A modified block Newton iteration for approximating an invariant subspace of a symmetric matrix

Ralf Lösche [1], Hubert Schwetlick*, Gisela Timmermann [1]

Technische Universität Dresden, Institut für Numerische Mathematik, 01062 Dresden, Germany

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Abstract

In this paper we propose a *Modified Block Newton Method* (MBNM) for approximating an invariant subspace $\mathscr{S}$ and the corresponding eigenvalues of a symmetric matrix A. The method generates a sequence of matrices $Z^{(k)}$ which span subspaces $\mathscr{S}_k$ approximating $\mathscr{S}$. The matrices $Z^{(k)}$ are calculated via a Newton step applied to a special formulation of the block eigenvalue problem for the matrix A, followed by a Rayleigh–Ritz step which also yields the corresponding eigenvalue approximations. We show that for sufficiently good initial approximations the subspaces $\mathscr{S}_k$ converge to $\mathscr{S}$ in the sense that $\sin \varphi_k$ with $\varphi_k := \angle(\mathscr{S}_k, \mathscr{S})$ Q-quadratically converges to zero under appropriate conditions.   © 1998 Elsevier Science Inc. All rights reserved.

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1. Introduction

This paper is concerned with the approximation of an invariant subspace $\mathscr{S}$ of a symmetric matrix A which belongs to an arbitrary set of eigenvalues provid-

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* Corresponding author.
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ed that this set is sufficiently separated from the rest of the spectrum and that a sufficiently good initial approximation to the target subspace is available.

The background for our studies are continuation techniques, see, e.g., [1,9]. These methods are used for solving parameter dependent nonlinear equations

$$H(u,t) = 0 \quad \text{with} \quad H: \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n. \tag{1}$$

In general, the solution set $\mathscr{L} = \{(u,t): H(u,t) = 0\}$ of (1) consists of one-dimensional paths. The invariant subspace corresponding to the zero eigenvalues of $A := \partial_u H(u,t)$ is needed to obtain information about the occurrence of singular points as, e.g., turning points, or simple bifurcation points. In order to detect, classify, and compute such singular points this invariant subspace has to be tracked along the solution path. Moreover, for some practically relevant classes of problems (1), the matrix A has only a few negative eigenvalues. So it makes sense to split A into a large positive definite part and a small part which corresponds to the negative, zero and small positive eigenvalues, see [10]. The related eigenvalue problem can be described as follows: For an one-parametric family of symmetric matrices $\{A(s) = \partial_u H(u(s), t(s))\}$ with $A(.): \mathbb{R} \to \mathbb{R}^{n,n}$ sufficiently smooth, find approximations to the invariant subspace $\mathscr{S}(s)$ corresponding to all nonpositive and a few small positive eigenvalues of $A(s)$. Starting at $(u_0, t_0) = (u(s_0), t(s_0)) \in \mathscr{L}$, an approximation to the subspace $\mathscr{S}(s_0)$ can be computed by subspace iteration, inverse subspace iteration, or Lanczos methods. Along the solution path the invariant subspace should be tracked by a local, fast convergent method. This directly leads to Newton-type methods which have superior local convergence properties over standard approaches like subspace iteration or Lanczos methods; for a discussion of the latter methods, see, e.g., [7]. Moreover, in the context of path following we can almost always provide sufficiently good initial approximations to ensure convergence.

Let A be a symmetric matrix and let the spectral decomposition of A be given by

$$AU = U\Lambda \quad \text{with a splitting} \quad U = [U_1|U_2], \quad \Lambda = \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix}, \tag{2}$$

where U is orthogonal, $U_1 \in \mathbb{R}^{n,p}, U_2 \in \mathbb{R}^{n,q}, p + q = n$. This implies

$$\begin{aligned} \Lambda_1 &= U_1^\mathsf{T} A U_1 &= \text{diag}(\lambda_1, \ldots, \lambda_p) \in \mathbb{R}^{p,p}, \\ \Lambda_2 &= U_2^\mathsf{T} A U_2 &= \text{diag}(\lambda_{p+1}, \ldots, \lambda_n) \in \mathbb{R}^{q,q}. \end{aligned}$$

We assume that the number q of columns in U_2 is small compared with the dimension n of the matrix A. Our aim is to find a set of vectors $Z = \{z_1, \ldots, z_q\}$, such that $\operatorname{im} Z \approx \operatorname{im} U_2 =: \mathscr{S}$.

Let z be an eigenvector of A with $\|z\| = 1$ and let μ be the corresponding eigenvalue. If not otherwise specified, the norm is always the Euclidean vector norm or the spectral norm of a matrix. Then the eigenpair (z, μ) satisfies

$$F(z, \mu) = \begin{bmatrix} Az - \mu z \\ z^\mathsf{T} z - 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{3}$$

This is a quadratic system of equations. In [6] it is shown, that (z, μ) is a regular solution of (3) in the sense that the Jacobian $\partial F(z, \mu)$ is nonsingular if and only if μ is a simple eigenvalue of A. Hence, if μ is simple, Eq. (3) can be solved by applying Newton's method as has been done by Unger, see [12]. The z-part of Newton's method is essentially equivalent to applying one step of inverse iteration with the shift μ_k where μ_k is the kth approximation to μ, see again [6]. By the way, the relation between both approaches has already been discussed in the classic text book [14] published in 1953.

Hence, if Λ_2 only consists of simple eigenvalues, each of them can be approximated individually by applying Newton's method to (3). However, if Λ_2 contains multiple or clustered eigenvalues, Newton's method will fail or have a very small region of convergence since the condition number of the Newton equations will be large. So we are looking for a block generalization which allows to handle multiple or clustered eigenvalues simultaneously as in standard subspace iteration techniques.

A straightforward generalization of (3) is

$$F(Z, M) = \begin{bmatrix} AZ - ZM \\ Z^\mathsf{T}Z - I_q \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \tag{4}$$

where $Z \in \mathbb{R}^{n \cdot q}, M \in \mathbb{R}^{q \cdot q}$, and $q > 1$. Suppose that Z with rank $Z = q$ spans the invariant subspace im U_2 belonging to Λ_2. Then we have $Z = U_2 S$ with a nonsingular $S \in \mathbb{R}^{q \cdot q}$, and Z solves the first block $AZ - ZM = 0$ of (4) with $M = S^{-1}\Lambda_2 S$. The orthonormality condition of the second block requires $S^\mathsf{T} S = I_q$, i.e., S has to be orthogonal, and any orthogonal S yields a solution (Z, M) of (4). Thus, the solution set of (4) is not uniquely determined, and the Jacobian $\partial F(Z, M)$ is necessarily singular.

In order to avoid this difficulty, we replace the orthonormality condition by the biorthogonality condition $W^\mathsf{T}Z - I_q = 0$ with a fixed matrix $W \in \mathbb{R}^{n \cdot q}$, rank $W = q$. This leads to the system

$$F_W(Z, M) := \begin{bmatrix} AZ - ZM \\ W^\mathsf{T}Z - I_q \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{5}$$

with $F_W : \mathbb{R}^{n \cdot q} \times \mathbb{R}^{q \cdot q} \to \mathbb{R}^{n + q \cdot q}$. In this case, again, $(Z, M) = (U_2 S, S^{-1}\Lambda_2 S)$ with nonsingular S solves the first block of (5), and the biorthogonality condition of the second block leads to $W^\mathsf{T}U_2 S = I_q$. Under the additional assumption

$$W_2 := W^\mathsf{T}U_2 \quad \text{nonsingular}, \tag{6}$$

S is uniquely determined as $S = W_2^{-1}$ so that (5) is solved by

$$Z_W^* = U_2 W_2^{-1}, \qquad M_W^* = W_2 \Lambda_2 W_2^{-1}. \tag{7}$$

When applying Newton's method to Eq. (5), one obtains the iteration

$$\bar{Z}^{(k+1)} = \bar{Z}^{(k)} - \Delta Z^{(k)}, \qquad \bar{M}^{(k+1)} = \bar{M}^{(k)} - \Delta M^{(k)} \tag{8}$$

with $(\Delta Z, \Delta M) := (\Delta Z^{(k)}, \Delta M^{(k)}) \in \mathbb{R}^{n,q} \times \mathbb{R}^{q,q}$ from the linearized equation

$$\partial F_W(\bar{Z}^{(k)}, \bar{M}^{(k)})(\Delta Z, \Delta M) = F_W(\bar{Z}^{(k)}, \bar{M}^{(k)}),$$

i.e., in each step one has to solve the linear system

$$\begin{aligned} A \, \Delta Z - \Delta Z \bar{M}^{(k)} - \bar{Z}^{(k)} \, \Delta M &= A \bar{Z}^{(k)} - \bar{Z}^{(k)} \bar{M}^{(k)}, \\ W^{\mathrm{T}} \Delta Z &= W^{\mathrm{T}} \bar{Z}^{(k)} - I_q. \end{aligned} \tag{9}$$

Note that the first block is a Sylvester equation with respect to ΔZ.

In general, Eq. (9) are coupled by the off-diagonal elements of $\bar{M}^{(k)}$ so that the efficient solution of the whole linear system causes difficulties. In order to avoid these problems we propose a *Modified Block Newton Method* (MBNM) which guarantees the matrices $\bar{M}^{(k)}$ to be diagonal so that (9) separates into q decoupled linear systems for the columns $\Delta z_i \in \mathbb{R}^n$ of ΔZ and $\Delta m_i \in \mathbb{R}^q$ of ΔM. Moreover, under appropriate assumptions, all these systems have uniformly bounded inverses.

This paper is organized as follows: In Section 2 the MBNM is described. A convergence analysis of the algorithm is given in Section 3. In Section 4 we provide some numerical examples illustrating the performance of the method and confirming the theoretical results from Section 3. Some conclusions are made in Section 5.

2. A modified block Newton method

As already mentioned in Section 1 one of the basic ideas of our approach is to work with iterates $(Z^{(k)}, M^{(k)})$ where the matrices $M^{(k)}$ are diagonal. This can be achieved by applying the modified Gram–Schmidt orthogonalization procedure followed by the Rayleigh–Ritz procedure to an arbitrary full rank approximation $\bar{Z}$. Recall that these two basic algorithms are defined as follows (for details see, e.g., [3] or [4]):

Modified Gram–Schmidt orthogonalization: $(\tilde{Z}, \tilde{R}) = \mathrm{orth}(\bar{Z})$

Input: $\bar{Z} \in \mathbb{R}^{n,q}$ with rank $\bar{Z} = q$
Output: $\tilde{Z} \in \mathbb{R}^{n,q}$ with $\tilde{Z}^{\mathrm{T}} \tilde{Z} = I_q, \tilde{R} \in \mathbb{R}^{q,q}$ upper triangular, $\bar{Z} = \tilde{Z}\tilde{R}$

Rayleigh–Ritz procedure: $(Z, M) = \mathrm{rr}(\tilde{Z})$

Input: $\tilde{Z} \in \mathbb{R}^{n,q}$ with $\tilde{Z}^{\mathrm{T}} \tilde{Z} = I_q$
Output: $Z \in \mathbb{R}^{n,q}, M = \mathrm{diag}(\mu_1, \ldots, \mu_q)$ with
            $\mathrm{im}\, Z = \mathrm{im}\, \tilde{Z}, Z^{\mathrm{T}} Z = I_q, M = Z^{\mathrm{T}} A Z$, i.e.,
            M is the diagonal matrix of Ritz values, and
            Z is the matrix of the corresponding Ritz vectors
            with respect to the subspace $\mathrm{im}\, \tilde{Z}$

Note that $\mathrm{im}\, \bar{Z} = \mathrm{im}\, \tilde{Z} = \mathrm{im}\, Z$.

We solve (9) starting with $(Z^{(k)}, M^{(k)})$, where $Z^{(k)}$ is orthonormal and $M^{(k)}$ is diagonal. However, we use only the Z-correction ΔZ to obtain $\bar{Z}^{(k+1)} = Z^{(k)} - \Delta Z$, but forget the M-correction ΔM. Instead, we apply the modified Gram–Schmidt orthogonalization procedure followed by the Rayleigh–Ritz procedure to get the new iterate $(Z^{(k+1)}, M^{(k+1)})$ with, again, orthonormal $Z^{(k+1)}$ and diagonal $M^{(k+1)}$. This is motivated by the fact that, for a given orthonormal basis, the Rayleigh–Ritz pairs are optimal in a certain sense, see [3,4].

Further, we choose the normalizing matrix W as $W = W^{(k)} := Z^{(k)}$ in iteration step k. Then the second block of (9) yields the simple orthogonality condition

$$Z^{(k)^{\mathrm{T}}} \Delta Z = 0. \tag{10}$$

Thus, we consider the sequence of problems

$$F_{W^{(k)}}(Z, M) := \begin{bmatrix} AZ - ZM \\ W^{(k)^{\mathrm{T}}} Z - I_q \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{$\mathrm{P_k}$}$$

with normalizing matrices $W = W^{(k)} := Z^{(k)}$ which change with k. Note that the problems $(\mathrm{P_k})$ have, in general, different solutions $(Z^*_{W^{(k)}}, M^*_{W^{(k)}})$ which depend on $W^{(k)}$, but all $Z^*_{W^{(k)}}$ span the same subspace $\mathscr{S} = \operatorname{im} U_2$, and all $M^*_{W^{(k)}}$ are similar to Λ_2 and so have the same eigenvalues $\sigma(\Lambda_2)$.

With these settings the Newton equations (9) reduce to the q decoupled systems

$$\begin{bmatrix} A - \mu_i^{(k)} I & Z^{(k)} \\ Z^{(k)^{\mathrm{T}}} & 0 \end{bmatrix} \begin{bmatrix} \Delta z_i^{(k)} \\ -\Delta m_i^{(k)} \end{bmatrix} = \begin{bmatrix} AZ^{(k)} - Z^{(k)} M^{(k)} \\ 0 \end{bmatrix} \mathbf{e}^i, \tag{11}$$

$i = 1, \ldots, q$, where $\mathbf{e}^i$ denotes the ith coordinate vector in $\mathbb{R}^q$.

Now we can formulate the algorithm.

Algorithm: *Modified Block Newton Method* (MBNM)
  Initialization:
    S0: Given an initial approximation $\bar{Z}^{(0)}$ with rank $\bar{Z}^{(0)} = q$,
       $\operatorname{im} \bar{Z}^{(0)} \approx \operatorname{im} U_2$, compute $(\tilde{Z}^{(0)}, \tilde{R}^{(0)}) = \mathtt{orth}(\bar{Z}^{(0)})$
       and $(Z^{(0)}, M^{(0)}) = \mathtt{rr}(\tilde{Z}^{(0)})$
       Set $k := 0$
  Iteration:
  while $\{Z^{(k)}$ does not satisfy a termination criterion$\}$
    S1: Determine the correction $\Delta Z^{(k)} = [\Delta z_1^{(k)}, \ldots, \Delta z_q^{(k)}]$ by solving the q
       decoupled linear systems (11)
    S2: Set $\bar{Z}^{(k+1)} := Z^{(k)} - \Delta Z^{(k)}$
    S3: Compute $(\tilde{Z}^{(k+1)}, \tilde{R}^{(k+1)}) = \mathtt{orth}(\bar{Z}^{(k+1)})$
    S4: Compute $(Z^{(k+1)}, M^{(k+1)}) = \mathtt{rr}(\tilde{Z}^{(k+1)})$
    S5: Set $k := k + 1$
  end

Note that for the special case $q = 1$ this algorithm reduces to the Rayleigh quotient iteration.

In the next section it will be shown that, under appropriate assumptions, all systems (11) have uniformly bounded inverses. This allows using iterative solvers in step S1 in the case that A is large and sparse. For a discussion of such methods which, in general, are of Krylov type, see, e.g., [2]. The subsequent steps S3 and S4 require $\sim nq^2$ and $\sim nq^2 + \sim q^3$ flops and, hence, have costs $O(n)$, since $q \ll n$. So the overall complexity of the algorithm is determined by the costs for solving the linear systems in step S1.

3. Convergence analysis

In this section the convergence behavior of the algorithm is investigated. We begin with the convergence analysis of the standard Newton iteration without the Rayleigh-Ritz procedure, applied to $F_W(Z, M) = 0$ with fixed W. We show that, for matrices W from a certain class B_{i_0}, there exists a uniformly regular solution of (5), and ∂F_W has a uniform Lipschitz constant. Then we apply a standard convergence result, see, e.g., [8]. Finally, we show that this result can be extended to the MBNM.

Throughout this section we assume that

(A1) the matrix $A \in \mathbb{R}^{n,n}$ be symmetric with spectral decomposition (2),

(A2) the spectra $\sigma(A_1)$ and $\sigma(A_2)$ be separated, i.e., $\sigma(A_1) \cap \sigma(A_2) = \emptyset$.

Assumption (A2) implies

$$\gamma := \min\{|\lambda_i - \lambda_j|: \ \lambda_i \in \sigma(A_1), \lambda_j \in \sigma(A_2)\} > 0 \tag{12}$$

for the *gap* γ between $\sigma(A_1)$ and $\sigma(A_2)$.

The convergence analysis of the MBNM strongly depends on the notion of the angle between subspaces. For two subspaces $\mathscr{X}, \mathscr{Y} \subset \mathbb{R}^n$, the *angle*, more precisely the *maximal angle* ϕ between $\mathscr{X}$ and $\mathscr{Y}$ is defined as

$$\phi = \angle(\mathscr{X}, \mathscr{Y}) := \max_{x \in \mathscr{X}}\{\min_{y \in \mathscr{Y}} \angle(x, y)\} \in \{0, \pi/2\},$$

where $\alpha = \angle(x, y)$ is the usual angle between two vectors x and y, i.e., $\alpha = \pi/2$ if $x^T y = 0$, and $\alpha \in [0, \pi]$ such that $\cos\alpha = x^T y / \|x\| \|y\|$, otherwise. In this paper we only consider subspaces $\mathscr{X}, \mathscr{Y}$ of equal dimension q, and for such subspaces one has $\angle(\mathscr{X}, \mathscr{Y}) = \angle(\mathscr{Y}, \mathscr{X}) = \angle(\mathscr{X}^\perp, \mathscr{Y}^\perp)$.

For characterizing and computing ϕ, let $X, X^\perp, Y, Y^\perp$ be orthonormal bases for $\mathscr{X}, \mathscr{X}^\perp, \mathscr{Y}, \mathscr{Y}^\perp$, respectively, such that the matrices $[X|X^\perp]$ and $[Y|Y^\perp]$ are orthogonal. Then $\|X^{\perp^T} Y\| \leqslant 1, \|X^T Y\| \leqslant 1$, and

$$\sin\phi = \|X^{\perp^T} Y\| = \|X^T Y^\perp\|. \tag{13}$$

$$\cos\phi = \begin{cases} 0 & \text{if } X^\mathsf{T}Y \text{ is singular,} \\ 1/\|(X^\mathsf{T}Y)^{-1}\| & \text{if } X^\mathsf{T}Y \text{ is nonsingular,} \end{cases} \tag{14}$$

where the norm is the spectral norm of a matrix. For a detailed discussion of the angle concept see, e.g., [3,11].

Throughout this section we identify $(X, Y) \in \mathbb{R}^{n,q} \times \mathbb{R}^{q,q}$ with $\begin{bmatrix} X \\ Y \end{bmatrix} \in \mathbb{R}^{n+q,q}$, and the spectral norm is denoted by $\|(X, Y)\|$ or $\left\| \begin{matrix} X \\ Y \end{matrix} \right\|$.

First we show that the Jacobian $\partial F_W(Z_W^*, M_W^*)$ has a uniformly bounded inverse if $\measuredangle(\mathrm{im}\,W, \mathrm{im}\,U_2)$ is bounded from $\pi/2$, cf. [5].
We define $\psi := \measuredangle(\mathrm{im}\,W, \mathrm{im}\,U_2)$ and

$$B_\varepsilon(U_2) := \{W \in \mathbb{R}^{n,q} : W^\mathsf{T}W = I_q, \sin\psi \leqslant \varepsilon\}.$$

Lemma 3.1. *Let* $(Z^*, M^*) := (Z_W^*, M_W^*)$ *be the solution of (5) given by (7). Let* $W \in B_{\varepsilon_0}(U_2)$ *with* $\varepsilon_0 < 1$. *Then the Jacobian* $\partial F^* := \partial F_W(Z_W^*, M_W^*)$ *is nonsingular, and there holds*

$$\|(\partial F^*)^{-1}\| \leqslant C \quad \forall W \in B_{\varepsilon_0}(U_2). \tag{15}$$

Proof. We will show that all solutions of

$$\begin{aligned} A\,\Delta Z - \Delta Z\,M^* - Z^*\Delta M &= X, \\ W^\mathsf{T}\Delta Z &= Y, \end{aligned} \tag{16}$$

with right-hand sides (X, Y) such that $\|(X, Y)\| \leqslant 1$ are bounded by a constant C which does not depend on W. Note that the condition $\|(X, Y)\| \leqslant 1$ implies $\|X\| \leqslant 1, \|Y\| \leqslant 1$.

Premultiplying U^T on the first equation of (16), rewriting the second equation of (16), and using (2) we obtain

$$AU^\mathsf{T}\Delta Z - U^\mathsf{T}\Delta Z M^* - U^\mathsf{T}Z^*\Delta M = U^\mathsf{T}X, \tag{17}$$

$$W^\mathsf{T}UU^\mathsf{T}\Delta Z = Y. \tag{18}$$

Using $\Delta Z_l := U_l^\mathsf{T}\Delta Z, X_l := U_l^\mathsf{T}X, W_l := W^\mathsf{T}U_l, l = 1, 2$, and (7) we then rewrite the above two Eqs. (17) and (18) in block form as:

$$A_1\,\Delta Z_1 - \Delta Z_1 M^* = X_1, \tag{19}$$

$$A_2\,\Delta Z_2 - \Delta Z_2 M^* - W_2^{-1}\Delta M = X_2, \tag{20}$$

$$W_1\,\Delta Z_1 + W_2\,\Delta Z_2 = Y. \tag{21}$$

Applying the results in [11] (p. 245, Exercises 1–4) on Eq. (19) yields

$$\|\Delta Z_1\| \leqslant \|\Delta Z_1\|_F \leqslant \frac{\|X_1\|_F}{\mathrm{sep}(A_1, M^*)} \leqslant \frac{\|X_1\|_F \|W_2\| \|W_2^{-1}\|}{|\sigma(A_1) - \sigma(M^*)|} \leqslant \frac{\sqrt{q}}{\gamma\cos\psi},$$

where $\text{sep}(A, B) := \min\{\|AX - XB\|_F \colon \|X\|_F = 1\} \leqslant \min |\sigma(A) - \sigma(B)|$.
Using (20) we obtain $\Delta Z_2 = W_2^{-1}(Y - W_1 \Delta Z_1)$, and

$$\|\Delta Z_2\| \leqslant \|W_2^{-1}\|(\|Y\| + \|W_1\| \|\Delta Z_1\|) \leqslant \frac{1}{\cos\psi}\left(1 + \frac{\sqrt{q}}{\gamma \cos\psi}\right).$$

By (20) and (21) we have $\Delta M = M^*(Y - W_1 \Delta Z_1) - (Y - W_1 \Delta Z_1)M^* - W_2 X_2$. Hence,

$$\|\Delta M\| \leqslant 2\|M^*\|(1 + \|\Delta Z_1\|) + 1 \leqslant \frac{2\|\Lambda_2\|}{\cos\psi}\left(1 + \frac{\sqrt{q}}{\gamma \cos\psi}\right) + 1.$$

Finally,

$$\|(\Delta Z, \Delta M)\| \leqslant \|\Delta Z_1\| + \|\Delta Z_2\| + \|\Delta M\| \leqslant 1 + \frac{\sqrt{q}}{\gamma \cos\psi}$$
$$+ \frac{1 + 2\|\Lambda_2\|}{\cos\psi}\left(1 + \frac{\sqrt{q}}{\gamma \cos\psi}\right) \leqslant C,$$

since $W \in B_{\varepsilon_0}(U_2)$, i.e. $\sin\psi \leqslant \varepsilon_0 < 1$ or $\psi \leqslant \vartheta < \pi/2$ with $\sin\vartheta = \varepsilon_0$.   □

Next we show that ∂F_W is Lipschitz continuous. Since F_W contains the only quadratic term $-ZM$, the second derivative is given by

$$\partial^2 F_W(Z, M)[(X_1, Y_1), (X_2, Y_2)] = -(X_1 Y_2 + X_2 Y_1, 0)$$

which implies

$$\|\partial^2 F_W(Z, M)\| \leqslant 2 \quad \forall (Z, M) \ \forall W,$$

and $L := 2$ is a Lipschitz constant for ∂F_W.

Thus, both the Lipschitz constant L of ∂F_W and the bound C for the inverse of $\partial F_W(Z_W^*, M_W^*)$ do not depend on the special choice of $W \in B_{\varepsilon_0}(U_2)$. Therefore, we can exploit well-known local convergence results for the Newton method, see, e.g., [8], applied to (5) *uniformly* with respect to $W \in B_{\varepsilon_0}(U_2)$.
We define $e^k := (\bar{Z}^{(k)} - Z_W^*, \bar{M}^{(k)} - M_W^*)$.

Proposition 3.2. *Let (A1), (A2) be satisfied. Then, for any $\varepsilon_0 < 1$ there exist constants $Q > 0$ and $\delta > 0$ with $\kappa := Q\delta < 1$ such that, for arbitrary fixed $W \in B_{\varepsilon_0}(U_2)$, there holds*
i) the matrix $W_2 = W^\mathsf{T} U_2$ is nonsingular,
ii) Eq. (5) is solved by $(Z_W^*, M_W^*) = (U_2 W_2^{-1}, W_2 \Lambda_2 W_2^{-1})$, and this solution is unique in the ball around (Z_W^*, M_W^*) with radius δ,
iii) Newton's method applied to (5) is well defined and generates a sequence $(\bar{Z}^{(k)}, \bar{M}^{(k)})$ such that

$$\|e^{k+1}\| \leqslant Q\|e^k\|^2 \leqslant \kappa\|e^k\|, \tag{22}$$

$k = 0, 1, \ldots,$ *provided that the initial pair* $(\bar{Z}^{(0)}, \bar{M}^{(0)})$ *satisfies*

$$\|e^0\| \leqslant \delta. \tag{23}$$

Especially, all Jacobians $\partial F_W(\bar{Z}^{(k)}, \bar{M}^{(k)})$ *are nonsingular.*

For the remainder of this section we fix $\varepsilon_0 < 1$, and $Q, \delta, \kappa = Q\delta < 1$ are supposed to be the constants from Proposition 3.2 which belong to this ε_0. For simplicity of notation we, further, define $\vartheta \in [0, \pi/2)$ by $\sin \vartheta = \varepsilon_0$.

In the MBNM, at iteration step k we perform only one standard Newton step for (5) using the normalizing matrix $W = W^{(k)} = Z^{(k)}$ and starting from the Ritz pair $(\bar{Z}^{(0)}, \bar{M}^{(0)}) := (Z^{(k)}, M^{(k)})$. For this case Proposition 3.2 states that, if $Z^{(k)} \in B_{\varepsilon_0}(U_2)$ and

$$\left\| \begin{matrix} Z^{(k)} - Z^*_{Z^{(k)}} \\ M^{(k)} - M^*_{Z^{(k)}} \end{matrix} \right\| \leqslant \delta, \tag{24}$$

then $\partial F_{Z^{(k)}}(Z^{(k)}, M^{(k)})$ is nonsingular, and the first Newton iterate

$$\bar{Z}^{(k+1)} = Z^{(k)} - \Delta Z^{(k)}, \qquad \bar{M}^{(k+1)} = M^{(k)} - \Delta M^{(k)}$$

is well defined and satisfies

$$\|\bar{Z}^{(k+1)} - Z^*_{Z^{(k)}}\| \leqslant \left\| \begin{matrix} \bar{Z}^{(k+1)} - Z^*_{Z^{(k)}} \\ \bar{M}^{(k+1)} - M^*_{Z^{(k)}} \end{matrix} \right\| \leqslant Q \left\| \begin{matrix} Z^{(k)} - Z^*_{Z^{(k)}} \\ M^{(k)} - M^*_{Z^{(k)}} \end{matrix} \right\|^2. \tag{25}$$

We want to prove an analogous result for the sines of the angles

$$\varphi_k := \measuredangle(\operatorname{im} Z^{(k)}, \operatorname{im} U_2), \quad \varphi_{k+1} := \measuredangle(\operatorname{im} Z^{(k+1)}, \operatorname{im} U_2).$$

First we show that condition (24) can be satisfied for sufficiently small $\sin \varphi_k$.

Lemma 3.3. *Let* $\varphi := \measuredangle(\operatorname{im} Z, \operatorname{im} U_2)$ *and* $M := Z^T A Z$. *Then*

$$\|Z - Z^*_Z\| \leqslant \frac{\sin \varphi}{\cos \varphi}, \tag{26}$$

$$\|M - M^*_Z\| \leqslant \left(\|\Lambda_1\| + \frac{\|\Lambda_2\|}{\cos \varphi} \right) \sin^2 \varphi. \tag{27}$$

Proof. Let $Z^\perp \in \mathbb{R}^{n, n-q}$ be an orthonormal basis of $(\operatorname{im} Z)^\perp$ such that the matrix $[Z|Z^\perp]$ is orthogonal. By $W_l := Z^T U_l, W_l^\perp := Z^{\perp T} U_l, l = 1, 2,$ and (7) with $W = Z$ we have

$$Z - Z^*_Z = -(I - ZZ^T)U_2 W_2^{-1} = -Z^\perp W_2^\perp W_2^{-1}.$$

Using (14) this implies

$$\|Z - Z^*_Z\| \leqslant \|Z^\perp\| \|W_2^\perp\| \|W_2^{-1}\| \leqslant \frac{\sin \varphi}{\cos \varphi}.$$

Analogously we obtain

$$
\begin{aligned}
M - M_Z^* &= W_1 \Lambda_1 W_1^{\mathrm{T}} + W_2 \Lambda_2 (W_2^{\mathrm{T}} W_2 - I) W_2^{-1} \\
&= W_1 \Lambda_1 W_1^{\mathrm{T}} - W_2 \Lambda_2 W_2^{\perp \mathrm{T}} W_2^{\perp} W_2^{-1},
\end{aligned}
$$

and, hence, by (13) and (14)

$$
\| M - M_Z^* \| \leqslant \left(\| \Lambda_1 \| + \frac{\| \Lambda_2 \|}{\cos \varphi} \right) \sin^2 \varphi. \qquad \square
$$

If we define

$$
\varepsilon_1 := \min \left\{ \varepsilon_0, \frac{\delta}{\tau} \right\}, \qquad \tau := \frac{1}{\cos \vartheta} + \left(\| \Lambda_1 \| + \frac{\| \Lambda_2 \|}{\cos \vartheta} \right) \sin \vartheta. \tag{28}
$$

and choose $Z^{(k)} \in B_{\varepsilon_1}(U_2)$, then from Lemma 3.3 we obtain

$$
\left\| \begin{matrix} Z^{(k)} - Z_{Z^{(k)}}^* \\ M^{(k)} - M_{Z^{(k)}}^* \end{matrix} \right\| \leqslant \tau \sin \varphi_k \leqslant \delta. \tag{29}
$$

Hence, Proposition 3.2 guarantees $\bar{Z}^{(k+1)}$ to be well defined and to satisfy

$$
\| \bar{Z}^{(k+1)} - Z_{Z^{(k)}}^* \| \leqslant Q\tau^2 \sin^2 \varphi_k \leqslant \kappa\tau \sin \varphi_k. \tag{30}
$$

Next we show that $\sin \varphi_{k+1}$ is bounded by a certain multiple of $\sin^2 \varphi_k$. Define

$$
\varepsilon_2 := \min \left\{ \varepsilon_1, \frac{1}{2\omega} \right\}, \quad \omega := \tau(1 + \kappa). \tag{31}
$$

Lemma 3.4. *For* $Z^{(k)} \in B_{\varepsilon_2}(U_2)$ *there holds*

$$
\sin \varphi_{k+1} \leqslant \frac{2\sqrt{3}}{3} Q\tau^2 \sin^2 \varphi_k. \tag{32}
$$

Proof. First we show that $\tilde{R}^{(k+1)}$ from Gram–Schmidt orthogonalization in step S3 of MBNM is nonsingular.

Recall that $\bar{Z}^{(k+1)} = \tilde{Z}^{(k-1)} \tilde{R}^{(k+1)}$ with $\tilde{Z}^{(k+1)^{\mathrm{T}}} \tilde{Z}^{(k+1)} = I_q$. From step S2 of MBNM and the orthogonality condition (10) we obtain

$$
\tilde{R}^{(k+1)^{\mathrm{T}}} \tilde{R}^{(k+1)} = \bar{Z}^{(k+1)^{\mathrm{T}}} \bar{Z}^{(k+1)} = I_q + F^{(k)} \tag{33}
$$

with $F^{(k)} := \Delta Z^{(k)^{\mathrm{T}}} \Delta Z^{(k)}$. Using (29), (30) and (31) we get

$$
\| \Delta Z^{(k)} \| \leqslant \| \bar{Z}^{(k+1)} - Z_{Z^{(k)}}^* \| + \| Z^{(k)} - Z_{Z^{(k)}}^* \| \leqslant \omega \sin \varphi_k \leqslant \frac{1}{2}
$$

and, hence,

$$
\| F^{(k)} \| \leqslant \| \Delta Z^{(k)} \|^2 \leqslant \frac{1}{4}. \tag{34}
$$

Thus, by the perturbation lemma $I_q + F^{(k)} = \tilde{R}^{(k+1)^T} \tilde{R}^{(k+1)}$ is nonsingular, and

$$\|\tilde{R}^{(k+1)^{-1}}\| = \|(I_q + F^{(k)})^{-1}\|^{1/2} \leqslant \left(\frac{1}{1 - \|F^{(k)}\|} \right)^{1/2} \leqslant \frac{2\sqrt{3}}{3}.$$

Finally, using $\tilde{Z}^{(k+1)} = \bar{Z}^{(k+1)} \tilde{R}^{(k+1)^{-1}}$ and (7) for $W = Z^{(k)}$ we rewrite $U_1^T \tilde{Z}^{(k+1)} = U_1^T (\bar{Z}^{(k+1)} - Z^*_{Z^{(k)}}) \tilde{R}^{(k+1)^{-1}}$. By (13) and (30) we end up with

$$\sin \varphi_{k+1} = \|U_1^T \tilde{Z}^{(k-1)}\| \leqslant \frac{2\sqrt{3}}{3} Q \tau^2 \sin^2 \varphi_k. \qquad \square$$

Now we set

$$\varepsilon_3 := \min \left\{ \varepsilon_2, \frac{\sqrt{3}}{2} \frac{\delta}{\tau^2} \right\} \tag{35}$$

and choose $Z^{(k)} \in B_{\varepsilon_3}(U_2)$. Then from (32) it follows that

$$\sin \varphi_{k+1} \leqslant \frac{2\sqrt{3}}{3} Q \tau^2 \varepsilon_3 \sin \varphi_k \leqslant \kappa \sin \varphi_k,$$

where $\kappa = Q \delta < 1$. Hence, if $Z^{(k)} \in B_{\varepsilon_3}(U_2)$ is satisfied for $k = 0$ which means that $\varphi_0 = \angle (\operatorname{im} \bar{Z}^{(0)}, \operatorname{im} U_2)$ satisfies $\sin \varphi_0 \leqslant \varepsilon_3$, then, by induction, the whole sequence $\{Z^{(k)}\}$ is well-defined, and $\sin \varphi_k$ goes to zero at least Q-linearly with factor $\kappa < 1$ and, moreover, Q-quadratically.

Summarizing the results proved above and setting

$$\varepsilon := \varepsilon_3 = \min \left\{ \varepsilon_0, \frac{\delta}{\tau}, \frac{1}{2\omega}, \frac{\sqrt{3}}{2} \frac{\delta}{\tau^2} \right\}, \quad \bar{Q} := \frac{2\sqrt{3}}{3} Q \tau^2$$

with fixed ε_0, constants $Q, \delta, \kappa = Q\delta < 1$ from Proposition 3.2, τ from (28), ω from (31), we obtain the following convergence theorem.

Theorem 3.5. *Suppose (A1), (A2) to be satisfied. Then there exist constants $\varepsilon \in (0,1)$ and $\bar{Q} > 0$ such that*
   i) MBNM is well defined for all initial approximations $\bar{Z}^{(0)} \in B_\varepsilon(U_2)$, i.e., for all $\bar{Z}^{(0)}$ with

$$\sin \varphi_0 = \sin \angle (\operatorname{im} \bar{Z}^{(0)}, \operatorname{im} U_2) \leqslant \varepsilon,$$

and for all k we have $Z^{(k)} \in B_\varepsilon(U_2)$,
   ii) there holds $\lim_{k \to \infty} \sin \varphi_k = 0$,
   iii) the convergence is Q-quadratic in the sense of

$$\sin \varphi_{k+1} \leqslant \bar{Q} \sin^2 \varphi_k \quad \forall k.$$

4. Numerical results

The algorithm MBNM has been tested on several examples of different sizes and spectra. As test matrices we used the 21×21 Wilkinson matrix, see [13], and the 21×21 Dingdong matrix from a MATLAB test matrix suite. The eigenvalues of these matrices are listed in Tables 1 and 2. The spectrum of the Wilkinson matrix contains no multiple eigenvalues, but clusters. The Dingdong matrix has multiple eigenvalues and clusters near $\pi/2$ and $-\pi/2$.

Further, we used a 961×961 Poisson matrix which corresponds to a discretization of the 2D-Laplacian on $[0, 1] \times [0, 1]$ with an equidistant grid of stepsize $h_x = h_y = h = 1/N$, $N = 32$. The eigenvalues $\lambda_{i,j}$ and the corresponding eigenvectors $z_{i,j}^{k,l}$ of the Poisson matrix are given by

$$
\begin{aligned}
\lambda_{i,j} &= 4 \sin^2\left(\tfrac{i\pi}{2N}\right) + 4 \sin^2\left(\tfrac{j\pi}{2N}\right) \\
z_{i,j}^{k,l} &= \sqrt{2} \sin\left(\tfrac{ik\pi}{N}\right) \sin\left(\tfrac{jl\pi}{N}\right) \qquad i,j,k,l = 1, \ldots, N-1.
\end{aligned}
$$

From the theory developed in the previous Section 3 we expect that the convergence behavior of the MBNM is mainly influenced by the gap γ of the spectrum and the quality of the initial basis $\bar{Z}^{(0)}$ measured by the angle φ_0 between $\operatorname{im} \bar{Z}^{(0)}$ and $\operatorname{im} U_2$. Therefore, we tested the method for its sensitivity with respect to these parameters.

A second aim of our test computations was the following: For updating an approximation to an invariant subspace by Newton-type methods there are basically two possibilities, namely the simultaneous updating of all directions using MBNM, or the individual updating of each eigenpair approximation by the standard Newton method applied to (3). We compared the convergence behavior of these methods. We also monitored the condition number of the matrices of the linear systems to be solved in both approaches.

Finally, we wanted to compare the MBNM with linearly convergent methods like direct or inverse subspace iteration. However, by using the latter methods only special sets of eigenvalues and subspaces can be computed. When using subspace iteration, the target eigenvalues have to be the dominant ones. Then, no linear systems have to be solved, and the convergence is linear with rate $|\lambda_{q+1}|/|\lambda_q|$, if the eigenvalues are numbered according to $|\lambda_n| \leqslant \cdots \leqslant |\lambda_{q+1}| < |\lambda_q| \leqslant \cdots \leqslant |\lambda_1|$. In the path following example mentioned in Section 1 the target set $\sigma(\Lambda_2)$ consists of all negative, zero and a few small positive eigenvalues. These eigenvalues can be made to (negative) dominant ones by a shift $A - \alpha I$ with appropriate $\alpha > 0$; in the simplest but not optimal case choose $\alpha \geqslant \rho(A)$. On the other hand, if the eigenvalues close to a given reference point $\beta \in \mathbb{R}$ are needed, inverse subspace iteration with $A - \beta I$ may be performed, which requires solving q linear systems with this matrix per step. For large scale problems (which we have in mind) iterative solvers are a must, and then the fixed shift β brings no gain over our MBNM with varying shifts

Table 1
Wilkinson matrix

i	λ_i
1	−1.1254415221199
2	0.2538058170966
3	0.9475343675292
4	1.7893213526950
5	2.1302092193625
6	2.9610588841857
7	3.0430992925788
8	3.9960482013836
9	4.0043540234408
10	4.9997824777429
11	5.0002444250019
12	6.0002175222571
13	6.0002340315841
14	7.0039517986163
15	7.0039522095286
16	8.0389411158142
17	8.0389411228290
18	9.2106786473049
19	9.2106786473613
20	10.7461941829033
21	10.7461941829033

since every system has to be solved separately. However, the coefficient matrices of MBNM have bounded condition numbers whereas the matrix $A - \beta I$ of inverse iteration will have large condition if β is close to an eigenvalue. The latter property will cause difficulty for the iterative solver, in general. Of course, if the dimension n is moderate and LU factorization can be computed, MBNM requires q such factorizations per step whereas in inverse iteration with fixed shift β only one factorization is needed in the beginning. However, the convergence will be slow, in general, since, unlike in the case $q = 1$, one shift β cannot approximate $q > 1$ eigenvalues of A simultaneously. Therefore, the observed fast convergence of inverse iteration in the case of $q = 1$ and good eigenvalue approximation β will be lost, in general.

In our test examples we used randomly perturbed exact eigenvectors of the matrix A as initial approximations. The computations demonstrate that sufficiently good initial approximations are needed to ensure convergence. How good these initial approximations have to be depends on the problem. As always for Newton type methods, there are, in general, no easily computable criteria for checking the quality of the initial approximation $Z^{(0)}$, so one has to use some heuristic strategies. For instance, if after a fixed number of Newton steps a reasonable convergence criterion is not satisfied, the initial approximations

Table 2
Dingdong matrix

i	λ_i
1	−1.570796326795
2	−1.570796326795
3	−1.570796326795
4	−1.570796326795
5	−1.570796326794
6	−1.570796326351
7	−1.570796142764
8	−1.570754532538
9	−1.565796135236
10	−1.318181891827
11	0.581130731802
12	1.529806267375
13	1.570298247299
14	1.570793333979
15	1.570796317052
16	1.570796326777
17	1.570796326795
18	1.570796326795
19	1.570796326795
20	1.570796326795
21	1.570796326795

should be improved by alternative methods which possess better global convergence properties like linearly convergent methods such as subspace iteration or inverse subspace iteration with appropriate shifts, see the discussion above. MBNM can also be used to refine eigenpair approximations obtained by Lanczos type methods.

All computations were done using MATLAB.

Problem 1 (*Wilkinson matrix*). In a first setup we split the spectrum between $\lambda_{17} = 8.038$ and $\lambda_{18} = 9.210$ such that $q = 4$ and

$$\sigma(\Lambda_1) = \{\lambda_1, \ldots, \lambda_{17}\},$$
$$\sigma(\Lambda_2) = \{\lambda_{18}, \ldots, \lambda_{21}\},$$
$$\gamma = 1.172.$$

The results of MBNM are shown in Table 3. We carried out three tests with different φ_0. The table shows the sine of φ_0, the spectral norm $\|R_0\|$ of the initial residual $R_0 := AZ^{(0)} - Z^{(0)}M^{(0)}$, the number K of Newton steps performed, the maximum of the condition numbers over all linear systems solved, the sine of $\varphi^* = \varphi_K$ when the iteration terminated, and the spectral norm $\|R^*\|$ of the corresponding residual.

Table 3
Setup 1 – MBNM

Test	$\sin\varphi_0$	$\|R_0\|$	K	$\text{cond}(\partial F)$	$\sin\varphi^*$	$\|R^*\|$
1	0.631	3.65	9	1.83×10^{11}	1.00	9.61×10^{-14}
2	0.568	2.93	5	4.44×10^1	2.11×10^{-8}	8.62×10^{-11}
3	0.351	1.50	4	2.41×10^1	2.98×10^{-8}	1.45×10^{-14}

In Test 1 MBNM actually found an invariant subspace which can be seen from the almost vanishing $\|R^*\|$. However, this subspace contains a direction orthogonal to the target subspace since $\sin\varphi^* = 1.0$.

In Tests 2 and 3 the method converged. As expected, better initial approximations required less iterations for the algorithm to terminate.

Then we rerun the computations with the standard Newton method for (3) individually applied to each of the four eigenpair approximations. Hereby we used the same initial approximations as for MBNM.

We obtained the following results:

Test 1:

- No convergence was obtained for the second eigenpair.
- $\|AZ^* - Z^*M^*\| = 0.59$
- The maximal condition number 2.199×10^{14} occurred while updating the second eigenpair.

Test 2:

- No convergence was obtained for the third eigenpair.
- $\|AZ^* - Z^*M^*\| = 0.54$
- The maximal condition number 1.149×10^{12} occurred while updating the first eigenpair.

Test 3:

- Convergence was obtained for all eigenpairs.
- $\|AZ^* - Z^*M^*\| = 2.396 \times 10^{-14}$
- The maximal condition number 3.282×10^{14} occurred while updating the fourth eigenpair.

The tests demonstrate the superior convergence properties of MBNM when the spectrum contains clusters. This is reflected in the larger convergence region compared with the standard Newton method applied to individual eigenpairs and the blowing up of the condition numbers.

In order to show the limits of the method with respect to the separation of the spectra, in a second setup the spectrum was split between $\lambda_{16} = 8.03894111581427$ and $\lambda_{17} = 8.03894112282902$, such that $q = 5$ and

$$\sigma(A_1) = \{\lambda_1, \ldots, \lambda_{16}\},$$

$$\sigma(A_2) = \{\lambda_{17}, \ldots, \lambda_{21}\},$$

$$\gamma = 7.01475 \times 10^{-9}.$$

Here we tested MBNM only. The standard Newton method gives qualitatively analogous results as in the first setup except that one more eigenpair approximation has to be updated.

The results for MBNM are shown inTable 4.

Again, in Test 1 of the second setup an invariant subspace was computed, but not the target one. In Tests 2 and 3 no convergence was obtained at all. Finally, in Tests 4 and 5 the initial approximations were sufficiently good for the method to converge.

The results of the second setup show that, as expected from theory, smaller gaps require better initial approximations for the algorithm to converge. Note, that the condition numbers are of size $1/\gamma \approx 1 \times 10^9$.

When applying subspace iteration (which is admissible since the target eigenvalues are the dominant ones) with the same initial approximations as in the previous tests it always converged. For the first setup about 200 steps of subspace iteration were needed to obtain a residual of the same size as the final residual of MBNM. In the second setup after 1000 steps the residual was of order 1×10^{-10} and did not change any more. This is due to the bad separation of the spectra and also due to roundoff errors.

Problem 2 (*Dingdong matrix*). In this test problem we wanted to verify the Q-quadratic convergence of $\sin\varphi_k$ to zero predicted by the theory. Therefore, we run MBNM and monitored $\sin\varphi_k$ and the spectral norm of the residual $\|R_k\|$ after each iteration step. The computations were done with different gaps whereby the initial approximations were chosen such that the method converged. In accordance with Problem 1, the initial approximations had to be chosen the better the smaller the gap was.

The results are shown in Table 5. Each setup corresponds to a certain splitting with a gap γ, and k is the iteration index of MBNM. Indeed, $\sin\varphi_k$ quadratically converges to zero. Due to roundoff errors in the computation of $\sin\varphi_k$ its numerical value never got as small as $\|R_k\|$ in the very last step of the algorithm. Note that $\|R_k\|$ is of order $\sin\varphi_k$.

Table 4
Setup 2 – MBNM

Test	$\sin\varphi_0$	$\|R_0\|$	K	$\mathrm{cond}(\partial F)$	$\sin\varphi^*$	$\|R^*\|$
1	0.292	2.010	7	1.66×10^9	1.00	6.49×10^{-14}
2	0.190	0.322	2 steps, break down			
3	0.162	0.165	2 steps, break down			
4	0.165	0.153	4	1.38×10^9	3.65×10^{-8}	1.03×10^{-14}
5	0.083	0.058	3	1.31×10^9	1.33×10^{-7}	1.32×10^{-12}

Table 5
$A = $ Dingdong (21). Results for different gaps

Setup	Splitting between		γ	k	$\sin \varphi_k$	$\|R_k\|$
1	-1.318181	0.581130	1.899311	0	5.37×10^{-1}	1.27
				1	2.72×10^{-1}	6.73×10^{-1}
				2	1.07×10^{-2}	3.10×10^{-2}
				3	7.52×10^{-5}	1.72×10^{-4}
				4	2.58×10^{-8}	3.16×10^{-9}
				5	3.33×10^{-8}	1.87×10^{-15}
2	0.581131	1.529806	0.948675	0	3.15×10^{-1}	8.88×10^{-1}
				1	6.14×10^{-2}	3.84×10^{-1}
				2	3.67×10^{-3}	7.38×10^{-2}
				3	1.31×10^{-5}	7.60×10^{-4}
				4	3.94×10^{-8}	6.77×10^{-7}
				5	3.65×10^{-8}	1.99×10^{-14}
3	1.529806	1.570298	0.040492	0	2.32×10^{-1}	6.99×10^{-1}
				1	2.37×10^{-2}	1.34×10^{-1}
				2	1.27×10^{-4}	2.91×10^{-3}
				3	3.33×10^{-8}	1.77×10^{-5}
				4	4.21×10^{-8}	7.47×10^{-9}
				5	2.11×10^{-8}	2.65×10^{-15}
4	1.570298	1.570793	0.000495	0	1.43×10^{-1}	4.48×10^{-1}
				1	5.10×10^{-3}	2.78×10^{-2}
				2	2.06×10^{-6}	1.43×10^{-4}
				3	2.58×10^{-8}	6.17×10^{-9}
				4	1.49×10^{-8}	1.21×10^{-12}

Since the MBNM can be considered as a generalization of the Rayleigh quotient iteration, which usually has cubic convergence, one may ask whether MBNM has the same property. However, all the numerical results obtained for $q > 1$ indicate only quadratic convergence.

Problem 3 (*Poisson matrix*). Here we worked with a large sparse Poisson matrix $A \in \mathbb{R}^{n,n}, n = 961$, coming from the discretization of the 2D-Laplacian on the unit square with an equidistant grid of stepsize $h = 1/32$. We wanted to compare MBNM, the standard Newton method individually applied to each eigenpair approximation, and inverse subspace iteration. In all tests the same initial approximations were used.

The 15 largest eigenvalues of A are given in Table 6. The target subspace was the subspace belonging to the 13 largest eigenvalues $\lambda_{949} \ldots \lambda_{961}$ which leads to the gap $\gamma = 4.768989 \times 10^{-2}$.

We solved the arising symmetric but indefinite linear systems by MINRES and, only for comparison, additionally monitored the condition number of the matrices.

Table 6
Eigenvalues of the Poisson matrix

i	λ_i
947	7.7616397364870
948	7.7616397364870
949	7.8093296258290
950	7.8093296258290
951	7.8277613429288
952	7.8381285183670
953	7.8381285183670
954	7.8754512322709
955	7.8754512322709
956	7.9042501248088
957	7.9042501248088
958	7.9231411216129
959	7.9519400141509
960	7.9519400141509
961	7.9807389066888

The results of MBNM are shown in Table 7. MBNM required 5 steps which correspond to solving $5 \times 13 = 65$ linear systems of dimension $n + q = 974$. The condition numbers of the systems were moderate.

Applying standard Newton method with the same initial approximations, convergence was obtained for 2 eigenpairs only. For the other eigenpairs, either MINRES was not able to solve the linear systems due to large condition numbers, or the Newton iteration itself did not converge.

Finally, we applied inverse subspace iteration with the shift $\beta = (\lambda_{961} + \lambda_{949})/2$, which is the value of the midpoint of the interval $[\lambda_{949}, \lambda_{961}]$ containing the target eigenvalues. Here, 50 iterations were needed to get a residual $\|R_k\|$ of the same order as the residual in the final step of MBNM. This corresponds to solving $50 \times 13 = 650$ linear systems of dimension $n = 961$.

Table 7
MBNM for the Poisson matrix

k	$\sin \varphi_k$	$\|R_k\|$	cond(∂F)	MINRES
0	2.698053×10^{-1}	2.111697		
1	1.394442×10^{-1}	1.837613×10^{-1}	1.279003×10^{3}	2221
2	5.872637×10^{-3}	3.657906×10^{-3}	1.747727×10^{2}	1603
3	4.856856×10^{-5}	1.448030×10^{-5}	1.633486×10^{2}	1461
4	8.940697×10^{-8}	2.090324×10^{-10}	1.633484×10^{2}	1180
5	7.742870×10^{-8}	1.862886×10^{-12}	1.633484×10^{2}	595

5. Conclusions

We conclude this paper with some comments on the pros and cons of the proposed *Modified Block Newton Method*. The main advantages of the MBNM are:

1. The method is locally and Q-quadratically convergent while subspace or inverse subspace iteration possess only linear convergence.

2. The matrices of all linear systems occurring in MBNM are nonsingular, and their condition numbers are uniformly bounded. This is of great importance when iterative methods are used for solving these systems. On the other hand, in inverse subspace iteration methods with a single, constant shift the condition number of the matrix may be arbitrarily large when the shift is close to an eigenvalue.

3. The eigenvalues corresponding to the target subspace can be arbitrarily distributed in the spectrum, in particular, they may be multiple or clustered. They need not lie in an interval or be extremal in modulus, but they only have to be sufficiently separated from the rest of the spectrum. Nevertheless, the convergence region of the algorithm depends on the size of the gap. The smaller the gap is, the better initial approximations are needed to ensure convergence.

4. The method can easily be implemented using different hardware and software since only basic linear algebra tasks have to be performed.

The method might have limited applicability because of its local convergence properties. However, it is well suited for classes of problems where sufficiently good initial approximation of the target subspace can easily be provided, like in path following problems. Moreover, it can be used as an efficient refinement tool in a second phase of hybrid algorithms which use globally convergent schemes as subspace iteration or inverse subspace iteration in their first phase.

Acknowledgements

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