Ruprecht-Karls-Universität Heidelberg
Faculty of mathematics and computer science
Institute of applied mathematics

Altering Rayleigh Quotient iteration for close eigenvalues using imaginary shifts

Bachelor Thesis

Author: Nils Friess

Supervisor: Prof. Dr. Robert Scheichl

Submitted: November 1, 2019

1 Introduction

In this chapter, we introduce the general problem by discussing an example that naturally arises in different physical applications. We will then define that basic notion of the Rayleigh quotient and derive the Rayleigh quotient iteration (RQI) algorithm. Finally, we provide an overview of the historic developments of RQI and give a summary of important results concerning the numerical analysis of RQI.

1.1 Motivation

1.2 General problem

We will now formulate the abstract problem that was derived in the last section. To that end, we will give a few basics facts and definitions from linear algebra.

Definition 1.1. Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a real matrix. A scalar $\lambda \in \mathbb{C}$ is called *eigenvalue* of $\mathbf{A}$ if there exists a nonzero vector $v \in \mathbb{C}^n$ such that

$$\mathbf{A}\mathbf{v} = \lambda \mathbf{v} \,. \tag{1.1}$$

The vector $\mathbf{v}$ is called an *eigenvector* of $\mathbf{A}$ associated with λ. The tuple $(\lambda, \mathbf{v})$ is called an *eigenpair*. The set of all eigenvalues of $\mathbf{A}$ is called the *spectrum* and is denoted by $\sigma(\mathbf{A})$.

In the following proposition we combine some basic facts on eigenvalues and eigenvectors of symmetric matrices.

Proposition 1.2. *Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a symmetric matrix. Denote by $\lambda_1, \lambda_2, \ldots, \lambda_n$ the eigenvalues of $\mathbf{A}$ with associated eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.*

(1) All eigenvalues of $\mathbf{A}$ are real.

(2) Eigenvectors of $\mathbf{A}$ form a basis of $\mathbb{R}^n$. Eigenvectors $\mathbf{v}_i$ and $\mathbf{v}_j$ to two distinct eigenvalues λ_i and λ_j are orthogonal. Hence, after normalisation, we can choose eigenvectors of $\mathbf{A}$ that form an orthonormal basis of $\mathbb{R}^n$.

(3) If $\mathbf{A}$ is non-singular the eigenvalues of $\mathbf{A}^{-1}$ are given by $\lambda_1^{-1}, \ldots, \lambda_n^{-1}$ with eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

(4) Let $\sigma \in \mathbb{R}$ an arbitrary scalar. Then the eigenvalues of $\mathbf{A} - \sigma\mathbf{I}$ are $\lambda_i - \sigma$ with eigenvectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$.

The eigenvalues λ_1 and λ_n are called *extreme* eigenvalues. The remaining eigenvalues $(\lambda_2, \ldots, \lambda_{n-1})$ are called *interior* eigenvalues.

A well-known fact from linear algebra states that all eigenvalues $\{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ of symmetric matrices, i. e. $\mathbf{A} = \mathbf{A}^T$, are real and that there exist eigenvectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n\}$ that form an orthogonal basis of $\mathbb{R}^n$.

We will often make the assumption that $\mathbf{A}$ is positive definite, denoted by $\mathbf{A} > 0$, which implies that all eigenvalues are positive. Usually, the eigenvalues will be labeled in ascending order of magnitude, i. e. if $\mathbf{A} > 0$ holds then

$$0 < \lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n .$$

1.3 Iterative methods for eigenvalue problems

In this section we introduce the *power method*, one of the most simple methods to compute eigenpairs of symmetric matrices. By simply altering the initial matrix $\mathbf{A}$ in the power method we arrive at the *inverse iteration* that allows us to compute eigenvalues close to a given value. This will then directly lead us to the *Rayleigh Quotient Iteration* (or *RQI*, for short).

1.3.1 Power method

The power method is based on generating the sequence $\mathbf{A}^k\mathbf{v}_0$ where $\mathbf{v}_0$ is a non-zero unit vector. Of course, $\mathbf{A}^k$ does not have to be computed explicitly since

$$\mathbf{A}^k\mathbf{x} = \mathbf{A}(\mathbf{A}(\dots\mathbf{A}(\mathbf{A}\mathbf{x})\dots)) .$$

The sequence $\mathbf{v}_k$ as generated in Algorithm 1.3 convergences to the eigenvector associated with the eigenvalue λ_n (under the assumption that λ_n is the unique dominant eigenvalue, cf. [Par98, Theorem 4.2.1]).

Algorithm 1.3: Power method

Input: Nonzero unit vector $\mathbf{v}_0$
for $k = 1, 2, \dots$ *until convergence* **do**
  $\tilde{\mathbf{v}}_k \leftarrow \mathbf{A}\mathbf{v}_{k-1}$
  $\mathbf{v}_k \leftarrow \tilde{\mathbf{v}}_k / \|\tilde{\mathbf{v}}_k\|$

1.3.2 Inverse Iteration

To compute the eigenvector associated to the smallest eigenvalue λ_1

1.4 History

A Proofs

Bibliography

[Par98] Beresford N. Parlett. *The Symmetric Eigenvalue Problem*. Upper Saddle River, NJ, USA: Prentice-Hall, Inc., 1998.