A SIMPLE EXTRAPOLATION METHOD FOR CLUSTERED EIGENVALUES

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Abstract. This paper introduces a simple variant of the power method. It is shown analytically and numerically to accelerate convergence to the dominant eigenvalue/eigenvector pair; and, it is particularly effective for problems featuring a small spectral gap. The introduced method is a one-step extrapolation technique that uses a linear combination of current and previous update steps to form a better approximation of the dominant eigenvector. The provided analysis shows the method converges exponentially with respect to the ratio between the two largest eigenvalues, which is also approximated during the process. An augmented technique is also introduced, and is shown to stabilize the early stages of the iteration. Numerical examples are provided to illustrate the theory and demonstrate the methods.

1. Introduction

The power method is a standard tool for capturing the dominant eigenvalue/eigenvector pair of a matrix. Its advantages include simplicity and ease of implementation. Since it relies only on repeated matrix-vector products, the method can be run without explicit formation of the underlying system matrix. Applications for recovering dominant eigenpairs include stability analysis of PDE systems [1], and principal component analysis (PCA), where often only the dominant eigencomponents are of interest [12]. However, the convergence of the method is proportional to the rate $r = |\lambda_2/\lambda_1|$, or $r^2$ in the Hermitian case [5, Chapter 8], where the eigenvalues are ordered by descending magnitude.

The purpose of this paper is to introduce an accelerated version of the power method based on a one-step extrapolation. This method is shown to demonstrate asymptotically exponential convergence with respect to the ratio $r$. It will be shown to improve convergence to the dominant eigenpair for positive semi-definite systems, where the ratio $r$ is close to unity. More generally, it will be shown in the numerical results to be effective on dominantly positive definite systems, where the eigenvalues of magnitude close to $\lambda_1$ are positive, but smaller eigenvalues may be of either sign.

Each eigenvector iterate $u_{k+1}$ is formed by a linear combination of $v_{k+1}$ and $v_k$, where $v_{k+1} = Au_{k+1}/\|u_{k+1}\|$. The most basic form of the iteration is $u_{k+1} = (1 - \gamma_k)v_{k+1} + \gamma_k v_k$, where $\gamma_k = \|d_k\|/\|d_{k-1}\|$, the residual $d_k$ is given by $u_k - x_{\lambda_k}^k$, $x_{\lambda_k}^k$ is the Rayleigh quotient, and $x_{\lambda_k}^k$ is the A-preimage of the accelerated $u_k$. The method requires the storage of two additional vectors, and does not require significant additional computations other than a Rayleigh quotient and residual norm at each iteration. The method is motivated by the idea that if the initial iterate $u_0$ is a linear combination of the first two eigenvectors, then the method converges exponentially by choice of an extrapolation parameter that approximates $-r^k$ at iteration $k$. This motivation will be given in detail in section 2, and an analysis of the extrapolation method will be given as the main result in section 3.

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Extrapolation methods to accelerate the power iteration have been of recurring interest over the past several decades. The well-known Aitken’s acceleration is discussed in the context of the power iteration in [13, Chapter 9], and more recently in [9, Chapter 5], the latter as applied to Markov matrices for PageRank computations. It is pointed out in [13, page 579], that

“It is suprisingly difficult to design an automatic programme which uses
Aitken’s process efficiently.”

It is also pointed out, however, that the process has “considerable value.” More recently, another extrapolation approach is presented in [12] in the context of a stochastic iteration for PCA. That method, first introduced in a deterministic setting, takes the form \( u_{k+1} = Au_k - \beta u_{k-1} \). The product \( \beta u_{k-1} \) is called a momentum term, with \( \beta \) the momentum parameter, due to its motivation by the heavy ball method of [11]. The ideal value of \( \beta \) is given as \( \lambda_2^2/4 \), and given this information, this method is shown to accelerate convergence of the power iteration for semi-definite problems, and particularly those featuring a small spectral gap. The method is sensitive to the value of \( \beta \), however, and as \( \lambda_2 \) is not generally available, it must be approximated to effectively run the method. A heuristic approach that performs an initial sequence of iterations to generate such an approximation is suggested in [12], but it is not guaranteed to produce a sufficiently good approximation of \( \lambda_2 \). The method presented in the present paper differs, as it generates a convergent sequence of approximations to \( \lambda_1 \) and \( r = \lambda_2/\lambda_1 \), as the method progresses.

The remainder of the paper is organized as follows. In section 1.1, the introduced simple and augmented extrapolation methods are stated. In section 2, the simple method, algorithm 2, is motivated by an idealized extrapolation algorithm that makes use of information such as the value of \( r \) that in general is \emph{a priori} unavailable. The main result, theorem 1 is presented in section 3, and shows that the idealized method of section 2 is well-approximated by the practical algorithm 2. Section 4 includes a discussion of the augmented method, algorithm 3, and numerical results are given in section 5.

1.1. Extrapolation algorithms. Define the inner product \((u,v)\) in the \(l_2\) sense for \(u,v \in \mathbb{R}^n\), by \((u,v) = u^Tv\), and let \(\| \cdot \|\) be the induced \(l_2\) norm. First, the power method is stated for notational convenience.

**Algorithm 1.** Power method

Choose \(u_0\), set \(h_0 = ||u_0||\) and \(x_0 = h_0^{-1}u_0\).

\[
\text{for } k = 0,1, \ldots \text{ do}
\]

\[
\begin{align*}
&\text{Set } u_{k+1} = Ax_k, \text{ and } h_{k+1} = ||u_{k+1}|| \\
&\text{Set } x_{k+1} = h_{k+1}^{-1}u_{k+1}, \lambda_k = (u_{k+1},x_k), \text{ and } d_{k+1} = u_{k+1} - \lambda_k x_k \\
&\text{STOP if } ||d_{k+1}|| < \text{tol}
\end{align*}
\]

end for

The first novel method introduced requires two power iterations to start, as two consecutive residuals are required to define each extrapolation parameter \(\gamma_k\). In the analysis that follows, \(m\) iterations of algorithm 1 will be used before the simple extrapolation method below is started.

**Algorithm 2.** Simple extrapolation

Choose \(u_0\) and set \(h_0 = ||u_0||\)

\[
\text{for } k = 0,1 \text{ do}
\]

\[
\begin{align*}
&\text{Set } x_k = h_k^{-1}u_k, \ u_{k+1} = v_{k+1} = Ax_k, \ h_{k+1} = ||u_{k+1}|| \\
&\text{Set } \lambda_k = (u_{k+1},x_k), \text{ and } d_{k+1} = u_{k+1} - \lambda_k x_k
\end{align*}
\]

end for

\[
\text{for } k = 2,3, \ldots \text{ do}
\]

\[
\begin{align*}
&\text{Set } x_k = h_k^{-1}u_k \\
&\ u_{k+1} = Ax_k
\end{align*}
\]
effectively replaces
is complicated by the
will be referred to as the simple method, and algorithm
2 will be called
Remark 1 (On algorithm
one-parameter family of methods where larger values of the parameter \( \eta \) reduce the influence of the extrapolation. In the remainder, algorithm 2 will be referred to as the simple method, and algorithm 3 will be called the augmented method.

Algorithm 3. Augmented extrapolation
Choose \( u_0 \) and parameter \( \eta \geq 1 \), and set \( h_0 = \|u_0\| \)
for \( k = 0, 1 \) do
Set \( x_k = h_k^{-1} u_k \), \( u_{k+1} = v_{k+1} = Ax_k \), \( h_{k+1} = \|u_{k+1}\| \)
Set \( \lambda_k = (u_{k+1}, x_k) \), \( d_{k+1} = u_{k+1} - \lambda_k x_k \)
end for
Set \( p_1 = (v_2 - u_1, x_1) \)
for \( k = 2, 3, \ldots \) do
Set \( x_k = h_k^{-1} u_k \)
\( v_{k+1} = Ax_k \)
\( p_k = (v_{k+1} - u_k, x_k) \)
Compute \( \gamma_k = -(\|d_k\|^2 + p_k^2)^{1/2} / (\|d_{k-1}\|^2 + \eta p_{k-1})^{1/2} \)
Set \( u_{k+1} = (1 - \gamma_k) v_{k+1} + \gamma_k v_k \), \( h_{k+1} = \|u_{k+1}\| \)
\( x_k = (1 - \gamma_k) x_k + \gamma_k x_{k-1} \)
\( \lambda_k = (u_{k+1}, x_k) / (x_k, x_k) \)
\( d_{k+1} = u_{k+1} - \lambda_k x_k \)
STOP if \( \|d_{k+1}\| < \text{tol} \)
end for

Remark 1 (On algorithm 3). The \( \lambda_k \) are all true Rayleigh quotients for the accelerated iterates. The scalar quantities \( p_k \) are defined by \( p_k = (v_{k+1} - u_k, x_k) \). They are denoted by \( p \) because each is the projection of the difference between the latest extrapolated iterate and its image under \( A \), along the normalized iterate \( x_k \). Another view is

\[
p_k = (v_{k+1} - u_k, x_k) = (Ax_k - h_k x_k, x_k) = (Ax_k, x_k) - h_k,
\]

the difference between the pre-extrapolation Rayleigh quotient \( (Ax_k, x_k) \), and the norm of the previous accelerated iterate, both approximations of the dominant eigenvalue.

Some intuition on the parameter \( \eta \) in algorithm 3, can be gained by considering the limiting cases. If \( \eta \) is sufficiently large, then \( \gamma_k \) tends toward zero, by which algorithm 3 reduces to the algorithm 1. This helps to explain why algorithm 3 effectively replaces running some number \( m \) iterations of the power iteration before applying the simple extrapolation, algorithm 2, as done in the analysis below. A moderately chosen parameter \( \eta \) gradually increases the influence of the extrapolation at the beginning of the iteration, while its influence decreases as \( p_k \) is dominated by \( \|d_k\| \), as the first eigencomponent is resolved. Further detail is given in section 4.

The analysis of the simple extrapolation method of algorithm 2 which is presented below in section 3 is complicated by the \( l_2 \) normalization factors \( h_j \) and the inexactness
of \( \gamma_j \) as an approximation to \(-r^j\), where \( r = \mu/\lambda < 1 \) is the ratio of the first two eigenvalues, assumed to be positive. To motivate how the method works without these complications, an idealized analysis is next presented. The aforementioned complications are removed by normalizing by the principal eigenvalue \( \lambda \) rather that the \( l_2 \) norm of iterate \( u_j \), and by supposing \( \gamma_j \) is \(-r^j\). This is not possible for most practical purposes, where \( \lambda \) and \( r \) are a priori unknown. The notable exception is in PageRank algorithms, for which the (dominant) positive-definiteness is generally not satisfied, and for which appropriate accelerations have been well-developed elsewhere, for instance in \([4, 6, 8, 10]\) and \([9, \text{Chapter 5}]\), and the references therein. However, supposing this information were available, a classical extrapolation viewpoint illustrates how exponential convergence can be achieved starting from a linear combination of the first two eigenvectors. In section 4 and the numerical results of section 5, it will be illustrated that the starting vector need not be restricted to the first two eigencomponents.

2. Motivation: idealized extrapolation

Suppose \( m \) iterations of the power method have been run on \( v_0 = \varphi + c\psi \) with normalization \( v_k = \lambda^{-1}Av_k \), where \( \lambda \) and \( \mu \) are the first two leading eigenvalues with corresponding eigenvectors \( \varphi \) and \( \psi \). Let \( r = \mu/\lambda \). Then

\[
v_{m} = \varphi + cr^{m} \psi, \quad v_{m+1} = \varphi + cr^{m+1} \psi, \quad v_{m+2} = \varphi + cr^{m+2} \psi.
\]

Now let’s choose \( \gamma_{m+1} \) to form \( u_{m+2} = (1 - \gamma_{m+1})v_{m+2} + \gamma_{m+1}v_{m+1} \) to get a higher-order deterioration on the second eigencOMPONENT

\[
u_{m+2} = (1 - \gamma_{m+1})v_{m+2} + \gamma_{m+1}v_{m+1} = \varphi + ((1 - \gamma_{m+1})r + \gamma_{m+1})cr^{m+1} \psi.
\]

From (2.1), the choice \( \gamma_{m+1} = -r \) allows \( u_{m+2} = \varphi + cr^{m+3} \psi \), which improves on \( v_{m+2} \) by a factor of \( r \), and yields \( v_{m+3} = \varphi + cr^{m+4} \psi \). Notice that we could have chosen \( \gamma_{m+1} = -r/(1-r) \), to eliminate the entire second eigencOMPONENT. This, however, leads to a highly unstable method, particularly if \( r \) is close to one, which is the case we are most interested in. Repeat the process for \( \gamma_{m+2} \)

\[
u_{m+3} = (1 - \gamma_{m+2})v_{m+3} + \gamma_{m+2}v_{m+2} = \varphi + ((1 - \gamma_{m+2})r^2 + \gamma_{m+2})cr^{m+2} \psi.
\]

The choice of \( \gamma_{m+2} = -r^2 \) allows \( u_{m+3} = \varphi + cr^{m+6} \psi \), and \( v_{m+4} = \varphi + cr^{m+7} \psi \).

Continuing inductively, suppose

\[
u_{m+k} = \varphi + c(r^{m+1+\sum_{l=1}^{k-1} l}) \psi, \quad v_{m+k+1} = \varphi + c(r^{m+1+\sum_{l=1}^{k} l}) \psi.
\]

Then for \( \gamma_{k} = -r^{k} \) we have

\[
u_{m+k+1} = (1 - \gamma_{m+k})v_{m+k+1} + \gamma_{m+k}v_{m+k} = \varphi + ((1 - \gamma_{m+k})r^k + \gamma_{m+k}) (r^{m+1+\sum_{l=1}^{k-1} l}) \psi = \varphi + c(r^{m+1+\sum_{l=1}^{k+1} l}) \psi,
\]

\[
u_{m+k+2} = \varphi + c(r^{m+1+\sum_{l=1}^{k+1} l}) \psi.
\]

which completes the induction.

Next, we demonstrate that this idea works in a practical sense, by algorithm 2, where the extrapolation parameter \( \gamma_{m+k} \) is defined by \(-\|d_{m+k}\| / \|d_{m+k-1}\| \). As shown in the next section and numerically in section 5, this approximates \(-r^k \) up to \( O(r^{O(m-1)+k}) \), which is sufficient to obtain the exponential convergence seen above.

Remark 2. The choice of \( \gamma_{m+k} = -\|d_{m+k}\| / \|d_{m+k-1}\| \) is not the only possibility to give this approximation to \(-r^k \). One could also choose \( \tilde{\gamma}_{m+k} = -\|w_{m+k-1}\| / \|w_k\| \), where \( w_k = v_{k+1} - u_k \). Numerically, the two methods appear essentially equivalent, but the analysis was found to be simpler defining the extrapolation parameter in terms of the residuals.
3. **Analysis of simple extrapolation**

Suppose the power iteration, algorithm 1, is run for some given number of iterations $m$, before switching to the simple extrapolation, algorithm 2. As in section 2, we will suppose the initial iterate $u_0$ is some linear combination of the first two (dominant) normalized eigenvectors: $\varphi$ with eigenvalue $\lambda$, and $\psi$ with eigenvalue $\mu$. Let $r = \mu / \lambda$. In the analysis that follows, we will suppose $r > 1/2$. Supposing $u_0 = \varphi + c\psi$, for some $c \in \mathbb{R}$, after $n \geq 1$ power iterations

\[
\begin{align*}
  x_{n-1} &= (1 + c^2 r^{2(n-1)})^{-1/2} (\varphi + cr^{n-1}\psi) = \delta_{n-1}^{-1} (\varphi + cr^{n-1}\psi), \\
  u_n &= v_n = \lambda (1 + c^2 r^{2(n-1)})^{-1/2} (\varphi + cr^n\psi) = \lambda \delta_{n-1}^{-1} (\varphi + cr^n\psi), \\
  \lambda_{n-1} &= (u_n, x_{n-1}) = \lambda \frac{1 + c^2 r^{2n-1}}{1 + c^2 r^{2(n-1)}} = \lambda \delta_{n-1}^{-2} (1 + c^2 r^{2n-1})
\end{align*}
\]

where $\delta_n := (1 + c^2 r^{2n})^{1/2}$. The residual $d_n = u_n - \lambda_{n-1} x_{n-1}$ is then given by

\[
\begin{align*}
d_n &= \lambda \delta_{n-1}^{-1} \left\{ (\varphi + cr^n\psi) - \frac{1 + c^2 r^{2n-1}}{1 + c^2 r^{2(n-1)}} (\varphi + cr^{n-1}\psi) \right\} \\
&= \lambda \delta_{n-1}^{-1} \left\{ \varphi \left( 1 - \frac{1 + c^2 r^{2n-1}}{1 + c^2 r^{2(n-1)}} \right) + cr^n\psi \left( r - \frac{1 + c^2 r^{2n-1}}{1 + c^2 r^{2(n-1)}} \right) \right\} \\
&= \lambda (1 - r) cr^{n-1} \delta_{n-1}^{-3} \{ cr^n \varphi - \psi \}.
\end{align*}
\]

Similarly, $d_{n+1} = \lambda (1 - r) cr^n \delta_{n}^{-3} \{ cr^n \varphi - \psi \}$. Taking the ratio of $\|d_{n+1}\|$ and $\|d_n\|$ for $n = m$ to perform the first extrapolation, we have

\[
\frac{\|d_{m+1}\|}{\|d_m\|} = \frac{\lambda (1 - r) cr^{m-1}}{\delta_{m-1}^2} = \frac{\lambda (1 - r) cr^{m-1}}{1 + c^2 r^{2(m-1)}},
\]

which then yields

\[
\frac{\|d_{m+1}\|}{\|d_m\|} = r \frac{\delta_{m-1}^2}{\delta_m^2} = r \left( 1 + \frac{c^2 r^{2(m-1)}(1 - r^2)}{1 + c^2 r^{2m}} \right) = r \left( 1 + \varepsilon_{m+1}^d \right),
\]

where

\[
0 < \varepsilon_{m+1}^d = \frac{c^2 r^{2(m-1)}(1 - r^2)}{\delta_m^2} < c^2 r^{2(m-1)}(1 - r^2).
\]

The first accelerated iterate $u_{m+2} = (1 - \gamma_{m+1}) v_{m+2} + \gamma_{m+1} v_{m+1}$, is given by

\[
\begin{align*}
u_{m+2} &= \lambda \delta_{m+1}^{-1} \left\{ (1 - \gamma_{m+1}) (\varphi + cr^{m+2}\psi) + \gamma_{m+1} (\varphi + cr^{m+1}\psi) \right\} \\
&= \lambda \delta_{m+1}^{-1} \left\{ \varphi (1 - \gamma (1 - \delta_{m+1} / \delta_{m})) + cr^{m+1}\psi (r - \gamma_{m+1} (r - \delta_{m+1} / \delta_{m})) \right\}.
\end{align*}
\]

The expression for $u_{m+2}$ can be simplified using a little algebra, and the inequality $\sqrt{1 - x} = 1 - y$ for some $x/2 < y < x$, if $0 < x < 1$.

\[
1 - \delta_{m+1} / \delta_{m} = 1 - \left( \frac{1 + c^2 r^{2(m+1)}}{1 + c^2 r^{2m}} \right)^{1/2} = 1 - \left( \frac{1 - c^2 r^{2m}(1 - r^2)}{1 + c^2 r^{2m}} \right)^{1/2} = \varepsilon_{m+2}^u,
\]

where $0 < \varepsilon_{m+2}^u < c^2 r^{2m}(1 - r^2)$. From (3.7), it follows that

\[
r - \delta_{m+1} / \delta_{m} = r = (1 - \varepsilon_{m+2}^u).
\]
Applying (3.7) and (3.8) to (3.6) with $\gamma_{m+1} = -\|d_{m+1}\|/\|d_m\|$ expressed as (3.4), allows

$$u_{m+2} = \lambda \delta_{m+1}^{-1}\{\varphi(1 - \gamma_{m+1}^{\mu} u_{m+2}) + cr^{m+1} \psi (r - \gamma_{m+1}(r - 1 + \varepsilon_{m+2}^u))\}$$

$$= \lambda \delta_{m+1}^{-1}\{\varphi(1 + r\varepsilon_{m+2}(1 + \varepsilon_{m+1}^d)) + cr^{m+1} \psi (r + r(1 + \varepsilon_{m+2}^d)(r - 1 + \varepsilon_{m+2}^u))\}$$

(3.9) $$= \lambda \delta_{m+1}^{-1}\{\varphi(1 + r\varepsilon_{m+2}(1 + \varepsilon_{m+1}^d)) + cr^{m+2} \psi (-\varepsilon_{m+1}^d + (1 + \varepsilon_{m+2}^d)(r + \varepsilon_{m+2}^u))\}.$$

The term multiplying $\psi$ can be written as

$$cr^{m+3}\left(1 + \frac{\varepsilon_{m+2}^u}{r}(1 + \varepsilon_{m+1}^d) - \frac{1 - r}{r}\varepsilon_{m+1}^d\right),$$

which allows, for $r > 1/2$, and $m$ large enough so $c^2r^{2(m-1)}(1 - r^2) < 1$, that the accelerated iterate $u_{m+1}$ may be written as

$$u_{m+2} = \lambda \delta_{m+1}^{-1}\{\varphi(1 + \theta_{m+2}) + cr^{m+3}(1 + \eta_{m+2})\psi\},$$

$$0 < \theta_{m+2} < 2r\varepsilon_{m+2}^u < 2c^2r^{2m+1}(1 - r^2),$$

(3.10) $$|\eta_{m+2} < 2\varepsilon_{m+1}^d < 2c^2r^{2(m-1)}(1 - r^2).$$

Continuing the iteration up through the computation of $u_{m+3}$ before moving onto the inductive step, $x_{m+1}$ the (or a, if $A$ is singular) $A$-preimage of $u_{m+2}$, $x_{m+2}$ the $l_2$ normalization of $u_{m+2}$ from (3.10), and $v_{m+3}$ are given by given by

$$x_{m+1} = \delta_{m+1}^{-1}\{\varphi(1 + \theta_{m+2}) + cr^{m+2}(1 + \eta_{m+2})\psi\},$$

$$x_{m+2} = \delta_{m+2}^{-1}\{\varphi(1 + \theta_{m+2}) + cr^{m+3}(1 + \eta_{m+2})\psi\},$$

$$v_{m+3} = \lambda \delta_{m+1}^{-1}\{\varphi(1 + \theta_{m+2}) + cr^{m+4}(1 + \eta_{m+2})\psi\},$$

(3.11) $$\delta_{m+2} = \left((1 + \theta_{m+2})^2 + c^2r^{2(m+3)}(1 + \eta_{m+2})^2\right)^{1/2}.$$

The next Rayleigh quotient $\lambda_{m+1} = (u_{m+2}, x_{m+1}^*)/\|x_{m+1}^*\|^2$, is given by

(3.12) $$\lambda_{m+1} = \lambda \frac{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2}{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2}.$$

To expedite the process of computing the residual, first notice that

$$1 - \frac{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2}{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2} = \frac{(1 - r)c^2r^{2(m+2)}(1 + \eta_{m+2})^2}{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2},$$

(3.13) $$r - \frac{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2}{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2} = \frac{(r - 1)(1 + \theta_{m+2})^2}{(1 + \theta_{m+2})^2 + c^2r^{2(m+2)}(1 + \eta_{m+2})^2}.$$

Applying (3.13) along with the expansions (3.10)-(3.12), the residual $d_{m+2} = u_{m+2} - \lambda_{m+1} x_{m+1}^*$ is then

$$d_{m+2} = \lambda \frac{cr^{2(m+2)}(1 - r)(1 + \theta_{m+2})(1 + \eta_{m+2})}{\delta_{m+1} \delta_{m+2}} \times \left\{cr^{m+2}(1 + \eta_{m+2})\varphi + (1 + \theta_{m+2})\psi\right\},$$

and therefore its norm is

(3.14) $$\|d_{m+2}\| = \frac{\lambda c r^{2(m+2)}(1 - r)(1 + \theta_{m+2})(1 + \eta_{m+2})}{\delta_{m+1} \delta_{m+2}}.$$
Now, from (3.5) and (3.14) the next ratio of residual norms is given by

\[
\frac{\|d_{m+2}\|}{\|d_{m+1}\|} = r^2 \frac{(1 + \theta_{m+2})(1 + \eta_{m+2})\delta_m^2}{\delta_{m+1}\delta_{m+2}}
\]

\[
= r^2 \frac{(1 + \eta_{m+2})(1 + c^2 r^{2m})}{(1 + c^2 r^{2(m+1)})^{1/2}(1 + c^2 r^{2(m+3)})(1 + \eta_{m+2})^2/(1 + \theta_{m+2})^2)^{1/2}}
\]

(3.15)

\[
= r^2 \frac{(1 + \eta_{m+2})(1 + c^2 r^{2m})}{1 + \alpha c^2 r^{2(m+1)}},
\]

where \(\alpha\) lies in the interval between 1 and \(r^4(1 + \eta_{m+2})^2/(1 + \theta_{m+2})^2\). This last simplification is justified by the observation that both terms in the denominator of (3.15) are the square roots of positive perturbations of one. Then

\[
\frac{\|d_{m+2}\|}{\|d_{m+1}\|} = r^2 \left( 1 + \frac{\eta_{m+2}(1 + c^2 r^{2m}) + c^2 r^{2m}(1 - r^2 \alpha)}{1 + \alpha c^2 r^{2(m+1)}} \right) = r^2(1 + \varepsilon_{m+2}^d),
\]

(3.16) \[|\varepsilon_{m+2}^d| < 2\|\eta_{m+2}\| + c^2 r^{2m}(1 - r^2 \alpha) < c^2 r^{2(m-1)}(2(1 - r^2) + r^2(1 - r^2 \alpha)).\]

From the expressions for \(v_{m+2}\) and \(v_{m+3}\) in eqs. (3.1) and (3.10), respectively, the next extrapolated iterate \(u_{m+3} = (1 - \gamma_{m+2})v_{m+3} + \gamma_{m+2}\), can be written as

\[
u_{m+3} = \lambda \delta_{m+2}^{-1} \left\{ \varphi \left( (1 + \theta_{m+2}) - \gamma_{m+2} \left( (1 + \theta_{m+2}) - \frac{\delta_{m+2}}{\delta_{m+1}} \right) \right) 
\]

\[+ cr^{m+2} \psi \left( r^2(1 + \eta_{m+2}) - \gamma_{m+2} \left( r^2(1 + \eta_{m+2}) - \frac{\delta_{m+2}}{\delta_{m+1}} \right) \right) \right\}.
\]

(3.17)

Applying (3.15), the terms multiplying the principle eigenvector \(\varphi\) in (3.17) reduce to

\[
1 + \theta_{m+2}(1 - \gamma_{m+2}) - \gamma_{m+2} \left( 1 - \frac{\delta_{m+2}}{\delta_{m+1}} \right) = 1 + \theta_{m+2}(1 - \gamma_{m+2}) - r^2(1 + \theta_{m+2})(1 + \eta_{m+2})\delta_m^2 \left( \frac{1}{\delta_{m+1}\delta_{m+2}} - \frac{1}{\delta_{m+1}^2} \right)
\]

(3.18)

\[= 1 + \theta_{m+3}, \quad \theta_{m+3} = \mathcal{O}(r^{2m+1}).\]

Hereafter, we are concerned with tracking the perturbations in terms of powers of \(r\). The lowest-order term in (3.18) comes from \(\theta_{m+2}\), with a higher-order term of \(\mathcal{O}(r^{2(m+2)})\), resulting from \(r^2(\delta_{m+2}^{-1}\delta_{m+1} - \delta_{m+1}^{-2})\), by a similar calculation to that in (3.15). Together, (3.17) and (3.18) show the extrapolation does not do much damage to preserving the component of \(u_{m+3}\) along \(\varphi\). Next, consider the terms multiplying the second eigenvector \(\psi\), which the extrapolation is designed to reduce from \(\mathcal{O}(r^{m+4})\) (as in \(v_{m+3}\)) to \(\mathcal{O}(r^{m+6})\). Applying the expression for \(\gamma_{m+2} = -\|d_{m+2}\| / \|d_{m+1}\|\), from the first line of (3.15), allows

\[
r^2(1 + \eta_{m+2}) + \gamma_{m+2} \frac{\delta_{m+2}}{\delta_{m+1}} = r^2(1 + \eta_{m+2}) \left( 1 - (1 + \theta_{m+2}) \left( 1 + \frac{c^2 r^{2m}(1 - r^2)}{1 + c^2 r^{2m}} \right) \right)
\]

(3.19)

\[= r^4 \cdot \mathcal{O}(r^{2(m-1)}),
\]

and from (3.16), the remaining term satisfies \(\gamma_{m+2}r^2(1 + \eta_{m+2}) = r^4 \cdot \mathcal{O}(r^{2(m-1)})\). Putting these two estimates into (3.17) yields

\[
cr^{m+2} \left( r^2(1 + \eta_{m+2}) - \gamma_{m+2} \left( r^2(1 + \eta_{m+2}) - \frac{\delta_{m+2}}{\delta_{m+1}} \right) \right) = cr^{m+6} \cdot \mathcal{O}(r^{2(m-1)}).
\]

(3.20)
Summarizing, the extrapolated iterate \( u_{m+3} \) can be expressed as

\[
\begin{align*}
    u_{m+3} &= \lambda^j \delta_{m+2}^{-1} \{ (1 + \theta_{m+3}) \varphi + cr^{m+6} (1 + \eta_{m+3}) \psi \}, \\
    \theta_{m+3} &= \mathcal{O} \left( r^{2m+1} \right), \\
    \eta_{m+3} &= \mathcal{O} \left( r^{2(m-1)} \right).
\end{align*}
\]

(3.21)

The general inductive step is next shown in the following theorem.

**Theorem 1.** Let \( A \) be a positive semi-definite matrix with leading eigenvectors \( \varphi \) and \( \psi \) corresponding to eigenvalues \( \lambda \) and \( \mu \), with \( \lambda > \mu \) and \( r = \mu / \lambda > 1 / 2 \). Let \( u_0 = \varphi + c \psi \), and suppose \( m \) iterations of the power method, algorithm 1 are run before switching to the simple extrapolation method, algorithm 2, where \( m \) is large enough so that \( c^2 r^{2(m-1)} (1 - r^2) < 1 \). Then for \( j \geq 1 \), the extrapolation parameter \( \gamma_{m+j} = -\|d_{m+j}\| / \|d_{m+j-1}\| \) and the accelerated iterate \( u_{m+j} \) satisfy

\[
\begin{align*}
    \gamma_{m+j} &= -r^j (1 + \varepsilon_{m+j}^d), \\
    \varepsilon_{m+j}^d &= \mathcal{O} \left( r^{2(m-1)} \right), \\
    u_{m+j+1} &= \lambda \left\{ \varphi (1 + \theta_{m+j+1}) + r^{m+j+1} (1 + \eta_{m+j+1}) \right\},
\end{align*}
\]

with

\[
\begin{align*}
    \theta_{m+j+1} &= \mathcal{O} \left( r^{2m+1} \right), \\
    \eta_{m+j+1} &= \mathcal{O} \left( r^{2(m-1)} \right).
\end{align*}
\]

(3.22)

Proof. The base steps with \( j = 1 \) and \( j = 2 \) are established in the preceding discussion. There, and in the following, it will be shown that

\[
\begin{align*}
    u_{m+j+1} &= \lambda \delta_{m+j}^{-1} \left\{ \varphi (1 + \theta_{m+j+1}) + r^{m+j+1} (1 + \eta_{m+j+1}) \right\},
\end{align*}
\]

where for \( j \geq 2 \), \( \delta_{m+j} = 1 + \mathcal{O} \left( r^{2m+1} \right) \), which is sufficient to establish (3.22). Now, let us proceed inductively under the following hypotheses, where the indices \( J = m + j \), \( s = \sum_{l=1}^{j-1} l \), and \( t = s + j \), are introduced for notational brevity. Suppose, in accordance with (3.10) and (3.11), that

\[
\begin{align*}
    \gamma_{m+k} &= -r^k (1 + \varepsilon_{m+k}^d), \\
    \varepsilon_{m+k}^d &= \mathcal{O} \left( r^{2(m-1)} \right), \\
    u_{m+k+1} &= \lambda \delta_{m+k}^{-1} \left\{ \varphi (1 + \theta_{m+k+1}) + r^{m+k} (1 + \eta_{m+k+1}) \right\},
\end{align*}
\]

(3.23)

for \( k < j \), where the normalization factors are

\[
\delta_{m+k} = \left( (1 + \theta_{m+k})^2 + c^2 r^{2(m + \sum_{l=1}^{k} l)} (1 + \eta_{m+k})^2 \right)^{1/2}.
\]

(3.24)

We will proceed to compute \( \gamma_J = -\|d_J\| / \|d_{J-1}\| \), and the extrapolated iterate \( u_{J+1} \). From (3.23) and algorithm 2, we have

\[
\begin{align*}
    u_J &= \lambda \delta_{J-1}^{-1} \left\{ (1 + \theta_J) \varphi + cr^{m+t} (1 + \eta_J) \psi \right\}, \\
    x_{J-1}^\gamma &= \lambda \delta_{J-1}^{-1} \left\{ (1 + \theta_J) \varphi + cr^{m+t-1} (1 + \eta_J) \psi \right\}.
\end{align*}
\]

(3.25)

The Rayleigh quotient \( \lambda_{J-1} \) is then given by

\[
\lambda_{J-1} = \frac{(u_J, x_{J-1}^\gamma)}{(x_{J-1}, x_{J-1})} = \frac{(1 + \theta_J)^2 + c^2 r^{2(m+t)-1} (1 + \eta_J)^2}{(1 + \theta_J)^2 + c^2 r^{2(m+t-1)} (1 + \eta_J)^2}.
\]

(3.26)

The residual \( d_J \) is given from (3.25) and (3.26) by

\[
\begin{align*}
    d_J &= u_J - \lambda_{J-1} x_{J-1}^\gamma = \frac{\lambda}{\delta_{J-1}} \left\{ (1 + \theta_J)(1 - Z) + cr^{m+t-1} (1 + \eta_{m+z})(r - Z) \psi \right\},
\end{align*}
\]

(3.27)
where $Z$ is the ratio that multiplies $\lambda$ in the Rayleigh quotient (3.26). The factors $1 - Z$ and $r - Z$ are then

$$(1 - Z) = \frac{c^2r^{2(m+t-1)}(1 + \eta_j)^2(1 - r)}{(1 + \theta_j)^2 + c^2r^{2(m+t-1)}(1 + \eta_j)^2},$$

$$\tag{3.28} (r - Z) = \frac{(1 + \theta_j)^2(r - 1)}{(1 + \theta_j)^2 + c^2r^{2(m+t-1)}(1 + \eta_j)^2}.$$ Applying (3.28) to (3.27) yields the residual

$$\tag{3.29} d_j = \frac{\lambda(1 + \theta_j)(1 + \eta_j)(1 - r)c^{m+t-1}}{\delta_{j-1} (1 + \theta_j)^2 + c^2r^{2(m+t-1)}(1 + \eta_j)^2} \left\{ c^{m+t-1}(1 + \eta_{m+j})\varphi - (1 + \theta_j)\psi \right\},$$

with its norm given by

$$\tag{3.30} \|d_j\| = \frac{\lambda(1 + \theta_j)(1 + \eta_j)(1 - r)c^{m+t-1}}{\delta_{j-1} (1 + \theta_j)^2 + c^2r^{2(m+t-1)}(1 + \eta_j)^2} \left\{ c^{m+t-1}(1 + \eta_{m+j})\varphi - (1 + \theta_j)\psi \right\}.$$ It is useful to note the simplification, $(1 + \eta_{m+k})/(1 + \theta_{m+k}) = 1 + \varepsilon_k$, where $\varepsilon_k = O(r^{2(m-1)})$, $k = j - 1, j$. Then applying the same process for $\|d_{j-1}\|$, as (3.29)-(3.30), the ratio of residuals is given by

$$\tag{3.31} \frac{\|d_j\|}{\|d_{j-1}\|} = r^{t-s} \frac{(1 + \theta_j)(1 + \eta_j)}{(1 + \theta_{j-1})(1 + \eta_{j-1})} \times \frac{\delta_{j-2} ((1 + \theta_{j-1})^2 + c^2r^{2(m+s-1)}(1 + \eta_{j-1})^2)^{1/2}}{\delta_{j-1} ((1 + \theta_j)^2 + c^2r^{2(m+t-1)}(1 + \eta_j)^2)^{1/2}}
$$

$$= r^j \frac{(1 + \eta_j)}{(1 + \eta_{j-1})} \frac{\delta_{j-2} (1 + c^2r^{2(m+s-1)}(1 + \varepsilon_{j-1})^2)^{1/2}}{\delta_{j-1} ((1 + c^2r^{2(m+t-1)}(1 + \varepsilon_j)^2)^{1/2}}
$$

$$= r^j(1 + \varepsilon_j), \quad \varepsilon_j = O(r^{2(m-1)}),$$

where the lowest-order terms arise from $\eta_{m+k}$, $k = \{j-1, j\}$. This shows the first equation of (3.22).

The next extrapolated iterate is given by $u_{j+1} = (1 - \gamma_j) v_{j+1} + \gamma_j v_j$, where from the inductive hypothesis and algorithm 3

$$v_j = \lambda \delta_{j-1}^{-1} \left\{ (1 + \theta_{j-1}) \varphi + c^{m+s+1}(1 + \eta_{j-1})\psi \right\},$$

$$v_{j+1} = \lambda \delta_{j-1}^{-1} \left\{ (1 + \theta_j) \varphi + c^{m+t+1}(1 + \eta_j)\psi \right\}.$$ Then rearranging terms, $u_{J+1}$ can be written as

$$u_{j+1} = \lambda \delta_{j-1}^{-1} \left\{ \varphi \left( (1 + \theta_j) - \gamma_j \left( (1 + \theta_j) - (1 + \theta_{j-1}) \frac{\delta_j}{\delta_{j-1}} \right) \right) \right\} + \psi c^{m+s+1} \left( r^j (1 + \eta_j) - \gamma_j \left( r^j (1 + \eta_j) - (1 + \eta_{j-1}) \frac{\delta_j}{\delta_{j-1}} \right) \right).$$

Applying $\gamma_j = -\|d_j\|/\|d_{j-1}\|$, given by (3.31), the coefficient multiplying $\varphi$ can be written as $(1 + \theta_{J+1})$, with perturbation $\theta_{J+1} = O(r^{2m+1})$, where the lowest order term is inherited from $\theta_j$.

Looking more carefully at the terms multiplying $\psi$, we first want to see the sum of the first and third terms multiplying $\psi c^{m+s+1}$ in (3.32), is of order at least $r^{2(J-1)}$. Then after factoring $r^{2j}$ out of the entire expression, the remaining terms will be of order
Similarly to the base case in (3.19), the expression for $\gamma_J$ from the next-to-last line of (3.31) will be used to cancel like factors of $\eta_{J-1}$.

\[
r^j(1 + \eta_J) + \gamma_J(1 + \eta_{J-1})\frac{\delta_J}{\delta_{J-1}} = r^j(1 + \eta_J) \left(1 - \frac{\delta_{J-2}\delta_J}{\delta^2_{J-1}} \cdot \left(1 + \frac{c^2r^{2(m+s-1)}(1 + \varepsilon_{J-1})^2}{1 + c^2r^{2(m+t-1)}(1 + \varepsilon_J)^2} \right)^{1/2} \right).
\]  

(3.33)

The square-rooted term of (3.33) is easily seen to reduce to a term of the form $1 + \mathcal{O}(r^{2(m+s-1)})$. Defining $s_0 = \sum_{j=0}^{J-2}$, the term contributing the lowest-order perturbation $\delta_{J-2}\delta_J/\delta^2_{J-1}$, can be understood by the factorization

\[
\left(1 + \frac{c^2r^{2(m+s)}(1 + \varepsilon_J)^2}{1 + c^2r^{2(m+s)}(1 + \varepsilon_{J-1})^2} \right)^{1/2} \cdot \frac{(1 + \theta_{J-2})(1 + \theta_J)}{(1 + \theta_{J-1})^2},
\]

(3.34)

where for the $j = 3$ case, $\theta_{J-2} = \theta_{m+1} = 0$. The first ratio of (3.34) produces a term of the form $1 + \mathcal{O}(r^{2m})$, where $2s_0 - j \geq -1$ for $j \geq 3$, so the perturbation is of order at least $r^3 \cdot \mathcal{O}(r^{2m})$. The remaining term also produces a perturbation of at least order $r^{2m-1}$ for $j > 3$, and of order $r^{2(m-1)}$ for $j = 3$. For $j = 3$, this is because $\theta_{m+3}$ and $\theta_{m+2}$ are both $1 + \mathcal{O}(r^{2(m+1)}) = 1 + r^3 \cdot \mathcal{O}(r^{2(m-1)})$. For $j > 3$ we have

\[
(1 + \frac{\theta_{J-2} - \theta_{J-1}}{1 + \theta_{J-1}})^2 = 1 + \frac{(\theta_J - \theta_{J-1}) - (\theta_{J-1} - \theta_{J-2}) + (\theta_J\theta_{J-2} - \theta_{J-1}^2)}{(1 + \theta_{J-1})^2},
\]

(3.35)

the lowest-order term of which is $(\theta_{J-1} - \theta_{J-2})$. Both terms in the difference are of order $r^{2m+1}$, and may be analyzed as follows. For $k \geq 3$, the term multiplying $\varphi$ in the iterate $u_{m+k}$ is given (cf. (3.32)) by

\[
\lambda \delta_{m+k-1}^{-1} \left(1 + \theta_{m+k-1} \right) \left(1 + \theta_{m+k-1} \right) \left(1 + \theta_{m+k-2} \right) \delta_{m+k-2} \right) = r^{2j} \cdot \mathcal{O}(r^\nu), \text{ with } \nu \geq 2(m-1).
\]

Finally, from (3.31), and the inductive hypothesis on $\eta_{m+j}$, the remaining term of (3.32) that multiplies $\psi cr^{m+s+1}$, satisfies

\[
-g_J r^{2j} (1 + \eta_J) = r^{2j} (1 + \epsilon_J^2) (1 + \eta_J) = r^{2j} \left(1 + \mathcal{O}(r^{2(m-1)})\right).
\]

Putting everything together into (3.32), and noting that $m + s + 2j + 1 = m + t + (j + 1)$, we have

\[
u_{J+1} = \lambda \delta_J^{-1} \left\{ \varphi(1 + \theta_{J+1}) + r^{m+t+(j+1)}(1 + \eta_{J+1}) \right\},
\]

(3.36)

\[
\theta_{J+1} = \mathcal{O}(r^{2m+1}), \quad \eta_{J+1} = \mathcal{O}(r^{2(m-1)}),
\]

which establishes (3.22). \qed
4. Augmenting the Simple Method

In this section we discuss the motivation behind the augmented method, algorithm 3. The key, and only substantial, difference between the augmented method and the simple method of algorithm 2, is the use of the projection \( p_k := (u_{k+1} - u_k, x_k) = (Ax_k, x_k) - h_k \) to compute the extrapolation parameter

\[
\gamma_k = -\left( \|d_k\|^2 + p_k^2 \right)^{1/2}/\left( \|d_{k-1}\|^2 + (\eta p_{k-1})^2 \right)^{1/2}.
\]

The parameter \( \gamma_k \) for the augmented method features a user-defined tuning parameter \( \eta \geq 1 \). Large values of \( \eta \) reduce the effect of the extrapolation; and, as discussed below, more moderate values can help resolve transient modes earlier in the iteration. For general initial iterates, the quantity \( \gamma_k \) generally decreases as the algorithm converges, though the behavior need not be monotone. With \( \eta \) chosen well, the augmented method often provides faster convergence than the simple method to the correct eigenvector. As demonstrated in sections 5.1 and 5.2, if \( \eta \) is chosen too large, the iteration remains stable but takes longer to converge.

To better understand the distinction between the simple and augmented algorithms, we may examine the difference between one step of each. If the simple method is run without any preliminary power iterations beyond the first two, then both algorithms have the same \( u_1 \) and \( u_2 \), and it makes sense to compare outcomes for \( u_3 \).

Suppose \( A \) be a nondefective \( n \times n \) matrix, with spectrum

\[
\frac{\mu_1, \mu_1, \ldots, \mu_1, \mu_{J+1}, \ldots, \mu_M, \ldots, \mu_N}{J}
\]

where \( \mu_1 > \mu_{J+1} \geq \ldots \mu_N \geq 0 \), and let an initial iterate \( u_0 \) be

\[
u_0 = \sum_{i=1}^{J} c_i \phi_i + c_M \phi_M + \sum_{i>J, i \neq M}^{N} c_i \phi_i,
\]

where the \( \phi_i \) are normalized and mutually orthogonal eigenvectors of \( A \). The length of the initial vector satisfies

\[
h_0^2 = \sum_{i=1}^{J} c_i^2 + c_M^2 + \sum_{i>J, i \neq M}^{N} c_i^2.
\]

The index \( M \) is associated with the largest magnitude component, \( |c_M| \), in the initial vector.

We will evaluate \( u_3 \) starting from this initial iterate \( u_0 \) for both algorithm 3 and algorithm 2. The first two iterates \( u_{k+1}, \ k = 0, 1 \), are then

\[
(4.1) \quad u_{k+1} = \frac{1}{h_k} Au_k = \frac{1}{\prod_{j=0}^{k} h_j} \left[ \mu_1^{k+1} \sum_{i=1}^{J} c_i \phi_i + \mu_M^{k+1} c_M \phi_M + \sum_{i>J, i \neq M}^{N} \mu_i^{k+1} c_i \phi_i \right],
\]

with Rayleigh quotients

\[
\lambda_k = \frac{1}{h_k^2} (Au_k, u_k) = \frac{1}{(\prod_{j=0}^{k} h_j)^2} \left[ \mu_1^{2k+1} \sum_{i=1}^{J} c_i^2 \phi_i + \mu_M^{2k+1} c_M^2 \phi_M + \sum_{i>J, i \neq M}^{N} \mu_i^{2k+1} c_i^2 \phi_i \right].
\]

The first two residual vectors \( d_{k+1} = u_{k+1} - (\lambda_k/h_k) u_k \) are then

\[
d_{k+1} = \frac{1}{h_k} \left[ \mu_1^k \sum_{i=1}^{J} (\mu_i - \lambda_1) c_i \phi_i + \mu_M^k (\mu_M - \lambda_1) c_M \phi_M + \sum_{i>J, i \neq M}^{N} \mu_i^k (\mu_i - \lambda_1) c_i \phi_i \right].
\]
The projection $p_1$ is $p_1 = (Ax_1, x_1) - h_1 = \lambda_1 - h_1$, and the projection $p_2$ is
$$p_2 = \left( \frac{1}{h_2} Au_2 - u_2, \frac{1}{h_2} u_2 \right) = \frac{1}{h_2^2} (Au_2, u_2) - h_2 = \lambda_2 - h_2.$$

For the first extrapolated step of each method, keeping track of the two different methods $u^{acc}$, where $acc = \{s, au\}$ for the simple and augmented methods respectively, we have
$$\gamma_2^{su} = -\left[\|d_2\|^2 + |p_2|^2\right]^{1/2} / \left[\|d_1\|^2 + \eta^2 |p_1|^2\right]^{1/2}, \quad \gamma_2^{su} = -\left[\|d_2\| / \|d_1\|\right]$$
$$u_3^{acc} = \frac{1}{h_2} (1 - \gamma_2^{acc}) Au_2 + \gamma_2^{acc} h_1 Au_1.$$

In particular, from (4.1), the components of $u_3^{acc}$ which lie in the dominant eigenspace for each method are
\begin{equation}
\text{proj}_{\text{span}(\phi_1,...,\phi_j)} u_3^{acc} = \mu_2^{acc} \frac{\gamma_2^{acc} h_0 h_1 h_2}{j=1} \sum c_i(h_2 - \mu_1) \phi_i
\end{equation}

The ratio of norm of these two projections is then nothing but the ratio of the extrapolation parameters $\|\text{proj}_{\text{span}(\phi_1,...,\phi_j)} u_3^{su}/\|\text{proj}_{\text{span}(\phi_1,...,\phi_j)} u_3^{su}\| = \gamma_2^{su}/\gamma_2^{su}$. When this ratio is larger than one, $u_3^{su}$ yields a better approximation to $\mu_1$ in its Rayleigh quotient. This is satisfied when
$$\frac{\gamma_2^{su}}{\gamma_2^{su}} = \frac{\|d_2\|^2 + |p_2|^2}{\|d_2\|^2} > 1 \quad \text{iff} \quad \frac{|p_2|}{|p_1|} > \eta |d_1|.$$

Similarly to (4.2), the projection onto the eigenspace with the largest initial coefficient is given by
\begin{equation}
\text{proj}_{\text{span}(\phi_M)} u_3^{acc} = \left( \frac{\mu_M}{\mu_1} \right)^2 \frac{\gamma_2^{acc} h_0 h_1 h_2}{c_M(h_2 - \mu_M) \phi_M
\end{equation}

If $|c_M| >> |c_i|$, as
$$|c_M| \left( \frac{\mu_M}{\mu_1} \right)^k << |c_i|,$$
the augmented method magnifies the difference between the growth in the dominant and principle subdominant component. As the iteration continues and subdominant modes are sequentially suppressed, the iteration reduces essentially to simple method. Its behavior is then described well by algorithm 2.

5. Numerical results

In this section we present numerical results that illustrate the theory and demonstrate the presented methods. The first two examples illustrate convergence rates predicted by the theory, and robustness with respect to initial conditions. The next two examples demonstrate use of the algorithms for finite element discretizations of Neumann and Steklov eigenvalue problems.

5.1. Example 1: Benchmarking. We will start by looking at a simple problem to verify and illustrate the theory. Then we will look at three benchmark examples using matrices of different sizes.

First, consider the simple method algorithm 2, started after $m = 10$ power iterations, applied to the diagonal matrix $A = \text{diag}([1,0.9,0.5,...,0.5])$. In the following results, $A$ is $50 \times 50$, but the number of padding entries of 0.5 appears inconsequential. The iteration is started with $u_0$ a vector of ones. Table 1 shows $\gamma_{j+1}/\gamma_j$ which according to theorem 1 should be approximately $r = 0.9$; $u(2)/r^{1+...+j}$, the component of the approximate eigenvector in the second eigendirection, normalized by $r^{\sum_{l=1}^{j-1}}$, which should be approximately constant; and, the residual $\|d_j\|$. Each of the quantities behaves as predicted, with the second eigencomponent decaying a little faster as the algorithm converges. This simple
| $j$ | 1  | 2  | 3  | 4  | 5  | 6  | 7  |
|-----|----|----|----|----|----|----|----|
| $\gamma_j/\gamma_{j-1}$ | -  | 0.912 | 0.899 | 0.887 | 0.886 | 0.893 | 0.899 |
| $u(2)/r^{1+\ldots+j}$ | 0.304 | 0.309 | 0.310 | 0.308 | 0.305 | 0.302 | 0.299 |
| $\|d_j\|$ | 2.4e-02 | 1.8e-02 | 1.2e-02 | 7.0e-03 | 3.7e-03 | 1.8e-03 | 7.5e-04 |

| $j$ | 8  | 9  | 10 | 11 | 12 | 13 | 14 |
|-----|----|----|----|----|----|----|----|
| $\gamma_j/\gamma_{j-1}$ | 0.900 | 0.899 | 0.898 | 0.900 | 0.905 | 0.909 | 0.899 |
| $u(2)/r^{1+\ldots+j}$ | 0.295 | 0.291 | 0.287 | 0.285 | 0.281 | 0.266 | 0.200 |
| $\|d_j\|$ | 2.9e-04 | 9.9e-05 | 3.0e-05 | 8.5e-06 | 2.2e-06 | 5.0e-07 | 9.9e-08 |

Table 1. The ratio of consecutive extrapolation parameters, the component along the second exact eigenvector scaled by $r^{1+\ldots+j}$, and the norm of the residual for a diagonal matrix with $r = 0.9$.

Next we demonstrate the simple extrapolation method algorithm 2 and the augmented method algorithm 3 compared to the power method algorithm 1. In each of these tests, algorithm 2 is started after $m = 40$ initial power iterations, and the augmented method is run with parameter $\eta = 40$. This part of the example demonstrates the methods on benchmark problems of three different sizes.

- Matrix 1 is the Wilkinson matrix $W_{21+}$, which can be generated in Matlab by `gallery('wilk',21)`. It is a tridiagonal matrix with pairs of nearly equal eigenvalues. The largest eigenvalues are approximately $10.746$, and all but one of the eigenvalues are positive, with the negative eigenvalue approximately $-1.125$.
- Matrix 2 is a diagonal matrix of order $n = 1000$, with leading eigenvalue 1 and remaining eigenvalues equally spaced between 0.75 and 0.999, defined in Matlab by `diag(v)`, with $v = [1, \text{linspace}(0.75, 0.999, 1000)]$.
- Matrix 3 is a sparse matrix of order $n = 102158$, from a finite element problem describing temperature in a steel cylinder. It has $r \approx 0.9975$. This matrix is available as `thermomech_TC`, from the SuiteSparse matrix collection [3].

Figure 1 shows the residual histories for each of these three matrices starting from an initial vector $u_0 = [1, 1, \ldots, 1]$.

On each of these examples both the simple and augmented acceleration outperform the power method; and, the augmented method demonstrates the exponential convergence predicted from the theory. The simple method shows more oscillatory behavior in the second two cases, as additional eigencodeponents play a dominant role, and are subsequently damped, as the iterations progress.
As a demonstration of robustness with respect to initial data, algorithms 1 to 3 are run on Matrix 1, 2 and 3, starting with 100 different initial vectors \( u_0 \) determined by the Matlab command \texttt{rand(n,1)-0.5}. The augmented method algorithm 3 is run with three different values of the tuning parameter \( \eta = \{20, 40, 80\} \). As above, the simple method is started after 40 initial power iterations. Runs were terminated after a maximum of 6000 iterations. The average number of iterations to residual convergence of \( \text{tol} = 10^{-7} \) is reported in table 2. The results show general agreement with those shown in fig. 1, demonstrating the methods are not overly sensitive to choice of initial iterate. The last three columns of table 2 show the computation with the three different values of \( \eta \) in the augmented method. We see that there does appear to be a best value for each problem, but the method is not overly sensitive to the choice. Problems with many components competing for dominance, like Matrix 2, appear to benefit from larger values, while problems featuring larger spectral gaps like Matrix 3 (see the performance of the power method in fig. 1) may show better efficiency with smaller values.

5.2. Example 2: Bad initial data. We illustrate section 4 with some simple but extreme tests starting with bad initial data. Figure 2, shows the performance of the three algorithms on \( A = \text{diag}(\{1, 2, 0.01\}) \) with an initial iterate of \( u_0 = [0.01, 0.01, 10^{9}] \), and the parameter \( \eta = 1 \). The simple iteration is started without any additional power iterations. The initial iterate \( u_0 \) has its largest component in the wrong direction. Starting with iterate 3, the scale factors \( \gamma_k \) are different for the two methods, and these in turn lead to different dynamics for the eigenvector approximations. But, we see the augmented and simple effectively forcing successive approximations to align with the dominant eigenvector direction \([0, 1, 0]\).

The next example again features an extremely poor initial iterate. Additionally, the matrix \( A = \text{diag}(\{1.01, 1.0, 0.01\}) \), features a small spectral gap. Here, \( u_0 = [0.01, 0.01, 1, 10^{9}] \), so \( c_M = 10^{9} \), corresponds to the eigenvalue 0.01, and the coefficient \( c_1 \) corresponding to the leading eigenvalue is 0.01.

The sequence of approximate (normalized) eigenvectors generated by each method are presented componentwise in fig. 3, to give a detailed view of how the methods compare.
Both simple on the left. The eigenvalues $\mu$ we obtain that the nearest discrete eigenvalue as converge to $5439$. The power iteration has a larger error, with the located eigenvalue agreeing with the augmented and simple methods to $10^{-11} \pi^2$, but with a much larger residual, suggesting an inaccurate approximation to the eigenvector.

All methods quickly resolve the initially bad data, by damping out the fourth component (right plot) within the first few iterations, meanwhile increasing the component in the dominant direction (left plot). The two accelerated methods are much more efficient (center plot) at damping out the second component, corresponding to the second eigenvalue, which is close to the first.

### 5.3. Laplace-Neumann eigenvalues on the unit square

In this example, we seek a specific Neumann eigenvalue on the unit square $\Omega$, i.e., eigenpairs of

$$
-\Delta u_m = \mu_m u_m, \quad x \in \Omega, \quad \frac{\partial u_m}{\partial n} = 0, \quad x \in \Gamma.
$$

The eigenvalues $\mu_m$ are of the form $(k^2 + \ell^2)\pi^2, k, \ell = 0, 1, 2, \ldots$. The first several eigenvalues, scaled by $\pi^2$ for easier reading, are $0, 1, 1, 2, 2, 4, 4, 5, 5, 8, 9, 9, \ldots$.

We discretize the domain $\Omega$ using a $P_2$ Lagrange finite element method within the FreeFem++ library [7], using 20 nodes per side on the boundary. This leads to the discrete linear system $Kx = \mu Mx$, where $K$ and $M$ are the usual finite element stiffness and mass matrices, both of which are sparse and symmetric and of size $1681 \times 1681$. With the relatively coarse mesh, we only expect the lower eigenmodes to be captured to high accuracy. We also note some eigenvalues occur with multiplicity 2. For this problem, the stiffness matrix is singular, and the eigenvector corresponding to $\lambda = 0$ is a constant function on $\Omega$, which explains the initially very small residual when the iteration is started with an initial iterate of ones.

We first implement our accelerated methods using $A = M \backslash K$, with $\eta = 10$, $\text{tol} = 1e-10$, a starting iterate of $u = \text{ones}(N,1)$, and a maximum of 400 iterations. We do not expect the largest discrete eigenvalue to be very close to the continuous one of a similar size ($5426 \pi^2$) since the discretization is coarse. Both the augmented and simple methods converge to $5439.464585998008 \pi^2$. The power method converges to a similar value, but with a much larger residual, suggesting greater inaccuracy in the eigenvector. The results are shown in fig. 4 on the left.

We next implement our accelerated method to locate the eigenvalue closest to the pair at $20\pi^2$. Using Matlab’s eig with an shift of $20.01\pi^2$ and the default tolerance of $10^{-14}$, we obtain that the nearest discrete eigenvalue as $\mu_h = 20.009477014838016 \pi^2$. We run our method on $A = (K - \text{shift} \times M) \backslash M$, with $\eta = 10$, $\text{tol} = 1e-10$, and a maximum of 400 iterations. The progression of the methods are shown in fig. 4 (right). Both simple and augmented methods quickly recover from the initial data along the component of the zero eigenvalue and demonstrate exponential convergence. The simple method converges to the same eigenvalue as the augmented method. The power iteration has a larger error, with the located eigenvalue agreeing with the augmented and simple methods to $10^{-11} \pi^2$, but with a much larger residual, suggesting an inaccurate approximation to the eigenvector.
We recall here the algorithms presented in this paper assume the first few dominant eigenvalues are positive. When applying a shift, this condition is easily violated, particularly early in the spectrum. So, for instance, if we seek the eigenvalues of the Neumann problem closest to $4\pi^2$ by using the true eigenvalue as a shift, the methods do not work.

Our final FEM example is for the Neumann eigenproblem when $\Omega$ consists of two squares of sides length 2, connected by a thin channel of thickness 0.01 and length 2, with 30 grid points per edge of the polygon, shown in fig. 5. In this instance, the eigenfunctions are not guaranteed to be regular, and we expect some eigenvalues to have high multiplicity.

We set the maximum number of iterations to 1300. Using $P_2$ Lagrange elements, we are lead to a $5461 \times 5461$ sparse system $Kx = \mu h Mx$. Matlab’s eigs yields the largest eigenvalue as $\approx 20081.60885\pi^2$. The simple and augmented methods yield the same eigenvalue, as does the power method; in this instance, the residual is least when using the augmented strategy. The residual histories for the three methods are shown in fig. 6, along with a comparison between the residual and projection used to compute the extrapolation parameter $\gamma$, in the augmented method.

5.4. Steklov eigenvalues. In this last example, we examine the behavior of our acceleration scheme on an eigenvalue problem involving the eigenvalues of a dense, and possibly ill-conditioned matrix.

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with a Lipschitz piecewise-smooth boundary $\Gamma$. The general Steklov eigenvalue problem can be stated as: find $u_m \in H^1(\Omega), \lambda_m \in \mathbb{R}$ so that

$$\Delta u_m = 0, \quad \forall x, \in \Omega, \quad \frac{\partial u_m}{\partial n} = \lambda_m u_m, \quad \forall x, \in \Gamma,$$

for eigenvalues $\lambda_m$ and eigenfunction $u_m$. The system (5.2) is called the Steklov problem, and $\lambda_m$ and $u_m$ are called Steklov eigenvalues and eigenfunctions. We note this spectrum
Figure 6. Residual histories for highest computed eigenvalue in the channel example (left), and the residual $\|d_k\|$ compared to the projection $p_k$ used in the augmented method.

Figure 7. Residual histories (left) and the residual $\|d_k\|$ compared to the projection $p_k$ used in the augmented method, for the Steklov problem.

coincides with that of the Dirichlet-to-Neumann operator $\Lambda : H^{3/2}(\Gamma) \to H^{-3/2}(\Gamma)$, given by $\Lambda u = \partial_n(\mathcal{H}u)$, where $\mathcal{H}u$ denotes the unique harmonic extension of $u \in H^{3/2}(\Gamma)$ to $\Omega$.

A particularly elegant and accurate (in the sense of approximation) strategy for computing $\lambda_m$ is via boundary integral strategies. We shall employ a modified single layer strategy. A modified formulation is based on the ansatz

$$\begin{align*}
\int_{\Gamma} \Phi(x-y)\varphi(y)\,ds(y) + \varphi & \in \Omega,
\end{align*}$$

based on the average of the density $\varphi = |\Gamma|^{-1} \int_{\Gamma} \varphi(y)\,ds(y)$, as suggested in [2, Equation 7.58]. Here $\Phi$ denotes the fundamental solution for the Laplacian. We introduce the operators $S : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ and $T : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ as

$$
S[\varphi] := \int_{\Gamma} \Phi(x-y)\varphi(y)\,ds(y), \quad x \in \Gamma, \quad T[\varphi] := \int_{\Gamma} \frac{\partial \Phi(x-y)}{\partial n(x)}\varphi(y)\,ds(y), \quad x \in \Gamma.
$$

Taking into account well known expressions (see e.g. [2]) for the jump of the single layer potential and its normal derivative across $\Gamma$, the eigenvalue problem (5.3) is reduced to a system of integral equations

$$
(\mathcal{T} + \frac{1}{2}I) [\varphi - \varphi] = \lambda (S[\varphi - \varphi] + \varphi), \quad x \in \Gamma,
$$

for the eigenvalue $\lambda$ and density $\varphi$. This system is discretized using a Fourier spectral strategy. The resultant discrete generalized eigenvalue problem is to find $\lambda \in \mathbb{R}, c \in \mathbb{R}^N$ such that $Ac = \lambda Bc$, where $B$ is invertible (thanks to the modification of the single layer). Both matrices are dense.

We take $\Omega$ to be the unit disk, and use $N = 32$ collocation points on $\Gamma$. The true eigenvalues are known to consist of the countable set $0, 1, 1, 2, 2, 3, 3, \ldots$; with the discrete
strategy used, we expect the largest eigenvalue we approximate to be close to 16. This is indeed the case. All three tested methods locate the eigenvalue correct to 14 digits. (We have used a tolerance of $10^{-10}$). The rapid decay of the residual is evident in the accelerated methods (see fig. 7, left). Once again, since $\lambda = 0$ is an eigenvalue (corresponding to the constant eigendensity case), and our starting iterate of a vector of ones leads to an initial near-zero residual. The somewhat oscillatory convergence behavior is due to interference from eigencomponents other than the first two most dominant ones. This suggests that introducing an extrapolation technique with greater depth that is designed to reduce multiple components at each step (instead of just the second-most dominant) may lead to smoother convergence. Figure 7 on the right compares the residual to the projection used in the augmented method. Similarly to the previous example (see fig. 6, right), here the projection $p_k$ of the update along the approximate eigenvector, converges at a better rate than the full residual; in contrast, however, it achieves a tolerance of $10^{-15}$, when the residual is reduced to $10^{-10}$.

6. Conclusion

In this paper we introduced and analyzed algorithm 2, a simple method to accelerate the power iteration. We proved the method features exponential convergence if the initial iterate has components of only two eigenvectors. We further introduced algorithm 3, which modifies the simple method to help stabilize the early stages of the iteration. Both methods are one-step extrapolation techniques which form the accelerated iterates from a linear combination of the two most recent update steps. The extrapolation parameter is computed by a ratio of residuals, and requires minimal additional computation beyond a residual norm and Rayleigh quotient at each iteration. The methods are shown numerically to be robust with respect to initial iterate, and to substantially improve performance in the case where the spectral gap is small.

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