THE MODIFIED RAYLEIGH QUOTIENT ITERATION*

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Abstract

The Rayleigh Quotient Iteration (RQI) is a very popular method for computing eigenpairs of symmetric matrices. It is a special kind of inverse iteration method using the Rayleigh Quotient as shifts. Unfortunately, poor initial approximations may render RQI to slow convergence or even to divergence, In this paper we suggest two kinds of numbers each of which can be used instead of the Rayleigh Quotient as a shifts in the RQI. We call the iteration using the new shifts the Modified Rayleigh Quotient Iteration (MRQI). It has been proved that the MRQI always converges and its convergence rate is cubic.

§ 1. Introduction

The Rayleigh Quotient Ieration is a very popular method for computing eigenpairs of symmetric matrices. It is a special kind of inverse iteration method using the Rayleigh Quotient as shifts. Let A be a N by N real symmetric matrix. Its eigenvalues are $\lambda_1, \lambda_2, \cdots, \lambda_N$, and ordered in nondecreasing order i.e. $\lambda_1 \leqslant \lambda_2 \leqslant \cdots \leqslant \lambda_N$. The unit vector $y_i (i=1, 2, \cdots, N)$ is the eigenvector corresponding to eigenvalue λ_i.

The RQI for finding an eigenpair of A is as follows:

Pick a unit vector x_1; then for $k=1, 2, \cdots$ repeat the following:

1. Compute $\rho_k = (Ax_k, x_k)/(x_k, x_k)$.
2. If $A-\rho_k$ is singular, then solve $(A-\rho_k)x_{k+1}=0$ for unit vector x_{k+1}. (ρ_k, x_{k+1}) is an eigenpair of A and stop. Otherwise, solve the equation $(A-\rho_k)y_{k+1}=x_k$ for y_{k+1}.
3. Normalize, i.e. $x_{k+1}=y_{k+1}/\|y_{k+1}\|$.
4. If $\|y_{k+1}\|$ is big enough, then (ρ_{k+1}, x_{k+1}) is an approximate eigenpair and stop.

It was proved that if $\lim_{k\to\infty} x_k = x$ is an eigenvector of A, then the convergence rate is cubic [4, p.72]. Unfortunately, when the initial vector x_1 is poor, the sequence $\{x_k\}$ will not have a limit. Although the sequence $\{\rho_k\}$ has a limit ρ, yet ρ may not be an eigenvalue of A. If we give a small perturbation to the above initial vector x_1, and let $x_1+\varepsilon$ be a new initial vector, then thesequence $\{x_k(x_1+\varepsilon)\}$ will be convergent. However, it converges very slowly.

The drawback of the RQI makes one consider some variants of the RQI and in this paper we suggest two kinds of modified Rayleigh Quotient Iteration. One is called MRQI-W and the other, MRQI-RW. The MRQI-W, MRQI-RW differ with the RQI only in the shifts.

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The MRQI–W runs as follows:

1. Pick a unit vector x_1, $1\to k$.
2. Compute $\rho_k=(Ax_k, x_k)$, $r_k=Ax_k-\rho_k x_k$, $b_k=\|r_k\|$.
3. If $b_k<\varepsilon$ then goto 5.
4. Compute $a_k=(Ar_k, r_k)/b_k^2$, $d_k=(a_k-\rho_k)/2$,

$$\omega_k=\rho_k-(\operatorname{sign} d_k)b_k^2/[|d_k|+(d_k^2+b_k^2)^{1/2}].$$

Solve $(A-\omega_k I)x_{k+1}=\tau_k x_k$ for x_{k+1}, where the number τ_k makes $\|x_{k+1}\|=1$. $k+1\to k$ goto 2.

5. (ρ_k, x_k) is an approximate eigenpair of A.

The MRQI–RW runs as follows:

1. Pick a unit vector x_1, $1\to k$.
2. Compute $\rho_k=(Ax_k, x_k)$, $r_k=Ax_k-\rho_k x_k$, $b_k=\|r_k\|$.
3. If $b_k<\varepsilon$ then goto 5.
4. Compute $a_k=(Ar_k, r_k)/b_k^2$, $d_k=(a_k-\rho_k)/2$,

$$c_k=\|Ar_k-a_k r_k-b_k^2x_k\|/b_k,$$

$$\delta_k=\rho_k,\ \text{if } 2b_k^2<c_k^2,$$

$$\delta_k=\omega_k=\rho_k-(\operatorname{sign} d_k)b_k^2/[|d_k|+(d_k^2+b_k^2)^{1/2}],\ \text{if } 2b_k^2\geqslant c_k^2.$$

Solve $(A-\delta_k I)x_{k+1}=\tau_k x_k$ for x_{k+1}, where the number τ_k makes $\|x_{k+1}\|=1$. $k+1\to k$ goto 2.

5. (ρ_k, x_k) is an approximate eigenpair of A.

In this paper it is proved that the sequence $\{(\rho_k, x_k)\}$ produced by MRQI–W or MRQI–RW always converges to (λ_i, y_i), an eigenpair of A, and the rate of convergence is almost cubic or cubic respectively. Estimates of the bound of $|\rho_k-\lambda_i|$ and $\sin\theta_k$ are also given, where $\cos\theta_k=(x_k, y_i)$.

The norm and inner product (x, y) are in the sense of space l_2. The vector e_i is the i-th column of identity matrix of order N.

§ 2. Main Results

Let $\{s_k\}$ be a real number sequence. We call the following algorithm MRQI–$\{s_k\}$:

1. Pick a unit vector x_1, $1\to k$.
2. Compute $\rho_k=(Ax_k, x_k)$, $r_k=Ax_k-\rho_k x_k$, $b_k=\|r_k\|$,

$$a_k=(Ar_k, r_k)/b_k^2,\quad c_k=\|Ar_k-a_k r_k-b_k^2x_k\|/b_k.$$

3. If $b_k<\varepsilon$ then goto 5.
4. Solve equation $(A-s_kI)x_{k+1}=\tau_k x_k$ for x_{k+1}. The number τ_k makes $\|x_{k+1}\|=1$. $k+1\to k$ goto 2.
5. (ρ_k, x_k) is an approximate eigenpair of A and stop.

When $s_k=\omega_k=\rho_k-(\operatorname{sign} d_k)b_k^2/[|d_k|+(d_k^2+b_k^2)^{1/2}]$ MROI–$\{s_k\}$ is MRQI–W and when

$$s_k=\delta_k=\rho_k,\ \text{if } 2b_k^2<c_k^2 \text{ and } s_k=\delta_k=\omega_k,\ \text{if } 2b_k^2\geqslant c_k^2$$

MRQI–$\{s_k\}$ is MRQI–RW

For any initial vector x_1, there is an orthogonal matrix

$$W=[x_1, s_2, \cdots, s_N]$$