solver. Suppose that $\mu_1 \ll \mu_n$ and $\mu_{n-1} = \mu_n(1 - \varepsilon)$ for some $1 \gg \varepsilon > 0$. Then we have*

$$\kappa = \frac{\mu_n - \mu_1}{\mu_n - \mu_{n-1}} = \frac{1 - \frac{\mu_1}{\mu_n}}{1 - \frac{\mu_{n-1}}{\mu_n}} \sim \frac{1}{\varepsilon}.$$

Thus the convergence rate becomes

$$\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \sim \frac{1 - \sqrt{\varepsilon}}{1 + \sqrt{\varepsilon}} \sim 1 - 2\sqrt{\varepsilon}.$$

Compared to the power iteration case (5.9), we have gained a square root in the convergence rate.

A similar estimate can be obtained for the lowest eigenvalue of the matrix A, provided that we now assume a gap between μ_1 and μ_2, and that in the iterative Arnoldi algorithm, the lowest eigenvalue is computed instead of the largest one.

Corollary 5.8. *Let A be a Hermitian matrix with eigenvalues $\mu_1 < \mu_2 \leq \cdots \leq \mu_n$. Let q_1 be an eigenvector associated to μ_1. Let $(\lambda^{(m)}, y^{(m)})$ be the result of the iterative Arnoldi algorithm* `which=smallest` *(Algorithm 5.3) starting with the vector y. Suppose that $\langle q_1, y \rangle \neq 0$. Then* *there exists a constant $C > 0$ independent of m such that the error on the approximated eigenvalue $\lambda^{(m)}$ given after m steps of the iterative Arnoldi algorithm is given by*

$$0 \leq \lambda^{(m)} - \mu_1 \leq C \frac{\mu_n - \mu_1}{T_m\left(\frac{\mu_n + \mu_2 - 2\mu_1}{\mu_n - \mu_2}\right)^2} \leq 4C(\mu_n - \mu_1)\left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1}\right)^{2m}, \tag{5.19}$$

where T_m is the m-th Chebyshev polynomial of the first kind and $\kappa = \frac{\mu_n - \mu_1}{\mu_2 - \mu_1}$.

Proof. Apply Theorem 5.6 to the matrix $-A$. □