The extrapolated modified Aitken iteration method applied to σ_1-ordered systems of linear equations

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The extrapolated Aitken iteration method as applied to σ_2-ordered systems of linear equations was proposed and analyzed by Evans (1963), who showed that with a suitable choice of extrapolation factor, together with Chebyshev acceleration, an asymptotic rate of convergence superior to that of S.O.R. may be obtained for certain problems.

The present paper applies the above method to σ_1-ordered systems of linear equations, and the analysis concerning the extrapolation and Chebyshev acceleration of the iterative procedure is discussed. The theoretical results derived for the asymptotic rate of convergence for both the σ_1 and σ_2-orderings are confirmed by numerical examples.

We seek the solution vector $\boldsymbol{x}$ to the equation

$$\boldsymbol{Ax} = \boldsymbol{d} \tag{1}$$

where $\boldsymbol{A}$ is a given $(N \times N)$ symmetric, positive definite matrix, and $\boldsymbol{x}$, $\boldsymbol{d}$ are $(N \times 1)$ vectors. We shall assume that $\boldsymbol{A}$ has the form $\boldsymbol{I}$–$\boldsymbol{L}$–$\boldsymbol{U}$, where $\boldsymbol{L}$ and $\boldsymbol{U}$ are, respectively, lower and upper triangular matrices with zero diagonal entries, and $\boldsymbol{I}$ is the identity matrix. Since $\boldsymbol{A}$ is symmetric, $\boldsymbol{L}$ is $\boldsymbol{U}^T$.

The extrapolated modified Aitken iteration method for a σ_2-ordered system of linear equations (Evans, 1963) is defined by the equations

$$(\boldsymbol{I} - \omega\boldsymbol{L})(\boldsymbol{I} - \omega\boldsymbol{U})\hat{\boldsymbol{x}}^{(n+1)} = [\omega^2\boldsymbol{LU} + (1 - \omega)\boldsymbol{I}]\boldsymbol{x}^{(n)} + \omega\boldsymbol{d} \tag{2a}$$

and

$$\boldsymbol{x}^{(n+1)} = \boldsymbol{x}^{(n)} + \alpha_n(\hat{\boldsymbol{x}}^{(n+1)} - \boldsymbol{x}^{(n)}) + \beta_n(\boldsymbol{x}^{(n)} - \boldsymbol{x}^{(n-1)}), \tag{2b}$$

where the optimum ω_2 is that value of ω which minimizes the spectral radius of $\boldsymbol{Q}(\omega)$, where

$$\boldsymbol{Q}(\omega) \equiv \boldsymbol{I} - \omega(\boldsymbol{I} - \omega\boldsymbol{U})^{-1}(\boldsymbol{I} - \omega\boldsymbol{L})^{-1}\boldsymbol{A}, \tag{3}$$

the error operator of equation (2*a*).

Furthermore, it was shown that the optimum ω satisfies the quartic equation

$$\frac{2}{\omega_2} = \frac{\tau_n}{P_n} + \frac{\tau_1}{P_1} \tag{4}$$

where

$$\tau_s = \boldsymbol{\psi}_s^T\boldsymbol{A}\boldsymbol{\psi}_s, \quad s = 1, n$$

$$k_s = \boldsymbol{\psi}_s^T\boldsymbol{LU}\boldsymbol{\psi}_s$$

$$P_s = 1 - \omega_2(1 - \tau_s) + \omega_2^2 k_s,$$

and $\boldsymbol{\psi}_1$ and $\boldsymbol{\psi}_n$ are the eigenvectors corresponding to the algebraically highest and lowest eigenvalues of $\boldsymbol{Q}(\omega)$ when $\omega = \omega_2$.

Finally, the Chebyshev acceleration parameters are given by

$$\alpha_0 = 1$$

and

$$\alpha_n = \frac{2}{\delta}\frac{T_n(\delta^{-1})}{T_{n+1}(\delta^{-1})}, \quad \beta_n = \frac{T_{n-1}(\delta^{-1})}{T_{n+1}(\delta^{-1})}, \quad n = 1, 2, \ldots \tag{5}$$

where $\delta = \dfrac{1 - V}{1 + V}$ and $V = \dfrac{1}{2(\omega_2^{-1} - 1) + 2\omega_2 k_1 + \tau_1}$

is the spectral radius of $\boldsymbol{Q}(\omega_2)$.

Since the optimum extrapolation factor and the Chebyshev acceleration parameters are not simple to estimate, the use of the above proposed iteration for practical applications is severely limited.

We now apply a similar iterative procedure, i.e. equation (2), but this time further assume that the matrix $\boldsymbol{A}$ possesses Property A (Young, 1954). Hence the system of equations given by (1) is σ_1-ordered and we can write

$$\boldsymbol{A} \equiv \boldsymbol{I} - \boldsymbol{B} \equiv \begin{bmatrix} \boldsymbol{I}_1 & -\boldsymbol{U}^* \\ -\boldsymbol{L}^* & \boldsymbol{I}_2 \end{bmatrix}, \tag{6}$$

$$\boldsymbol{L} \equiv \begin{bmatrix} 0 & 0 \\ \boldsymbol{L}^* & 0 \end{bmatrix} \text{ and } \boldsymbol{U} \equiv \begin{bmatrix} 0 & \boldsymbol{U}^* \\ 0 & 0 \end{bmatrix},$$

where $\boldsymbol{U}^*$ is an $(m \times r)$ submatrix, $\boldsymbol{L}^*$ is an $(r \times m)$ submatrix, $\boldsymbol{I}_1$, $\boldsymbol{I}_2$ are $(m \times m)$ and $(r \times r)$ identity submatrices, respectively, and $m + r = N$.

Now, the analysis given earlier simplifies in the following manner when we take into consideration the special property possessed by the matrix $\boldsymbol{A}$. For, if λ is an eigenvalue of $\boldsymbol{Q}(\omega)$ and $\boldsymbol{\psi} = \begin{vmatrix} \boldsymbol{y} \\ \boldsymbol{z} \end{vmatrix}$ is the corresponding eigenvector, we have the usual eigenvector statement

$$\boldsymbol{Q}(\omega)\boldsymbol{\psi} = \lambda\boldsymbol{\psi}$$

or $$[(1 - \omega)\boldsymbol{I} + \omega^2\boldsymbol{LU}]\boldsymbol{\psi} = \lambda(\boldsymbol{I} - \omega\boldsymbol{L})(\boldsymbol{I} - \omega\boldsymbol{U})\boldsymbol{\psi}. \tag{7}$$

If we take advantage of the relationships given by (6), equation (7) further simplifies to

$$\boldsymbol{I}(1 - \omega)\boldsymbol{y} = \lambda\boldsymbol{I}\boldsymbol{y} - \lambda\omega\boldsymbol{U}^*\boldsymbol{z}$$

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$$[(1-\omega)\boldsymbol{I}+\omega^2\boldsymbol{L}^*\boldsymbol{U}^*]z=-\lambda\omega\boldsymbol{L}^*y+\lambda(\boldsymbol{I}+\omega^2\boldsymbol{L}^*\boldsymbol{U}^*)z. \tag{8}$$

Eliminating y, we have

$$\lambda^2\boldsymbol{I}z+\{\lambda[\omega^3\boldsymbol{L}^*\boldsymbol{U}^*-2\omega^2\boldsymbol{L}^*\boldsymbol{U}^*-2(1-\omega)\boldsymbol{I}] +(1-\omega)([1-\omega]\boldsymbol{I}+\omega^2\boldsymbol{L}^*\boldsymbol{U}^*)\}z=0. \tag{9}$$

Now it is easily shown that the non-zero eigenvalues of $\boldsymbol{B}$ occur in pairs, i.e. $\pm u_i$ $(i=1,2,\ldots m)$, where m is less than or equal to the number of rows in $\boldsymbol{L}^*$ or $\boldsymbol{U}^*$. Furthermore, the eigenvalues of $\boldsymbol{L}^*\boldsymbol{U}^*$ are precisely u_i^2 $(i=1,2,\ldots m)$ or zero.

Therefore, the relationship

$$\lambda^2+\lambda[\omega^3u_i^2-2\omega^2u_i^2-2(1-\omega)] +(1-\omega)(1-\omega+\omega^2u_i^2)=0 \tag{10}$$

must hold between the eigenvalues of the Jacobi iteration matrix $\boldsymbol{B}$ and the eigenvalues of the extrapolated Aitken iteration matrix $\boldsymbol{Q}(\omega)$.

Our main concern in extrapolating the basic iterative method (2) is to choose a value of ω which results in a minimization of the spectral radius of $\boldsymbol{Q}(\omega)$ and from the above paragraph, it follows that the spectral radius of the extrapolated Aitken iteration is related to the spectral radius of the basic Jacobi iteration by the following equation

$$\lambda^2+\lambda[\omega^3u_1^2-2\omega^2u_1^2-2(1-\omega)] +(1-\omega)(1-\omega+\omega^2u_1^2)=0. \tag{11}$$

The discriminant of the quadratic (11) is given by

$$\omega^2u_1^2[4(1-\omega)^2+\omega^2u_1^2(\omega-2)^2]$$

which is >0 for all $\omega\neq 0$ and $u_i\neq 0$. Therefore, the roots of the quadratic (11) are always real for all values of u_i $(i=1,2,\ldots m)$.

Further, the iteration defined by equation (2) converges if $-1<\lambda<1$. The upper limit is satisfied when $\omega>0$, whilst the lower limit is attained when $\omega=\omega_f$, i.e. when

$$2u_1^2\omega_f^3-\omega_f^2(3u_1^2+1)+4\omega_f-4=0. \tag{12}$$

Since the coefficients of the quadratic equation (11) are not simple in form, it is difficult, for this iteration, to predict the form of variation of the eigenvalues λ with ω. In an earlier paper (Evans, 1963) the author proceeded empirically and calculated the values of λ for the lowest-order finite-difference representation of two model problems, namely

PROBLEM I: $$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0,\quad h^{-1}=5$$

in the unit square with prescribed boundary values; and

PROBLEM II: $$\frac{d^2\phi}{dx^2}=0,\quad h^{-1}=10,20$$

on a unit interval with prescribed terminal values.

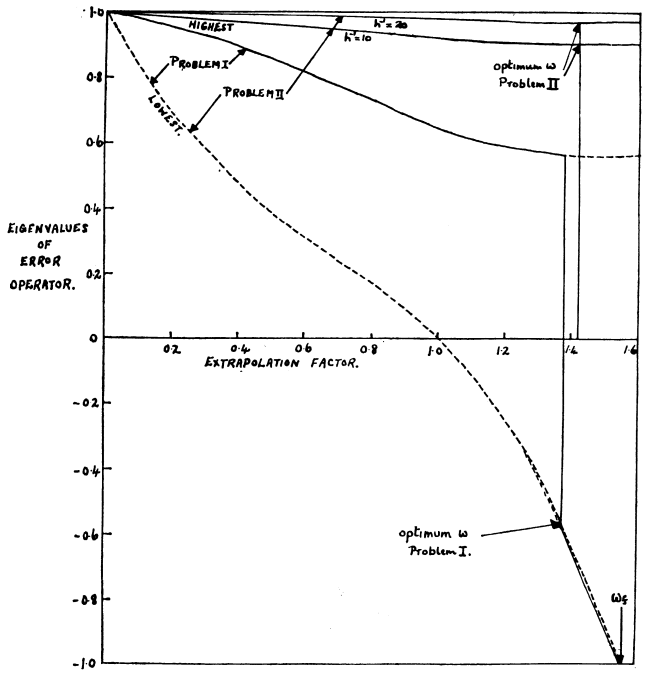

Fig. 1.—Extrapolated Aitken iteration: Problems I and II

Let us now choose the same two problems and proceed empirically as before. The results are displayed in Fig. 1. We observe that the lowest extreme values of λ are monotonic in ω, and convergence is achieved when ω lies in the range $0<\omega<\omega_f$, where ω_f is given by (12), whilst the highest extreme values of λ possess a minimum point within the range of convergence.

We further observe from Fig. 1 that the minimization process of the spectral radius of $\boldsymbol{Q}(\omega)$ is different for Problems I and II.

For Problem I, the minimization occurs when the extreme values of λ are equal in magnitude, but opposite in sign. This happens when the coefficient of λ in (11) is zero, i.e. when

$$\omega_1^3u_1^2-2\omega_1^2u_1^2+2\omega_1-2=0 \tag{13}$$

at which time the spectral radius of $\boldsymbol{Q}(\omega_1)$ is given by

$$\lambda=\pm[(\omega_1-1)(1-\omega_1+\omega_1^2u_1^2)]^{1/2}$$

which, by the use of equation (12), can be further simplified to

$$\lambda=\pm[1-\omega_1^2(1-u_1^2)]^{1/2}. \tag{14}$$

Thus the optimum ω_1 is given by (13) which can be easily verified to have at least one real root in the range $1<\omega<2$.

For Problem II, the minimization occurs when the largest eigenvalue λ_1 is minimized, i.e. when $\frac{d\lambda_1}{d\omega}=0$.

Differentiating λ_1, we find that this occurs when the spectral radius of $\boldsymbol{Q}(\omega_1)$ is given by

$$\lambda_1 = 1 - \frac{2\omega_1(1 - u_1^2)}{3\omega_1^2 u_1^2 - 4\omega_1 u_1^2 + 2}. \quad (15)$$

Substituting this value of λ_1 into (11), we obtain the result that the optimum ω_1 satisfies the quartic equation

$$3u_1^2\omega_1^4 - 4u_1^2\omega_1^3 - 4\omega_1^2 + 8\omega_1 - 4 = 0. \quad (16)$$

It can be shown that (16) has at least one real root in the range $1 < \omega < 2$. We can further simplify equation (15) with the aid of (16) to obtain the spectral radius of $\boldsymbol{Q}(\omega_1)$ as

$$\lambda_1 = 1 - \frac{\omega_1(1 - u_1^2)}{1 + 2(1 - \omega_1^{-1})^2}. \quad (17)$$

Similarly, λ_2 the lowest eigenvalue of $\boldsymbol{Q}(\omega_1)$ is obtained from equation (11).

If we assume $\lambda_2 = -\lambda_1$ for the purpose of providing simple bounds for the Chebyshev acceleration process the equations (5) are valid; otherwise the parameters of the Chebyshev acceleration are given by

$$\alpha_n = \frac{4}{(b-a)}\frac{T_n(\gamma)}{T_{n+1}(\gamma)}; \quad \beta = \frac{T_{n-1}(\gamma)}{T_{n+1}(\gamma)}, \quad (18)$$

where $\gamma = [(b + a)/(b - a)]$ and a and b are the smallest and largest eigenvalues of the matrix $\boldsymbol{I} - \boldsymbol{Q}(\omega)$.

Thus, summarizing the results derived in this section, we have shown that when the extrapolated Aitken iteration method is applied to σ_1-ordered systems of linear equations, the optimum extrapolation factor which minimizes the spectral radius of the error operator is a simple root ($1 < \omega < 2$) of a linear cubic equation when $u_1 \leqslant 0{\cdot}9$, and a root of a quartic equation when $u_1 > 0{\cdot}9$, the coefficients of both equations depending upon the largest eigenvalue u_1 of the associated Jacobi iteration.

Consequently, the extrapolation and Chebyshev acceleration parameters can be determined very easily from an estimate of the largest eigenvalue of the Jacobi iteration matrix. The iterative method, therefore, is much more easily defined than in the case with σ_2-ordering. Thus it appears that the asymptotic rates of convergence may be greatly affected by different consistent orderings, which is not true for the S.O.R. method. Lynn (1964) has recently shown that similar results are valid for the S.S.O.R. method.

For the practical application of the extrapolated Aitken method we now proceed on similar lines as for the S.O.R. method. After an initial estimate of the largest eigenvalue of the Jacobi iteration matrix u_1, the optimum parameter ω_1 is determined by solving the appropriate equation (13) or (16) using the Newton–Raphson method with a starting approximation $\omega_1^{(0)} \approx 1{\cdot}4$. In practice only 3 to 5 applications of this process are required if we assume convergence to be sufficient when

$$|\omega_1^{(m+1)} - \omega_1^{(m)}| < 0{\cdot}01.$$

Immediately ω_1 is known, the spectral radius λ can be determined from (14) or (17), and the Chebyshev acceleration parameters from (5) or (18), to define the complete iterative process.

Asymptotic rates of convergence for the extrapolated Aitken iteration with σ_1-ordering are obtained when we assume $u_1 = 1 - \varepsilon$, where $\varepsilon \ll 1$. It is easily verified from (16) that $\omega_1 = \sqrt{2}$ is a close approximation to the optimum extrapolation factor, whilst the spectral radius given by (17) is $1 - (\sqrt{2} + 1)\varepsilon$. The asymptotic rate of convergence of the complete iteration process (2) is not less than $2{\cdot}2\varepsilon^{1/2}$, which compares slightly unfavourably with the S.O.R. method, whose convergence rate is $2\sqrt{2}\varepsilon^{1/2}$. Finally, the range of convergence of the iterative process (2) is given by $0 < \omega < 1{\cdot}54$, since $1{\cdot}55$ can be shown to be a close approximation to a root of (12).

Experimental programs were written for the Manchester University Atlas computer to perform the procedures discussed in this paper. Fig. 1 shows the highest and lowest eigenvalues of the error operator plotted as functions of ω for the σ_1-ordering for both Problems I and II, whilst Figs. 2, 3 and 4 show the asymptotic rates of convergence for both the σ_1 and σ_2-orderings of the extrapolated Aitken iteration method compared with that of the S.O.R. method for each problem. The asymptotic rates of convergence of all three processes at the optimum ω are given in Table 1, from which we can establish that the σ_1-ordering compares unfavourably with the S.O.R. method, as predicted by theoretical considerations. The results for the σ_2-ordering agree with the theoretical considerations given elsewhere (Evans, 1963). Furthermore, the ranges of convergence of the extrapolated Aitken method for the σ_1 and σ_2-orderings can be verified both experimentally and theoretically to be $1{\cdot}55$ and $1{\cdot}5$, respectively.

The relative efficiency of the extrapolated Aitken method to the S.O.R. method will now be discussed. The amount of work done at each mesh point for the

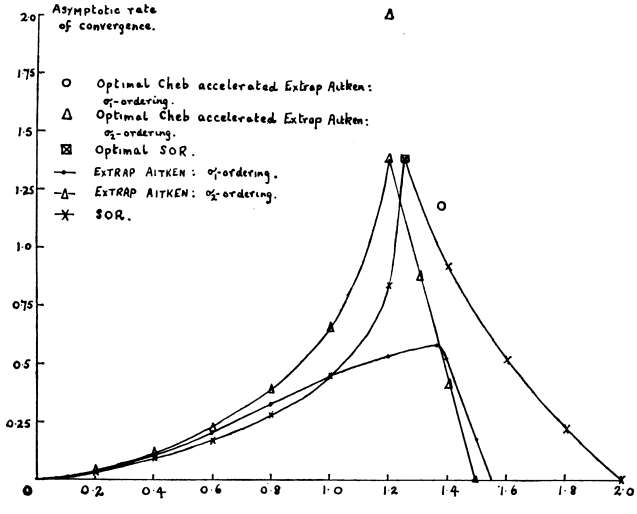

Fig. 2.—Asymptotic rates of convergence: Problem I

Table 1

Optimized rates of convergence

METHOD	PROBLEM I, $h^{-1} = 5$	PROBLEM II, $h^{-1} = 10$	PROBLEM II, $h^{-1} = 20$
Chebyshev accelerated extrapolated Aitken, σ_1-ordering ($\omega = \omega_1$)	1·178 $\omega_1 = 1{\cdot}38$ $\lambda_1 = 0{\cdot}563$	0·428 $\omega_1 = 1{\cdot}42$ $\lambda_1 = 0{\cdot}903$	0·224 $\omega_1 = 1{\cdot}42$ $\lambda_1 = 0{\cdot}973$
Chebyshev accelerated extrapolated Aitken, σ_2-ordering ($\omega = \omega_2$)	2·063 $\omega_2 = 1{\cdot}2$ $\lambda_2 = 0{\cdot}25$	0·470 $\omega_2 = 1{\cdot}38$ $\lambda_2 = 0{\cdot}608$	0·301 $\omega_2 = 1{\cdot}46$ $\lambda_2 = 0{\cdot}806$
Optimized S.O.R. ($\omega = \omega_b$)	1·386 $\omega_b = 1{\cdot}25$ $\lambda_b = 0{\cdot}25$	0·580 $\omega_b = 1{\cdot}5603$ $\lambda_b = 0{\cdot}5603$	0·301 $\omega_b = 1{\cdot}7406$ $\lambda_b = 0{\cdot}7406$

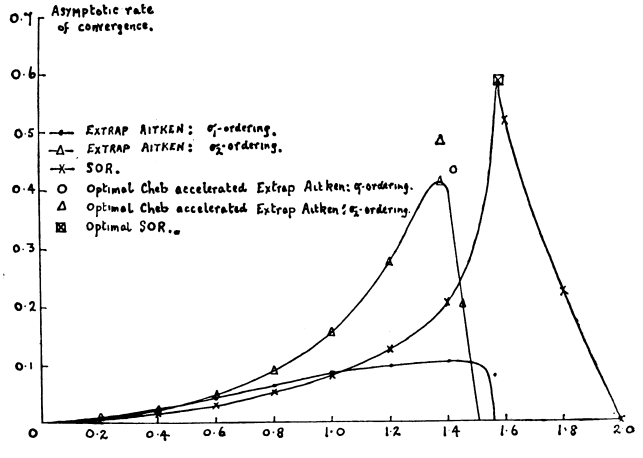

Fig. 3.—Asymptotic rates of convergence: Problem II, $h^{-1}=10$

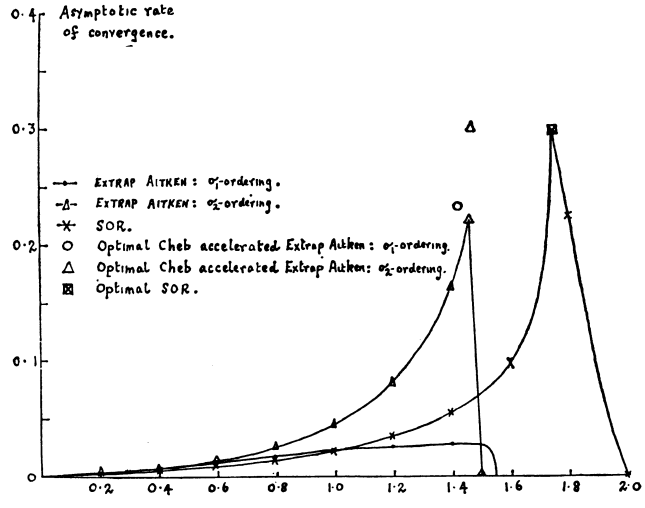

Fig. 4.—Asymptotic rates of convergence: Problem II, $h^{-1}=20$

general 5-point finite-difference equation is 5 multiplications and 6 additions for the S.O.R. method, but 8 multiplications and 8 additions for the σ_1-ordering and 7 multiplications and 7 additions for the σ_2-ordering of the extrapolated Aitken method. Thus the new method compares unfavourably in efficiency by approximately 50%.

Finally, the author wishes to thank the referee whose criticisms and comments have greatly improved this paper.

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