THE MODIFIED RAYLEIGH QUOTIENT ITERATION*

JIANG ER-XIONG (蒋尔雄)
(Fudan University, Shanghai, China)

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 $s_k = (Ar_k, r_k)/b_k^2$, $d_k = (a_k - \rho_k)/2$,

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

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 $a_k = (Ar_k, r_k)/b_k^2$, $d_k = (a_k - \rho_k)/2$,

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

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

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

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 $\rho_k = (Ax_k, x_k)$, $r_k = Ax_k - \rho_k x_k$, $b_k = \|r_k\|$,

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

3. If $b_k < \varepsilon$ then goto 5.
4. Solve equation $(A - s_k I)x_{k+1} = \tau_k x_k$ 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 $s_k = \omega_k = \rho_k - (\text{sign } d_k) b_k^2 / [|d_k| + (d_k^2 + b_k^2)^{1/2}]$ MROI–$\{s_k\}$ is MRQI–W and when

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

MRQI–$\{s_k\}$ is MRQI–RW

For any initial vector x_1, there is an orthogonal matrix

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

where x_1 is the first column of W such that

$$W^TAW=T_1=\begin{bmatrix} \alpha_1^{(1)} & \beta_1^{(1)} & & \\ \beta_1^{(1)} & \alpha_2^{(1)} & \beta_2^{(1)} & \\ & \ddots & \ddots & \beta_{n-1}^{(1)} \\ & & \beta_{n-1}^{(1)} & \alpha_n^{(1)} \end{bmatrix}$$

is a symmetric tridiagonal matrix. We can get W and T_1 by using the Lanczos process.

For any $\{s_k\}$, we apply the QL algorithm to T_1 with shifts s_k as follows:

$$T_k-s_kI=Q_kL_k,$$
$$T_{k+1}=L_kQ_k+s_kI$$

where Q_k is an orthogonal matrix and L_k is a lower triangular matrix. It is well known that the $\{T_k\}$ is one of sequence of symmetric tridiangonal matrices. Let

$$T_k=\begin{bmatrix} \alpha_1^{(k)} & \beta_1^{(k)} & & \\ \beta_1^{(k)} & \alpha_2^{(k)} & \beta_1^{(k)} & \\ & \ddots & \ddots & \beta_{n-1}^{(k)} \\ & & \beta_{n-1}^{(k)} & \alpha_n^{(k)} \end{bmatrix}.$$

There is a relationship between MRQI-$\{s_k\}$ and $\{T_k\}$.

Theorem 1. *If no s_k is an eigenvalue of A, then the following propositions hold for $k=1, 2,\cdots$:*

1. $\rho_k=\alpha_1^{(k)}$.
2. $b_k=\|r_k\|=\beta_1^{(k)}$.
3. $a_k=(Ar_k, r_k)/(r_k, r_k)=\alpha_2^{(k)}$, if $r_k\neq 0$.
4. $c_k=\|Ar_k-a_kr_k-b_k^2x_k\|/b_k=\beta_2^{(k)}$, if $r_k\neq 0$.
5. *Let $P_k=WQ_1Q_2\cdots Q_k$. Then $x_{k+1}=P_ke_1$.*

Proof. When $k=1$,

$$\alpha_1^{(1)}=(T_1e_1, e_1)=(W^TAWe_1, e_1)=(Ax_1, x_1)=\rho_1,$$
$$r_1=Ax_1-\rho_1x_1=AWe_1-\rho_1We_1=W(W^TAWe-\rho_1e_1)$$
$$=W(T_1e_1-\alpha_1^{(1)}e_1)=W(0,\beta_1^{(1)}, 0, \cdots, 0)^T.$$

So $b_1=\|r_1\|=\beta_1^{(1)}$ and $s_2=r_1/\|r_1\|$.

From $WT_1=AW$, we have

$$\beta_2^{(1)}s_3=As_2-\alpha_2^{(1)}s_2-\beta_1^{(1)}x_1.$$

Hence

$$\beta_2^{(1)}=\|Ar_1-a_1r_1-b_1^2x_1\|/\|r_1\|.$$

By the QL algorithm, we know[3, Lemma 1]

$$(T_1-s_1I)q_1^{(1)}=l_{11}^{(1)}e_1$$

where $q_1^{(1)}$ is the first column of Q_1 and $l_{11}^{(1)}$ is the first diagonal element of L_1. So

$$(W^TAW-s_1I)q_1^{(1)}=l_{11}^{(1)}e_1,$$
$$(A-s_1I)Wq_1^{(1)}=l_{11}^{(1)}We_1=l_{11}^{(1)}x_1$$

and $x_2=Wq_1^{(1)}=WQ_1e_1$.

Therefore all propositions of Theorem 1 hold for $k=1$. Now suppose they hold when $k=j$. We prove they are valid when $k=j+1$.

$$T_{j+1}=Q_j^T Q_{j-1}^T Q_{j-2}^T \cdots Q_1^T T_1 Q_1 Q_2 \cdots Q_j = P_j^T A P_j, \tag{1}$$

$$\alpha_1^{(j+1)}=(T_{j+1}e_1,\ e_1)=(AP_je_1,\ P_je_1)=(Ax_{j+1},\ x_{j+1})=\rho_{j+1}.$$

From

$$r_{j+1}=Ax_{j+1}-\rho_{j+1}x_{j+1}=AP_je_1-\rho_{j+1}P_je_1=P_j(T_{j+1}e_1-\alpha_1^{(j+1)}e_1)$$
$$=P_j(0,\ \beta_1^{(j+1)},\ 0,\ \cdots,\ 0)^T,$$

we have

$$\beta_1^{(j+1)}=\|r_{j+1}\|=b_{j+1}$$

and

$$r_{j+1}=\beta_1^{(j+1)}P_je_2,$$
$$a_{j+1}=(Ar_{j+1},\ r_{j+1})/(r_{j+1},\ r_{j+1})=(AP_je_2,\ P_je_2)$$
$$=(T_{j+1}e_2,\ e_2)=\alpha_2^{(j+1)}.$$

From (1)

$$\beta_2^{(j+1)}P_je_3=AP_je_2-\alpha_2^{(j+1)}P_je_2-\beta_1^{(j+1)}P_je_1$$
$$=Ar_{j+1}/\|r_{j+1}\|-\alpha_2^{(j+1)}r_{j+1}/\|r_{j+1}\|-\beta_1^{(j+1)}x_{j+1}$$
$$=(Ar_{j+1}-\alpha_2^{(j+1)}r_{j+1}-b_{j+1}^2x_{j+1})/\|r_{j+1}\|.$$

Hence

$$\beta_2^{(j+1)}=\|Ar_{j+1}-\alpha_2^{(j+1)}r_{j+1}-b_{j+1}^2x_{j+1}\|/\|r_{j+1}\|=c_{j+1}.$$

By the QL algorithm, we have

$$(T_{j+1}-s_{j+1}I)q_1^{(j+1)}=l_{11}^{(j+1)}e_1 \tag{2}$$

where $q_1^{(j+1)}$ is the first column of Q_{j+1} and $l_{11}^{(j+1)}$ is the first diagonal element of L_{j+1}. Using (1) we get

$$(P_j^TAP_j-s_{j+1}I)q_1^{(j+1)}=l_{11}^{(j+1)}e_1$$

i.e.

$$(A-s_{j+1}I)P_jq_1^{(j+1)}=l_{11}^{(j+1)}P_je_1,$$
$$(A-s_{j+1}I)P_jQ_{j+1}e_1=l_{11}^{(j+1)}x_{j+1}.$$

So

$$P_jQ_{j+1}e_1=P_{j+1}e_1=x_{j+2}.$$

Theorem 2. *For any unit initial vector x_1, if no ω_k is an eigenvalue of A and the sequence $\{(\rho_k,\ x_k)\}$ produced by MRQI-W, then there is an eigenpair $(\lambda_i,\ y_i)$ of A, such that*

$$\lim_{k\to\infty}(\rho_k,\ x_k)=(\lambda_i,\ y_i).$$

Furthermore,

$$|\rho_k-\lambda_i|\le b_k^2/\sigma, \quad \text{where } \sigma=\min_{\lambda_j\ne\lambda_i}|\lambda_j-\rho_k|,$$
$$\sin\theta_k=b_k/\sigma \quad \text{where } \cos\theta_k=(x_k,\ y_i)$$

and

$$\lim_{k\to\infty}b_k=0, \quad b_{k+1}=M_kb_k^3c_k^2/|a_k-\omega_k|,$$

where M_k is a bounded numcer, $|M_k| <$constant.

Proof. For matrix A and vector x_1, there is a symmetric tridiagonal matrix T_1, such that

$$W^T A W = T_1$$

whrer $W = [x_1, s_2, \cdots, s_n]$ is an orthogonal matrix. By Theorem 1, implementation of MRQI-W to A means that of the QL algorithm with shift ω_k to T_1. Because

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

$$\rho_k = \alpha_1^{(k)},\ d_k = (\alpha_2^{(k)} - \alpha_1^{(k)})/2,\ b_k = \beta_1^{(k)},$$

ω_k is just the Wilkinson shift [4]. By Wilkinson's result [5], [1], we have

$$b_k = \beta_1^{(k)} \to 0.$$

By the result of [1], we have

$$\beta_1^{(k+1)} = M_k (\beta_1^{(k)})^3 (\beta_2^{(k)})^2 / |\alpha_2^{(k)} - \omega_k|$$

i.e.

$$b_{k+1} = M_k (b_k)^3 (c_k)^2 / |a_k - \omega_k|$$

where $|M_k| <$constant. Because ρ_k is the Rayleigh Quotient of A and x_k, from $Ax_k - \rho_k x_k = r_k$, we know there is an eigenpair (λ_i, y_i) of A, such that[4, p.222]

$$|\rho_k - \lambda_i| \leq \|r_k\|^2/\sigma = b_k^2/\sigma \tag{3}$$

where $\sigma = \min\limits_{\lambda_j \neq \lambda_i} |\lambda_j - \rho_k|$, and $|\sin\theta_k| \leq \|r_k\|/\sigma = b_k/\sigma$

where $\cos\theta_k = (x_k, y_i)$.

It is known from [1], [2] that for k large enough, λ_i in inequality (3) is independent of k. So using $b_k \to 0$ we have

$$(\rho_k, x_k) \to (\lambda_i, y_i).$$

Theorem 3. *For any unit initial vector x_1, if no δ_k is an eigenvalue of A and the sequence $\{(\rho_k, x_k)\}$ is produced by MRQI-RW, then there is an eigenpair (λ_i, y_i) of A, such that*

$$\lim_{k\to\infty} b_k = 0,$$

$$b_{k+1} = M_k b_k^3, \quad |M_k| < \text{constant},$$

$$b_{k+1} < b_k, \text{ if } b_k \neq 0$$

and

$$\lim_{k\to\infty} (\rho_k, x_k) = (\lambda_i, y_i).$$

Furthermore

$$|\rho_k - \lambda_i| \leq b_k^2/\sigma, \quad \text{where } \sigma = \min_{\lambda_k \neq \lambda_j} |\lambda_j - \rho_k|,$$

$$|\sin\theta_k| \leq b_k/\sigma, \quad \text{where } \cos\theta_k = (x_k, y_i).$$

Proof. In the case of MRQI-RW, $s_k = \delta_k$, where δ_k is just the RW shift of the QL algorithm[3]. By the result of [3], we have

$$\lim_{k\to\infty} b_k = 0 \text{ and } b_{k+1} = M_k b_k^3,\ |M_k| < \text{constant}.$$

Now let us prove $b_{k+1} < b_k$ if $b_k \neq 0$. From [3].

$$\begin{aligned}\hat{l}_{11}^2 &< l_{11}^2/(q_{11}^2+q_{21}^2+q_{31}^2)\\ &< [(1-k)^2\beta_1^2+(1+k)\beta_2^2]\beta_1^2/[(1+k)\beta_1^2+\beta_2^2] = \beta_1^2\end{aligned} \tag{4}$$

where

$$k=\begin{cases}0, \text{ if } 2\beta_1^2\leq\beta_2^2,\\ 1, \text{ if } 2\beta_1^2>\beta_2^2,\end{cases}$$

and

$$\hat{\beta}_1^2 = l_{11}^2(q_{21}^2+q_{31}^2+\cdots+q_{n1}^2). \tag{5}$$

There are two cases only: $q_{11}^2+q_{41}^2+\cdots+q_{n1}^2\neq 0$ and

$$q_{11}^2+q_{41}^2+\cdots+q_{n1}^2=0.$$

In case 1, from (4) and (5),

$$\hat{\beta}_1^2<\beta_1^2, \text{ i.e. } b_{k+1}<b_k.$$

In case 2, from $q_{11}=0$, we have $q_{21}^2+q_{31}^2+\cdots+q_{n1}^2=1$ and $\hat{\beta}_1^2=\hat{l}_{11}^2$. On the other hand

$$\hat{T}=LQ+\delta I.$$

We have $\hat{\beta}_1=l_{11}q_{12}$; so $|q_{12}|=1$ and $q_2=\pm e_1$. In this case $q_1=q_{21}e_2+q_{31}e_3$ and

$$\hat{\beta}_1=q_1^T T q_2=(q_{21}e_2+q_{31}e_3)^T(\pm\alpha_1 e_1\pm\beta_1 e_2)=\pm\beta_1 q_{21}.$$

So if $|q_{21}|<1$, then $\hat{\beta}_1<\beta_1$; if $|q_{21}|=1$, $q_{31}=0$. From the third equation of $(T-\delta I)$ $q_{11}=l_{11}e_1$, we obtain

$$\beta_2 q_{21}+(\alpha_3-\delta)q_{31}+\beta_3 q_{41}=0.$$

Thus $\beta_2=0$ and $2\beta_1^2>\beta_2^2$ holds except when $\beta_1=0$. Hence $k=1$, $l_{11}=0$ and $\hat{\beta}_1=0$. This means that $\hat{\beta}_1^2<\beta_1^2$ i.e. $b_{k+1}<b_k$.

The other part of the theorem can be proved similarly as Theorem 2.

Comment. If s_k (ω_k or δ_k) is an eigenvalue of A, then x_{k+1} computed from equation

$$(A-s_kI)x_{k+1}=\tau_k x_k$$

in the practice, is an approximate eigenvector of A. (ρ_{k+1}, x_{k+1}) is an approximate eigenpair. This will be illustrated by an example in the next section.

§ 3. Numerical Examples

Let

$$A=HDH, \quad D=\mathrm{diag}(1, 2, 3, 4, 5, 6, 7, 8, 9, 10)$$

where $H=1-2uu^T$ and u is a unit random vector,

$$u=(0.0761301 \quad 0.0235906 \quad 0.1520517 \quad 0.2882251 \quad 0.2825532$$
$$0.2212344 \quad 0.3890589 \quad 0.6627968 \quad 0.2896246 \quad 0.2900421)^T.$$

We want to find an eigenpair of A. The computational results at Honewell DPS-8 at single precision are as follows:

1. $x_1=(0.3287396,\ 0.0328171,\ 0.4509322,\ 0.4133724,\ 0.0329908\ 0.4545829,$
$0.3441579,\ 0.0963663,\ 0.4240890,\ 0.0363405)^T,$

$$\rho_1=7.1257992, \quad \|r_1\|=b_1=2.24620670.$$

a. Use RQI, after 6 iterations we get

$$\rho_6=6.9999999,$$

$$x_6=(0.0592382,\ 0.0183563,\ 0.1183141,\ 0.2242731,\ 0.219859\ 0.1721465,\ -0.6972663,\ 0.5157341,\ 0.2253620,\ 0.2256869)^T,$$

$$\|r_6\|=0.00000027.$$

b. Using MRQI-W, after 4 iteration we get

$$\rho_4=7.9999998,$$

$$x_4=(0.1009176,\ 0.0312715,\ 0.2015587,\ 0.3820692,\ 0.3745506,\ 0.2932668,\ 0.5157344,\ -0.1214010,\ 0.3839247,\ 0.3844776)^T,$$

$$\|r_4\|=0.00000095.$$

c. Using MRQI-RW, after 4 iterations we get

$$\rho_4=7.9999999,$$

$$x_4=(0.1009176,\ 0.0312715,\ 0.2015588,\ 0.3820693,\ 0.3745507,\ 0.2932670.\ 0.5157341,\ -0.1214007,\ 0.3839245,\ 0.3844780)^T,$$

2. $x_1=(0.6963704,\ 0.7037799,\ -0.0214433,\ -0.0406473,\ -0.0398475,\ -0.0311999,\ -0.0548676,\ -0.0934718,\ -0.0408447,\ -0.409036)^T,$

$$\rho_1=1.5,\ \|r_1\|=b_1=0.5.$$

a. Using RQI, after 15 iterations we get

$$\|r_{15}\|=0.49883967.$$

It seems to be divergent or very slowly convergent.

b. Using MRQI-W

$$\omega_1=1$$

is an eigenvalue of A, but from equation $(A-\omega_1 I)x_2=\tau_1 x_1$ we get

$$x_2=(-0.9884084,\ 0.0035919,\ 0.0231514,\ 0.0438852,\ 0.0430216,\ 0.0336852,\ 0.0592382,\ 0.1009176,\ 0.0440983,\ 0.0441619)^T,$$

$$\rho_2=1,$$

(ρ_2, x_2) is a good approximate eigenpair.

c. Using MRQI-RW, we get the results similar to that using MRQI-W.

3. Give a small perturbation to the vector x_1 of 2.

$$x_1=(0.6964550,\ 0.7038226,\ -0.0212273,\ -0.0403840,\ -0.0398228,\ -0.0307639,\ -0.0544837,\ -0.0933525,\ -0.0402345,\ -0.0408472)^T,$$

$$\rho_1=1.5000234,\quad \|r_1\|=0.50003509.$$

a. Using RQI, after 13 iterations we get $\|r_{13}\|=0.00000004$ and

$$\|r_{12}\|=0.00047257,$$

$$\rho_{13}=2.00000000,$$

$$x_{13}=(-0.0035919,\ 0.998870,\ -0.0071740,\ -0.015988,\ -0.0133312\ -0.0104381,\ -0.0183563,\ -0.0312715,\ -0.0136648,\ -0.0136845)^T.$$

b. Using MRQI-W, after 2 iterations, we get

$$\rho_3=1.0000000,$$

$$x_3=(0.9884084,\ -0.0035919,\ -0.0231514\ -0.0438852,\ -0.0430216,$$

$-00.0336852, -0.0592382, -0.1009176, -0.0440983, -0.0441619)^T,$

$$\|r_3\| = 0.00000002.$$

c. Using MRQI-RW, after 2 iterations we get ρ_3, x_3, $\|r_3\|$ which are the same as produced by MRQI-W.

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