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Variational Rayleigh Quotient Iteration Methods for a Symmetric Eigenvalue Problem

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Abstract. New versions of Rayleigh quotient iteration (RQI) methods for a symmetric eigenvalue problem have been investigated. *A posteriori* choice of an additional shift in RQI is proposed from variational considerations. Convergence for an arbitrary initial approximation and a decrease in the norm of residuals which is not worse than a geometric progression with a common ratio of $1/\sqrt{2}$ are proved. The model numerical experiments showed a certain superiority of the new version over the classic one in computing the extreme eigenvalues.

Keywords: symmetric eigenvalue problem, Rayleigh quotient iteration, variational methods.

AMS(MOS) subject classification: 65F15, 65F10.

1 Introduction

One of the most familiar methods of finding several eigenvalues and eigenvectors of a symmetric matrix A is an inverse iteration method

$$u_{k+1} = (A - \sigma I)^{-1} u_k, \quad k = 0, 1, \ldots, \tag{1.1}$$

where the vector u_k is an approximation to the eigenvector, and σ is a certain shift.

The properties of convergence of the method with fixed σ are well studied, *e.g.*, in [4, 6].

One of the modifications of the inverse iteration method is the Rayleigh quotient iteration method (RQI). The role of σ is played here by the Rayleigh quotient:

$$u_{k+1} = (A - \rho_k I)^{-1} u_k, \tag{1.2}$$

where

$$\rho_k = \rho(u_k) = \frac{(Au_k, u_k)}{(u_k, u_k)}$$

is the Rayleigh quotient for the vector u_k.

The RQI method has a high asymptotic rate of convergence. Late in the 1950s Ostrowski [5] showed that RQI converges asymptotically with a cubic rate. A detailed investegation of the RQI method is carried out in Parlett's book [6].

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In case of a poor choice of the initial approximation, RQI can converge very slowly or even diverge. Batterson and Smillie [1] showed that a set of vectors u_0, for which the values u_k in (1.2) do not converge to the eigenvector subspace, has zero measure.

There are known modifications of the RQI method allowing us to avoid divergence. Jiang Er-Xiong [3] suggests using $\rho_k + \delta_k$ as a shift, where δ_k is the function dependent on the vector of residual for the corresponding vector u_k. It is stated that the method converges regardless of the choice of the initial approximation while asymptotically cubic convergence retains.

It is sometimes advantageous to combine RQI with other methods. Szyld [7] proposes to use RQI for improving the approximation to the eigenvector obtained by the inverse iteration method (1.1) and formulates a quality criterion for an approximation in method (1.1) which, being initial for RQI, ensures RQI convergence to the nearest eigenvalue. The ideas of this work are developed in [2].

In Section 1.7 of book [4] the version of the RQI method with an additional shift γ_k is proposed:

(1.3)
$$u_{k+1} = (A - \rho(u_k)I)^{-1}u_k + \gamma_k u_k,$$

and the estimate of the rate of $\rho(u_k)$ convergence to the extreme eigenvalue for corresponding γ_k is derived. The best *a priori* choice of γ_k is found on the basis of this estimate. This choice involves estimates for the spectrum bounds which are rarely known in practice.

The aim of this paper is to find, on the basis of optimizing the value $\rho(u_{k+1})$, a practically realizable *a posteriori* method of choosing γ_k in (1.3), for a symmetric matrix A, which improves the convergence properties of the classic RQI method with, essentially, the same computational time per iteration.

2 The Monotone Rayleigh Quotient Iteration Method

The method in (1.3) with a step γ_k chosen for each iteration according to the condition of either the maximum or the minimum value $\rho(u_{k+1})$ will be called the monotone Rayleigh quotient iteration method. In the first case it will be called the monotone method RQI+, in the second case the monotone method RQI-. We shall derive explicit formulas for the appropriate values γ_k and $\rho(u_{k+1})$.

We shall consider a single step of the iterative process (1.3)

$$u' = (A - \rho(u)I)^{-1}u + \gamma u,$$

where A is a symmetric matrix, u is a normalized vector, and γ is a certain parameter. Hereafter, it is supposed for simplicity that $\rho(u)$ is never accurately equal to an eigenvalue, so that the matrix $A - \rho(u)I$ is nondegenerate.

We shall investigate the dependence of the Rayleigh quotient $\rho' = \rho(u')$ on γ.

Let us introduce the designation $B = B(u) = (A - \rho(u)I)^{-1}$. We have

$$u' = Bu + \gamma u,$$

(2.1)
$$\rho' = \rho(u') = \rho(u) + \frac{(Bu,u) + 2\gamma}{(Bu,Bu) + 2\gamma(Bu,u) + \gamma^2}.$$

This equality provides a technique for computing the Rayleigh quotient for a successive approximation of the method (1.3) without multiplying the matrix A by the vector.

The values γ_+ and γ_-:

(2.2)
$$\gamma_{+,-} = \gamma_{+,-}(u) = \frac{-(Bu,u) \pm \sqrt{4(Bu,Bu) - 3(Bu,u)^2}}{2}$$

are the positions of extrema for the Rayleigh quotient $\rho(u')$ in (2.1). We have

$$\gamma_+\gamma_- = (Bu,u)^2 - (Bu,Bu) < 0,$$

by virtue of the Cauchy–Schwarz–Bunyakowski inequality. Here the inequality is strict, since an equality would imply the parallelism of vectors Bu and u. This is impossible, because, in case of the nondegenerate matrix $A-\rho(u)I$, the vector u is not an eigenvector for the matrix A and, hence, for $B=(A-\rho(u)I)^{-1}$ as well. Consequently,

$$\gamma_- < 0 < \gamma_+. \tag{2.3}$$

Let us find the extreme values of Rayleigh quotient (2.1) corresponding to γ_+ and γ_-:

$$\begin{aligned} \rho_+ =&\rho(u,\gamma_+) = \rho(u) + \frac{(Bu,u)+2\gamma_+}{(Bu,Bu)+2\gamma_+(Bu,u)+\gamma_+^2} \\ =&\rho(u) + \frac{2}{(Bu,u)+\sqrt{4(Bu,Bu)-3(Bu,u)^2}} \\ =&\rho(u) - \frac{1}{\gamma_-} > \rho u. \end{aligned} \tag{2.4}$$

Thus, γ_+ ensures the maximum value for Rayleigh quotient (2.1). Similarly, γ_- corresponds to the minimum value of (2.1) and

$$\rho_- = \rho(u,\gamma_-) = \rho(u) - \frac{1}{\gamma_+} < \rho(u). \tag{??'}$$

Ritz' vectors

$$\begin{aligned} u'_+ =&Bu+\gamma_+u, \\ u'_- =&Bu+\gamma_-u, \end{aligned} \tag{2.5}$$

and the values ρ_+ and ρ_- form the characteristic pairs of projection [6]of the matrix A on the subspace Span (u, Bu).

We shall denote $\|u_+{}'\|^2$ by γ_+ and γ_-:

$$\begin{aligned} \|u'_+\|^2 =&(Bu,Bu)+2\gamma_+(Bu,u)+\gamma_+^2 \\ =&2(Bu,Bu) - \frac{3}{2}(Bu,u)^2 + \frac{1}{2}(Bu,u)\sqrt{4(Bu,Bu)-3(Bu,u)^2} \\ =& -\gamma_-(\gamma_+-\gamma_-). \end{aligned} \tag{2.6}$$

Analogously

$$\|u'_-\|^2 = \gamma_+(\gamma_+-\gamma_-). \tag{2.7}$$

Let us formulate the monotone RQI+ method.

The RQI+ method:

We choose a certain normalized vector as an initial approximation u_0 and calculate ρ_0, *viz.*, the Rayleigh quotient for it. Subsequent approximations are calculated by the formulas

$$\begin{aligned} B_ku_k =&(A-\rho_kI)^{-1}u_k, \\ u_{k+1} =&\tau_k(B_ku_k+\gamma_{+k}u_k), \\ \rho_{k+1} =&\rho_k - \frac{1}{\gamma_{-k}}, \end{aligned} \tag{2.8}$$

where $\gamma_{\pm k} = \gamma_\pm(u_k)$ in (2.2), $\tau_k = (-\gamma_{-k}(\gamma_{+k}-\gamma_{-k}))^{-1/2}$.

The RQI- method ensuring a decrease in the Rayleigh quotient ρ_k is formulated in a similar way.

3 Properties of the Monotone RQI Method

Since the RQI+ and RQI- methods are similar, only the properties of the RQI+ method are investigated in this section.

By contradiction it is not difficult to prove

Theorem 3.1. *Regardless of the choice of the initial approximation u_0 a sequence of Rayleigh quotients ρ_k in (2.8) converges to some eigenvalue of the matrix A.*

Of major importance is

Lemma 3.1. *Let the eigenvalue λ_i of the matrix A be the limit of a sequence ρ_k, and λ_{i-1} be the preceding eigenvalue, $\lambda_{i-1} < \lambda_i$. We define $\hat{k}$ by the condition*

$$\rho_{\hat{k}} \geq \frac{\lambda_{i-1} + \lambda_i}{2}$$

then, $(B_k u_k, u_k) \geq 0$ when $k \geq \hat{k}$.

Proof. By virtue of the condition of the lemma,

$$\|B_k\| = \frac{1}{\min_j |\lambda_j - \rho_k|} = \frac{1}{\lambda_i - \rho_k}.$$

Taking into account that

$$\frac{1}{-\gamma_{k-}} = \rho_{k+1} - \rho_k \leq \lambda_i - \rho_k,$$

we have

$$\|B_k u_k\| \leq \|B_k\| \, \|u_k\| = \|B_k\| = \frac{1}{\lambda_i - \rho_k} \leq -\gamma_{k-}.$$

The explicit expression for γ_{k-} in (2.2) indicates that the inequality $\|B_k u_k\| \leq -\gamma_{k-}$ is equivalent to the required one $(B_k u_k, u_k) \geq 0$.□

Theorem 3.2. *Assume that the conditions of Lemma 3.1 are satisfied. Then, for $k \geq \hat{k}$, the norms of the residual vectors $r_k = r(u_k) = Au_k - \rho_k u_k$ corresponding to the vectors u_k obtained by the RQI+ method (2.8) decrease monotonically and*

$$\frac{\|r_{k+1}\|}{\|r_k\|} < \frac{1}{\sqrt{2}}.$$

The proof is given at the end of Section 5.

4 The Combined Rayleigh Quotient Iteration Method

The monotone RQI method lacks the property of a non-increase in residuals which is inherent in the RQI method. The norm of a residual vector can increase at the beginning of an iterative process. For instance, if the initial approximation u_0 is in the vicinity of some eigenvector of the matrix A and the Rayleigh quotient somewhat exceeds the corresponding eigenvalue, the RQI+ method will depart from this good eigenvector approximation. The combined method in which the iterations of the RQI+ and RQI- methods alternate depending on sgn (Bu, u) enables us to avoid this situation.

From (2.1), with $\gamma = 0$, it follows that sgn(Bu, u) specifies the direction of change in the Rayleigh quotient in the conventional RQI method (1.2). With the same sign is connected

Theorem 4.1. *Let $\|u\| = 1$. We shall consider vectors u_+ and u_- in (2.5) and the corresponding residuals*

$$r_+ = \frac{Au_+ - \rho(u_+)u_+}{\|u_+\|}, \quad r_- = \frac{Au_- - \rho(u_-)u_-}{\|u_-\|}.$$

Let $\|r_+\| \neq 0$ and $\|r_-\| \neq 0$. If $(Bu,u) > 0$, then $\|r_+\| < \|r_-\|$. If $(Bu,u) < 0$, then $\|r_+\| > \|r_-\|$.

Proof. We shall introduce the designation $r = Au - \rho(u)u$. With the aid of (2.4) we obtain

$$\gamma_-\|u_+\|r_+ = (\gamma_- + \gamma_+)u + \gamma_+\gamma_- r + Bu. \tag{4.1}$$

Similarly

$$\gamma_+\|u_-\|r_- = (\gamma_- + \gamma_+)u + \gamma_+\gamma_- r + Bu. \tag{4.2}$$

Taking advantage of the equality of the right-hand sides, we derive

$$\gamma_-\|u_+\|r_+ = \gamma_+\|u_-\|r_-.$$

Squaring it and taking into account (2.6), we arrive at

$$\frac{\|r_+\|^2}{\gamma_+^3} = \frac{\|r_-\|^2}{-\gamma_-^3}.$$

By virtue of (2.2)

$$\gamma_+ + \gamma_- = -(Bu,u). \tag{4.3}$$

When $(Bu,u) > 0$, we have $\gamma_+ < -\gamma_-$ and $\|r_+\| < \|r_-\|$. Analogously, when $(Bu,u) < 0$ we obtain $\|r_+\| > \|r_-\|$.

Thus, at each step of an iterative process it is preferable to choose the direction of a monotone method corresponding to $\operatorname{sgn}(Bu,u)$.

In order to formulate the combined Rayleigh quotient iteration (CRQI) method, we shall introduce new quantities γ_b (best) and γ_w (worst) equal to γ_+ and γ_- in (2.2), taking into account $\operatorname{sgn}(Bu,u)$:

$$\begin{aligned}\gamma_b &= \begin{cases}\gamma_+, & \text{for } (Bu,u) \geq 0,\\ \gamma_-, & \text{for } (Bu,u) < 0,\end{cases}\\ \gamma_w &= \begin{cases}\gamma_-, & \text{for } (Bu,u) \geq 0,\\ \gamma_+, & \text{for } (Bu,u) < 0.\end{cases}\end{aligned} \tag{4.4}$$

The CRQI method:

Choose the initial approximation u_0 and calculate $\rho_0 = \rho(u_0)$. Subsequent approximations are calculated by the formulas

$$\begin{aligned}B_k u_k &= (A - \rho_k I)^{-1} u_k,\\ u_{k+1} &= \tau_k(B_k u_k + \gamma_{bk} u_k),\\ \rho_{k+1} &= \rho_k - \frac{1}{\gamma_{wk}},\end{aligned} \tag{4.5}$$

where $\gamma_{b,wk} = \gamma_{b,w}(u_k)$ from (4.4), $\tau_k = (-\gamma_{wk}(\gamma_{bk} - \gamma_{wk}))^{-1/2}$.

Note that immediately from definition (2.2) it follows that

$$|\gamma_b| \leq \|Bu\| \leq |\gamma_w|. \tag{4.6}$$

5 Properties of the Combined Method

Theorem 5.1. *Regardless of the choice of the initial approximation u_0, the norms of residuals*

$$r_k = r(u_k) = Au_k - \rho_k u_k$$

corresponding to vectors u_k in (4.4), decrease monotonically, where

$$\frac{\|r_{k+1}\|}{\|r_k\|} < \frac{1}{\sqrt{2}}. \tag{5.1}$$

Proof. We shall consider a single step of the iterative process (4.5) in the form

$$u' = \tau(Bu + \gamma_b u), \qquad \|u\| = 1, \tag{5.2}$$

where $\tau = \|u'\|^{-1} = (\gamma_w(\gamma_w - \gamma_b))^{1/2}$ and γ_b, γ_w are from (4.4). From residual relations (4.1) we get

$$\|u'\|r' - u'/\gamma_w = u + \gamma_b r, \tag{5.3}$$

where r and r' are the residuals corresponding to u and u'. Taking into account that $(r', u') = (r, u) = 0$, we shall square relation (5.3):

$$\|u'\|^2/\gamma_w^2\{1 + \gamma_w^2\|r'\|^2\} = 1 + \gamma_b^2\|r\|^2.$$

Since $\|u'\|^2/\gamma_w^2 = 1 - \gamma_b/\gamma_w = 1 + |\gamma_b|/|\gamma_w| > 1$, from the equality

$$1 + \gamma_w^2\|r'\|^2 = \{1 + |\gamma_b|/|\gamma_w|\}^{-1} + \{1 + |\gamma_b|/|\gamma_w|\}^{-1}\gamma_b^2\|r\|^2$$

immediately follows the inequality

$$\frac{\|r'\|^2}{\|r\|^2} < \frac{\gamma_b^2/\gamma_w^2}{1 + |\gamma_b|/|\gamma_w|}.$$

By virtue of (4.6) we have

$$\frac{\gamma_b^2/\gamma_w^2}{1 + |\gamma_b|/|\gamma_w|} \le \frac{1}{2} \tag{5.4}$$

from which inequality (5.1) follows.□

This theorem shows that the CRQI method improves the property of monotonicity of the residuals

$$\frac{\|r_{k+1}\|}{\|r_k\|} \le 1$$

which is true for the conventional RQI method [6].

The very fact that the residual norms tend to zero does not guarantee convergence, since, unlike the monotone RQI method, the combined RQI method does not ensure the monotonicity of the Rayleigh quotient ρ_k. For proving the convergence we may apply

Lemma 5.1. *Assume that u_k and ρ_k are sequences obtained by the CRQI method (4.5), then,* $\lim_{k\to\infty} |\rho_{k+1} - \rho_k| = 0$.

Proof. For the residual $\rho_k = Au_k - \rho_k u_k = B_k^{-1}u_k$ we have

$$\|\rho_k\|\,\|B_k u_k\| \ge (r_k, B_k u_k) = (B^{-1}u_k, B_k u_k) = (u_k, u_k) = 1.$$

Since $|\gamma_{kw}| \ge \|B_k u_k\|$, by virtue of (4.6), we conclude

$$|\rho_{k+1} - \rho_k| = \frac{1}{|\gamma kw} \le \|r_k\|.\square$$

From Theorem 5.1 and Lemma 5.1 follows

Theorem 5.2. *Regardless of the choice of the initial approximation u_0, a sequence of Rayleigh quotients ρ_k obtained by the CRQI method* (4.5) *converges to a certain eigenvalue of the matrix A.*

In conclusion, we shall give

Proof of Theorem 3.2.

Note that for $(B_k u_k, u_k) > 0$ in (2.8) the iterations in the RQI+ method (2.8) and the CRQI method (4.5) coincide, and for the latter Theorem 5.1 is true.□

6 Influence of the Choice of ρ_k on the Course of the CRQI Method

It is possible that the value ρ_0 in the CRQI method does not coincide with the Rayleigh quotient on the vector u_0 but is chosen from some other considerations. Then, the subsequent values ρ_k are not Rayleigh quotients on the vectors u_k either.

We shall study the sensitivity of the CRQI method to the choice of ρ_k.

Let us write a single step in the CRQI method (4.5) with a perturbation in ρ_k in the form

$$u' = \tau(\tilde{B}u + \gamma_b u), \quad \tilde{\rho}' = \tilde{\rho} - 1/\gamma_w, \quad \tau = (\gamma_w(\gamma_w - \gamma_b))^{-\frac{1}{2}}, \quad \|u\| = 1,$$

where $\tilde{B}u = (A - \tilde{\rho}I)^{-1}u$, γ_b and γ_w are determined by formulas (4.3), replacing Bu by $\tilde{B}u$ in (2.2),(4.4), and $\tilde{\rho}$ is a certain quantity which, generally speaking, does not coincide with the Rayleigh quotient on the vector u. Suppose that the matrix $A - \tilde{\rho}I$ is nondegenerate. Since $\|u'\|^2 = \tau^{-1}$, as in (2.6), we obtain by analogy with (2.1) and (2.4):

$$\rho' = \rho(u') = \tilde{\rho}' + \frac{\gamma_b^2/\gamma_w^2}{1 + |\gamma_b|/|\gamma_w|}(\rho - \tilde{\rho}).$$

In spite of replacing Bu by $\tilde{B}u$ in (2.2), (4.4), relations (4.6) and (4.6) remain valid. We conclude that

$$|\rho' - \tilde{\rho}'| \leq \frac{1}{2}|\rho - \tilde{\rho}|.$$

Hence, in the CRQI method the error in choosing ρ_0 is eliminated in the course of iterations, and possible errors in the computation of ρ_k do not accumulate. This conclusion was validated in the numerical experiments.

7 Discussion of the Numerical Results

A number of numerical experiments on model problems in order to compare the efficiency of the classic RQI method and the CRQI method were conducted. Since the time required for a single iteration is the same both in the CRQI and RQI methods, only the rate of convergence for an identical initial approximation was compared.

While computing the maximum and minimum eigenvalues within the computer accuracy, 5-8 iterations were characteristic of the RQI method, whereas one or two fewer iterations were required in the CRQI method.

In the computation of the eigenvalues in the middle of the spectrum, the number of iterations increased, and CRQI was often even second to the RQI method.

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