Convergence Analysis of Waveform Relaxation Methods Using Pseudospectra

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Abstract

The performance of the waveform relaxation method for solving systems of ODEs depends largely on the choices that are made for splitting, size of time window and preconditioning. Although it is known that superlinear convergence is obtained on finite time windows, the convergence may be slow in the first few iterations. We propose the use of pseudospectra to analyze the convergence ratio of the first few iterations when waveform relaxation is applied to linear systems of ODEs. Through pseudospectral radii we can examine the effect of preconditioning and overlapping on the rate of convergence. We may also use this to estimate a suitable size of the time window. Numerical experiments performed on a system of ODEs arising from the discretization of an advection-diffusion equation confirm the validity of the obtained estimates.

1 Introduction

The progress in parallel computing has made competitive iterative techniques for the numerical solution of large systems of ODEs. Such an iterative approach, called waveform relaxation, was first proposed by Lerasmee [7] and Lerasmee et al. [8] for time domain analysis of metal oxide semiconductor digital circuits. Nevanlinna [12, 13] and Miekkala and Nevanlinna [10, 11] use the term dynamic iteration to distinguish these methods from static iterative schemes for the numerical solution of linear systems of equations.

It has been observed by many authors that the approach based on waveform relaxation can be quite competitive with the existing methods for differential systems if the resulting iterations converge quickly. Unfortunately, this is not always the case and many attempts have been made to accelerate the rate of convergence of these iterations. Nevanlinna [14], Skeel [18] and Lubich [9] investigate the possibility to accelerate waveform relaxation

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schemes by taking linear combinations of the iterates. Lubich [9] also observed that the techniques to accelerate the convergence of waveform relaxation can be applied in the Laplace transform domain. Vandewalle [22] investigated the acceleration of convergence by multigrid techniques in the context of waveform relaxation methods for parabolic partial differential equations. Pohl [15], Jeltsch and Pohl [5] and Frommer and Pohl [3] investigated the effect of overlapping of the components of the system on the speed of convergence of the resulting dynamic iterations. Burrage et al. [2] also tested this technique on the linear systems of differential equations resulting from semidiscretization of the one and two dimensional heat equation, and they observed that some modes of overlapping are very effective in the one dimensional case and lead only to a modest improvement in the two dimensional case. Spilling [19] considers preconditioning the differential system (on the left) with the hope that this may lead to a faster iterative process than that obtained by applying the waveform relaxation technique to the original problem. He also discusses how to construct a specific preconditioner for a differential system resulting from the application of pseudospectral methods to a one-dimensional hyperbolic partial differential equation. Preconditioning on the right was proposed by Burrage [1] and examined carefully by Burrage et al. [2] for linear differential systems. This technique proved to be very effective for linear systems approximating the heat equation in two space dimensions.

Nevanlinna [12] has proved superlinear convergence of dynamic iterations for linear differential systems on finite time intervals. He also demonstrated that the spectral radius of the convolution operator which defines the dynamic iterations is equal to zero irrespective of the splitting of the original differential system and as a consequence gives no information about the effect of splitting on the actual rate of convergence of the resulting iterations. To obtain such information, Nevanlinna [12] introduced exponential weights into the error estimates, and Miekkala and Nevanlinna [10] studied the convergence in the Banach spaces defined on the interval $[0, \infty)$.

The task of obtaining practical measures of the speed of convergence of dynamic iterations is not easy. Leimkuhler [6] introduced convergence ratios r_i computed as $(e_i/e_0)^{1/i}$ where e_i is the difference between the ith and $(i-1)$th iterates in the maximum norm. Due to the superlinear convergence, these ratios ultimately tend to zero as $i \to \infty$, but the first few of them give some information about the speed of convergence of the corresponding iterations. These ratios were also used by Burrage et al. [2] to compare the waveform relaxation schemes implemented in block Gauss-Jacobi mode with or without preconditioning and overlapping. These modes were denoted by BJ, PBJ, BJO, and PBJO.

Using Laplace transform techniques, Leimkuhler [6] also obtained computable estimates for a window of rapid convergence of waveform relaxation iterations in BJ mode applied to a linear second order model system. This technique was extended by Burrage et al. [2] to obtain similar estimates in the preconditioned and/or overlapped modes. However, these estimates, especially when applied to PBJ and PBJO modes are not very reliable and different techniques for comparing the relative merits of different modes are needed.

In this paper we propose one such technique which is based on using the notion of ϵ-pseudospectra of matrices as introduced by Trefethen [20]. For this purpose, the integral operator which defines the continuous time waveform relaxation iterations is first approximated by a composite trapezoidal rule which leads to an iteration process in a finite dimensional space. The realistic convergence rates can then be related to the ϵ-pseudospectral radii of the corresponding iteration matrix (see Trefethen [21]). By considering these ϵ-pseudospectral radii for the different splittings, modes, and time window sizes, we can explain the observed behaviour of the dynamic iterations in many cases. This technique seems to provide more accurate information about the respective convergence rates than that based on the Laplace transform approach presented in Burrage et al. [2]. The finite dimensional iteration matrices corresponding to the BJ and BJO modes are block Toeplitz. For such matrices, efficient techniques for estimating the pseudospectra were introduced by Reichel and Trefethen [17]. The iteration matrices corresponding to the PBJ and PBJO modes do not have the block Toeplitz structure and the computation of ϵ-pseudospectral radii is more costly.

2 Preconditioning and overlapping

In this section we will describe the technique of preconditioning the differential system on the right and overlapping the components of the system. Consider the linear problem

$$
(2.1) \qquad \begin{cases} y'(t) + Q\, y(t) = g(t), & t \in [0,T], \\ y(0) = y_0, \end{cases}
$$

where Q is a consant matrix of dimension n. The waveform relaxation iterations corresponding to the splitting of the matrix Q into

$$
Q = M - N
$$

are defined by

$$
(2.2) \qquad \begin{cases} \dfrac{d}{dt} y^{(k+1)}(t) + M\, y^{(k+1)}(t) = N\, y^{(k)}(t) + g(t), \\ y^{(k+1)}(0) = y_0, \end{cases}
$$

$t \in [0,T]$, where $y^{(0)}$ is a given initial guess usually chosen as $y^{(0)}(t) = y_0$, $t \in [0,T]$. The technique of preconditioning (on the right) consists of applying the waveform relaxation to the differential system

$$
(2.3) \qquad \begin{cases} z'(t) + B(t)\, z(t) = e^{-Nt} g(t), & t \in [0,T], \\ z(0) = y_0 \end{cases} ,
$$

$t \in [0,T]$, where the matrix $B(t)$ is defined by

$$
B(t) = e^{-Nt}\, M\, e^{Nt}.
$$

This system is obtained from (2.1) by making the transformation

$$
z(t) = e^{-Nt}\, y(t).
$$

Splitting the matrix $B(t)$ into

$$B(t) = M - N(t),$$

where M corresponds to the original splitting of the matrix Q and

$$N(t) = M - e^{-Nt} M e^{Nt},$$

leads to the following dynamic iteration scheme applied to (2.3)

$$\begin{cases} \frac{d}{dt} z^{(k+1)}(t) + M\, z^{(k+1)}(t) = N(t) z^{(k)}(t) + e^{-Nt}\, g(t), \\ z^{(k+1)}(t) = y_0, \end{cases} \tag{2.4}$$

$t \in [0, T]$, with a given initial guess $z^{(0)}$. The technique described above was briefly introduced in Burrage [1] and examined in detail in Burrage et al. [2], where the following error bound was obtained

$$\|z^{(\nu)} - z\|_T \le \sum_{i=0}^{\infty} \frac{A_i^{\nu} T^{\nu(i+1)}}{((i+1)!)^{\nu} \nu!}, \tag{2.5}$$

$\nu = 0, 1, \ldots$. Here, A_i are constants such that

$$\|e^{-Mt} \Delta_i\|_T \le A_i,$$

and Δ_i are commutators defined recursively by

$$\Delta_{i+1} = \Delta_i N - N \Delta_i,$$

$i = 0, 1, \ldots$, with $\Delta_0 = M$. As discussed in Burrage et al. [2] if the constants A_i do not grow too fast then a reasonable approximation to this bound is

$$\Psi_P(T, \nu) = \frac{A_1^{\nu}\, T^{2\nu}}{2^{\nu}\, \nu!}.$$

On the other hand, in the case of non-preconditioned iterations (2.2) the error bound takes the form

$$\Psi_N(T, \nu) = \frac{A_0^{\nu}\, T^{\nu}}{\nu!}$$

where A_0 is a constant such that

$$\|e^{-Mt} N\|_T \le A_0,$$

compare Nevanlinna [12]. These bounds suggest that the preconditioned waveform relaxation iterations (2.4) should converge faster than (2.2) at least for some $T^* < 2$. A similar conclusion can also be obtained by the error analysis in the Laplace transform domain. These conclusions were indeed confirmed by extensive numerical experiments presented in

Burrage et al. [2] on the linear systems approximating the heat conduction equation in one and two space variables.

We will now describe the technique of overlapping the components of the system as proposed by Pohl [15] and further studied by Jeltsch and Pohl [5], Frommer and Pohl [3], and Burrage et al. [2]. Assume that the matrix M that corresponds to the splitting of the matrix Q of dimension n has block diagonal structure with block sizes $b_1, b_2, \dots, b_r$ and that the blocks overlap by $o_1, o_2, \dots, o_{r-1}$ where all $o_i \geq 0$ and

$$\sum_{i=1}^{r} b_i - \sum_{i=1}^{r-1} o_i = n.$$

Put $\tilde{n} = \sum_{i=1}^{r} b_i$. It was demonstrated in [2] that the new system formed from (2.1) takes the form

$$\left\{ \begin{array}{l} \tilde{y}'(t) + \tilde{Q}(t)\tilde{y}(t) = \tilde{g}(t), \\ \tilde{y}(0) = \tilde{y}_0, \end{array} \right. \tag{2.6}$$

where $\tilde{Q} \in \mathbb{R}^{\tilde{n}\times\tilde{n}}$, $\tilde{y}(t)$, $\tilde{g}(t)$, $\tilde{y}_0 \in \mathbb{R}^{\tilde{n}}$, can be obtained from Q, $y(t)$, $g(t)$ and y_0, respectively, by a simple algorithm defined in [2]. It was also demonstrated in [2] that the speed of convergence of dynamic iterations applied to (2.6) is usually faster than the corresponding iterations applied to (2.1) and in many cases there is a dramatic improvement in performance. The iterates $\tilde{y}^{(k)}(t)$ can be mapped into the space $\mathbb{R}^n$ by the formula

$$y^{(k)}(t) = PE\tilde{y}^{(k)}(t),$$

where P and E are projection and weight matrices of appropriate dimensions.

In this paper we will analyze the relative performances of various modes of block-Jacobi methods by using the pseudospectral techniques advocated by Trefethen [21]. These modes will be denoted by BJ, PBJ, BJO and PBJO, where P stands for preconditioning and O for overlapping. These modes will be tested on the linear differential system obtained from an advection-diffusion equation by discretizing the space variables. This leads to a system of the form (2.1) with the matrix Q given by

$$Q = \begin{bmatrix} d & e & & & \\ c & d & e & & \\ & \ddots & \ddots & \ddots & \\ & & c & d & e \\ & & & c & d \end{bmatrix} \tag{2.7}$$

$d > 0$, $c < 0$, $e < 0$ and the function $g(t)$ determined by the boundary conditions for the advection-diffusion equation. This is explained in more details in Section 5. As demonstrated in [2] the error equation for the dynamic iterations (2.2) takes the form

$$\epsilon^{(k+1)}(t) = \int_0^t e^{M(s-t)} N \epsilon^{(k)}(s)ds, \quad k = 0, 1, \dots \tag{2.8}$$

where $\epsilon^{(k)}(t) = y(t) - y^{(k)}(t)$.

Observe that the matrix given by (2.7) is, in general, non-normal which may lead to additional numerical difficulties as compared with the normal case. By making the substitution

$$z = \Gamma y$$

with the matrix Γ defined by

$$\Gamma = \mathrm{diag}(1, \alpha, \alpha^2, \ldots, \alpha^{n-1}),$$

$\alpha = \sqrt{e/c}$, the problem (2.1) can be reduced to the linear system

$$\left\{ \begin{array}{ll} z'(t) + \tilde{Q}\, z(t) = \Gamma g(t), & t \in [0, T], \\ z(0) = \Gamma y_0, & \end{array} \right. \tag{2.9}$$

where the matrix $\tilde{Q} = \Gamma Q \Gamma^{-1}$ is normal. However this will *not* remedy the situation. Indeed, it can be easily verified that the corresponding splitting of the matrix $\tilde{Q}$ is

$$\tilde{Q} = \tilde{M} - \tilde{N}$$

with

$$\tilde{M} = \Gamma M \Gamma^{-1}, \qquad \tilde{N} = \Gamma N \Gamma^{-1}.$$

Observe also that $\sigma(M^{-1}N) = \sigma(\tilde{M}^{-1}\tilde{N})$. Multiplying the error equation (2.8) by Γ we obtain

$$\tilde{\epsilon}^{(k+1)}(t) = \int_0^t \Gamma e^{M(s-t)} \Gamma^{-1} \tilde{N} \tilde{\epsilon}^{(k)}(s) ds, \tag{2.10}$$

$k = 0, 1, \ldots$, where $\tilde{\epsilon}^{(k)}(t) = \Gamma \epsilon^{(k)}(t)$. Since

$$\Gamma e^{M(s-t)} \Gamma^{-1} = e^{\tilde{M}(s-t)}$$

the equation (2.10) takes the form

$$\tilde{\epsilon}^{(k+1)}(t) = \int_0^t e^{\tilde{M}(s-t)} \tilde{N} \tilde{\epsilon}^{(k)}(s) ds,$$

$k = 0, 1, \ldots$, which is the error equation of the dynamic iterations applied directly to (2.9) with the splitting $\tilde{Q} = \tilde{M} - \tilde{N}$. This means that the dynamic iterations $y^{(k)}$ with respect to (2.1) and $z^{(k)}$ with respect to (2.9) are related by $z^{(k)} = \Gamma y^{(k)}$ which has the same form as the relationship between z and y.

3 Approximation in finite dimension

In all the cases that we have considered, the error $\epsilon^{(k)} = y^{(k)} - y$ of the waveform relaxation iterations can be written as

$$\epsilon^{(k+1)} = \mathcal{K} \epsilon^{(k)},$$

where $\mathcal{K}$ is an integral operator of the form

$$\mathcal{K}y\,(t) = \int_0^t K(t,s)y(s)ds \tag{3.1}$$

and $K(t,s)$ is an $n \times n$ matrix defined and uniformly bounded in the region $\{(t,s) : 0 \leq t \leq T,\ 0 \leq s \leq t\}$. Our idea is to replace the integral by the composite trapezoidal rule and represent any function on $[0,T]$ by its values on the mesh $\{t_i\}_{i=0}^q$ where $t_i = ih$ and $h = T/q$. Thus, for each $i = 1,\ldots,q$ we approximate $\mathcal{K}y(t_i)$ by the sum

$$\mathcal{K}y\,(t_i) = \frac{h}{2}\left(K(t_i,t_i)y(t_q) + K(t_i,t_0)y(t_0)\right) + h\sum_{j=2}^{i-1} K(t_i,t_j)y(t_j).$$

We shall also make use of the fact that for waveform relaxation iterations we have $\epsilon^{(k)}(0) = 0$ for all $k \geq 0$. For a function $y(t)$ it is convenient to define the nq-vector $\tilde{y}$ as

$$\tilde{y} = (y(t_1)^T, \ldots, y(t_q)^T)^T$$

Now we can write the discrete iteration for the error as follows

$$\tilde{\epsilon}^{(k+1)} = \mathcal{K}_q\tilde{\epsilon}^{(k)},$$

where $\mathcal{K}_q$ is an $nq \times nq$ matrix constructed from $n \times n$ blocks in the following way

$$\mathcal{K}_q = \begin{bmatrix} \frac{1}{2}hK(t_1,t_1) & & & \\ hK(t_2,t_1) & \frac{1}{2}hK(t_2,t_2) & & \\ \vdots & \ddots & \ddots & \\ \vdots & & & \\ hK(t_q,t_1) & \ldots & hK(t_q,t_{q-1}) & \frac{1}{2}hK(t_q,t_q) \end{bmatrix}.$$

Clearly, to monitor the convergence of this approximate iterations we need to study the powers of $\mathcal{K}_q$. For normal or nearly normal matrices this can be accomplished by considering the spectral radius of $\mathcal{K}_q$ while this is impossible for non-normal matrices. For the moment we shall not try to assess the degree of non-normality of $\mathcal{K}_q$, but only point out the following: The spectral radius of $\mathcal{K}_q$ is simply the maximum of the spectral radius of each diagonal blocks, thus we have $\rho(\mathcal{K}_q) = \mathcal{O}(h)$ as $h \to 0$. Hence, for small h, the spectral radius of $\mathcal{K}_q$ gives little or no information about the speed of convergence of the iterations.

Observe also that in the case the integral operator $\mathcal{K}$ defined by (3.1) is of the form $K(t,s) = \hat{K}(t-s)$, then $K(t_i,t_{i-r}) = \hat{K}(rh)$, and the resulting matrix $\mathcal{K}_q$ is block Toeplitz. In particular, for the BJ case we get blocks of the form

$$\alpha_r hK(t_i,t_{i-r}) = \alpha_r he^{-rhM}N, \quad i = 1,\ldots,q,\ r = 0,\ldots,i-1, \tag{3.2}$$

where $\alpha_0 = 1/2$ and $\alpha_r = 1,\ r > 0$, and similarly for the BJO case, only with M and N replaced by $\tilde{M}$ and $\tilde{N}$ respectively. Unfortunately, for the preconditioned cases, this block Toeplitz structure is lost. Instead we obtain blocks of the form

$$\alpha_{i-j}hK(t_i,t_j) = \alpha_{i-j}he^{(j-i)hM}(M - e^{-hjN}Me^{hjN}), \quad i = 1,\ldots,q,\ j = 1,\ldots,i. \tag{3.3}$$

4 Convergence analysis using pseudospectra

The idea of pseudo-eigenvalues was introduced by Trefethen [20] under the name of ϵ-approximate eigenvalues. There are several equivalent definitions of a pseudo-eigenvalue, we shall only make use of the following three.

Definition. Let A be a complex $n \times n$ matrix. Given $\epsilon > 0$, the number $\lambda \in \mathbb{C}$ is an ϵ-pseudo-eigenvalue of A if one of the following equivalent conditions is satisfied:

(i) λ is an eigenvalue of $A + E$ for some matrix E with $\|E\| \leq \epsilon$.

(ii) For some n-vector u we have $\|(A - \lambda I)u\| \leq \epsilon \|u\|$.

(iii) The following inequality holds

$$\|(A - \lambda I)^{-1}\| \geq \frac{1}{\epsilon}. \tag{4.1}$$

To simplify our notation we henceforth assume that all norms without subscripts refer to to the 2-norm or the induced spectral norm when used on matrices. Clearly, the above definitions of ϵ-pseudo-eigenvalues may be used for any norm.

Consistently we shall call the set of all ϵ-pseudo-eigenvalues, $\Lambda_\epsilon(A)$, the ϵ-pseudo-spectrum of A, and $\rho_\epsilon(A) = \max\{|z| : z \in \Lambda_\epsilon(A)\}$ the ϵ-pseudospectral radius.

For normal matrices, the ϵ-pseudo-spectrum is simply the union of ϵ-balls around the eigenvalues. But for non-normal matrices, the spectrum can be quite sensitive to perturbations. It is well-known that the condition $\rho(A) < 1$ is equivalent to $\|A^k\| \to 0$ as $k \to \infty$, however the powers may become large for some finite k. This observation can be made precise through the use of ϵ-pseudospectra, see for instance [16]. The essence is that if a pseudo-eigenvalue jumps outside the unit disk for some ϵ, the maximum power norm will be approximately equal to $\max_\epsilon (\rho_\epsilon(A) - 1)/\epsilon$.

In our applications we usually have the situation that $\|\mathcal{K}_q^k\|$ does not become exceptionally large for any value of k, in fact quite frequently we observe a contractive behaviour, i.e. $\|\mathcal{K}_q^k\|$ decreasing monotonically with k. The use of pseudospectra is motivated by the observation that $\rho(\mathcal{K}_q)$ is much smaller than the rate of decay $\|\mathcal{K}_q^k\|/\|\mathcal{K}_q^{k-1}\|$ for small values of k. For this purpose we may use a result by Trefethen [21]: For all values of ϵ it holds that

$$\|\mathcal{K}_q^k\| \leq \frac{\rho_\epsilon(\mathcal{K}_q)^{k+1}}{\epsilon}. \tag{4.2}$$

The relevance of ϵ depends on k. In Section 5 we give a numerical illustration of this bound. Keeping ϵ fixed in (4.2) we see that the decay rate of the power norms can be approximated by the pseudospectral radius of $\mathcal{K}_q$.

There are a number of ways to estimate the pseudospectrum and the pseudospectral radius of a matrix. Some of them require a lot of computing resources and other can be unreliable. The simplest and most intuitive way is perhaps to use (i) in the definition. One simply computes random matrices E such that $\|E\| = \epsilon$ and then the eigenvalues of $A + E$. We found that with a modest number of perturbations (5–10) the resulting pseudospectral radius was sometimes significantly underestimated. The matrices $\mathcal{K}_q$ have their spectrum in a neighborhood of $z=0$ of size $\mathcal{O}(h)=\mathcal{O}(T/q)$. For large enough q we therefore assume that $\Lambda_\epsilon(A)$ is a connected set containing $z=0$. We can then use the resolvent condition (iii) from the definition. We search along rays $re^{i\theta}$ (with the parameter θ fixed) from $z=0$ and for each ray we estimate

$$\sup_r \{|z| : z = re^{i\theta} \text{ and } \|(A-zI)^{-1}\| \geq \frac{1}{\epsilon}\}. \tag{4.3}$$

For each ray, (4.3) clearly yields a lower bound for the pseudospectral radius of A. We found this method to be more reliable than the method of random perturbations. We believe that the key to success in using pseudoeigenvalues to estimate the speed of convergence of waveform relaxation lies in the ability to compute the pseudospectral radius in an efficient way. The problem with our approach is that it involves making computations with the matrices $\mathcal{K}_q$ which are of dimension nq. To gain understanding about the convergence of continuous waveform relaxation, we may wish to do this computations for fairly large values of q. Therefore it is important to find methods for estimating pseudospectra with complexity that is independent of q. We have not been able to find a way to do this in general for matrices of the form $\mathcal{K}_q$, but in the case of no preconditioning (BJ and BJO) we can use an estimate proposed by Reichel and Trefethen [17]. Let us consider the general type of upper triangular block Toeplitz matrices

$$A = \begin{bmatrix} A_0 & A_1 & A_2 & \dots & A_{q-1} \\ & A_0 & A_1 & \ddots & \vdots \\ & & \ddots & \ddots & A_2 \\ & & & \ddots & A_1 \\ & & & & A_0 \end{bmatrix} \tag{4.4}$$

where $A_i \in \mathbb{R}^{n\times n},\ i=0,\dots,q-1$. We define the symbol of A as the $n\times n$ matrix

$$P(z) = \sum_{k=0}^{q-1} A_k z^k,$$

and the set Δ_r by

$$\Delta_r = \{z \in \mathbb{C} : |z| \leq r\}.$$

Following Reichel and Trefethen [17], we have the following result.

Proposition. Let A be of the form (4.4). Then

$$\{\lambda \in \mathbb{C} : \lambda \text{ is an eigenvalue of } P(z) \text{ with } z \in \Delta_r\} \subseteq \Lambda_\epsilon(A),$$

where $r=(\epsilon/c_q)^{1/q}$ and $c_q = (\sum_{k=1}^{q-1}\|A_k\|_\infty \sum_{k=1}^{q-1}\|A_k\|_1)^{1/2}$.

Proof. For any $z \in \Delta_r$ define the vector $u = U \otimes (1, z, z^2, \dots, z^{q-1})^T$ where U is an eigenvector of $P(z)$ with corresponding eigenvalue $\lambda(z)$. We compute

$$Au = \lambda(z)u - z^q \cdot \begin{bmatrix} 0 & & & & & \\ A_{q-1} & 0 & & & & \\ & A_{q-1} & 0 & & & \\ \vdots & & \ddots & \ddots & & \\ A_2 & & & & & \\ A_1 & A_2 & \dots & & A_{q-1} & 0 \end{bmatrix} \cdot u.$$

We recall the inequality $\|T\| \le \sqrt{\|T\|_1 \|T\|_\infty}$ valid for any matrix T. Thus it is clear that the spectral norm of the above matrix must be bounded by c_q and we obtain

$$\|(A - \lambda(z))u\| \le |z|^q c_q \|u\| \le \epsilon \|u\|.$$

Hence, $\lambda(z) \in \Lambda_\epsilon(A)$. $\square$

We now consider the application of this proposition to the cases BJ and BJO. By letting z range over the disk Δ_r we obtain a family of symbols $P(z)$ whose spectral radii are lower bounds for the pseudospectral radius of our matrix $\mathcal{K}_q$. It may be difficult to estimate c_q, but again following [17], we observe that for large values of q this is not critical since $r = (\epsilon/c_q)^{1/q}$ will be close to one. Thus, we take $r = \epsilon^{1/q}$. For $\mathcal{K}_q$ taken from the BJ case (3.2) we obtain

$$P(z) = h \sum_{r=0}^{q-1} e^{-rhM} N z^r - \frac{1}{2} hN = h \left(I - z e^{-hM} \right)^{-1} \left(I - z^q e^{-TM} \right) - \frac{1}{2} hN.$$

This expression may still be difficult to analyze, but far less expensive to compute than the method of random perturbations to $\mathcal{K}_q$ (cf definition (i) for pseudoeigenvalues). Numerical experiments with this formula seems to suggest that it gives reasonable estimates for the pseudospectral radius as long as the blocks on the diagonal are normal.

5 Numerical results

The origin of our model problem is the advection-diffusion equation

$$u_t + a u_x = b u_{xx}, \quad t > 0, \ 0 < x < 1, \tag{5.1}$$

$b > 0$, with Dirichlet boundary conditions $u(0, t) = \phi_0(t)$ and $u(1, t) = \phi_1(t)$ and initial condition $u(x, 0) = f(x)$. We introduce a mesh $\{x_i\}_{i=0}^{n+1}$ where $x_i = i\Delta x$ and $\Delta x = 1/(n+1)$. We let $y_i(t)$, $i = 1 \dots, n$ be the approximation obtained for $u(x_i, t)$ from (5.1) when u_{xx} and u_x are replaced by finite differences. If we use central differences for u_{xx} and central, backward, or forward differences for u_x we get a system of ODEs

$$y'(t) + Q\, y(t) = g(t), \tag{5.2}$$

where Q is an $n \times n$ matrix of the form (2.7) and

$$g(t) = [-c\phi_0(t), 0, \ldots, 0, -e\phi_1(t)]^T.$$

The values of c, d and e appearing in Q depend on the type of differencing which is used for the term u_x. We can summarize this in the following table (compare also [4]).

	c	d	e
Central	$-\frac{a}{2\Delta x} - \frac{b}{\Delta x^2}$	$\frac{2b}{\Delta x^2}$	$\frac{a}{2\Delta x} - \frac{b}{\Delta x^2}$
Forward	$-\frac{b}{\Delta x^2}$	$-\frac{a}{\Delta x} + \frac{2b}{\Delta x^2}$	$\frac{a}{\Delta x} - \frac{b}{\Delta x^2}$
Backward	$-\frac{a}{\Delta x} - \frac{b}{\Delta x^2}$	$\frac{a}{\Delta x} + \frac{2b}{\Delta x^2}$	$-\frac{b}{\Delta x^2}$

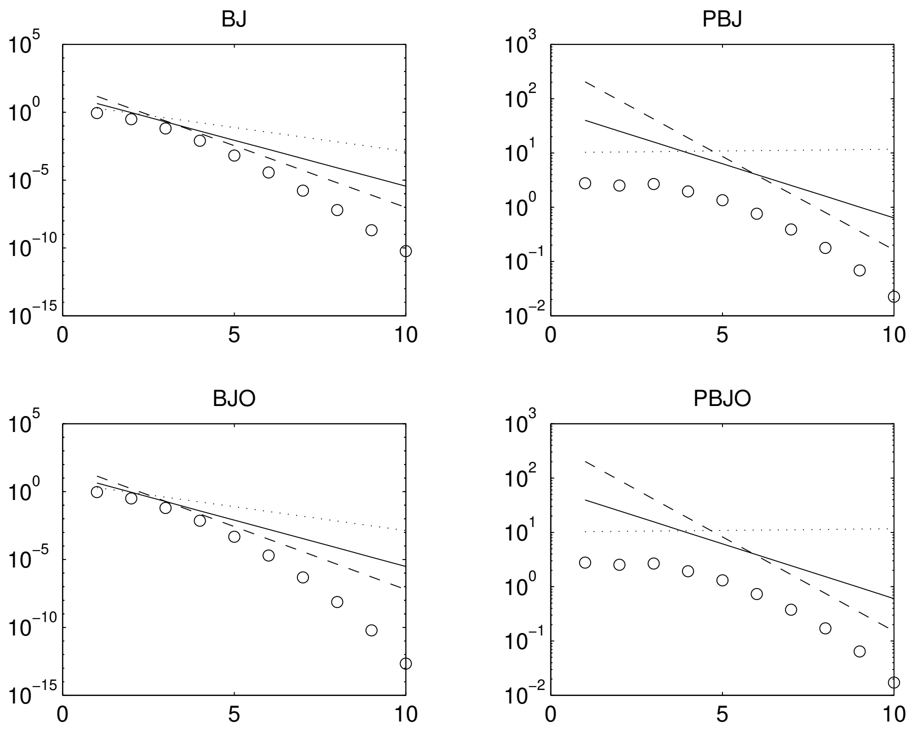

Figure 1: Power norms ('o') and $\rho_\epsilon(\mathcal{K}_q)^{k+1}/\epsilon$ in terms of k. Dotted line: $\epsilon = 0.1$, solid line: $\epsilon = 0.01$ and dashed line: $\epsilon = 0.001$.

We are particularly interested in the case where convection is dominating over diffusion in (5.1), that is $|a| >> b$. Following [4], in the numerical experiments to follow, we shall set $n = 24$, $a = 1$ and $b = 10^{-3.5}$. This results in a matrix Q which is highly non-normal.

Higham and Owren [4] study (5.1) supplied with a nonlinear reaction term and they find that the non-normality of the matrix Q severely affects the behaviour of the numerical scheme. In all the results presented here, the BJ and PBJ cases correspond to a splitting without overlapping and where the blocksizes are all equal to 2. In the BJO and PBJO cases we always use block sizes $b_1 = b_r = 3$ and $b_2 = \cdots = b_{r-1} = 4$ and overlaps $o_1 = \cdots = o_{r-1} = 2$ (compare Section 2).

We begin by illustrating the bound (4.2) given in Section 4. With parameters n, a, b as described above, we set $T = 0.1$ and $h = 0.01$ which corresponds to the number of trapezoidal points $q = 10$. We plot the first ten power norms of the resulting $\mathcal{K}_q$ and for $\epsilon \in \{0.1, 0.01, 0.001\}$ we plot $\rho_\epsilon(\mathcal{K}_q)^{k+1}/\epsilon$ in terms of k. The results are displayed in Figure 1 below.

We clearly see that the most relevant ϵ decreases as k increases. The bound (4.2) is quite sharp for the modes BJ and BJO but not as good for PBJ and PBJO.

In Figure 2 we plotted the error function of the first 6 iterates for (5.2) for all four modes of waveform relaxation.

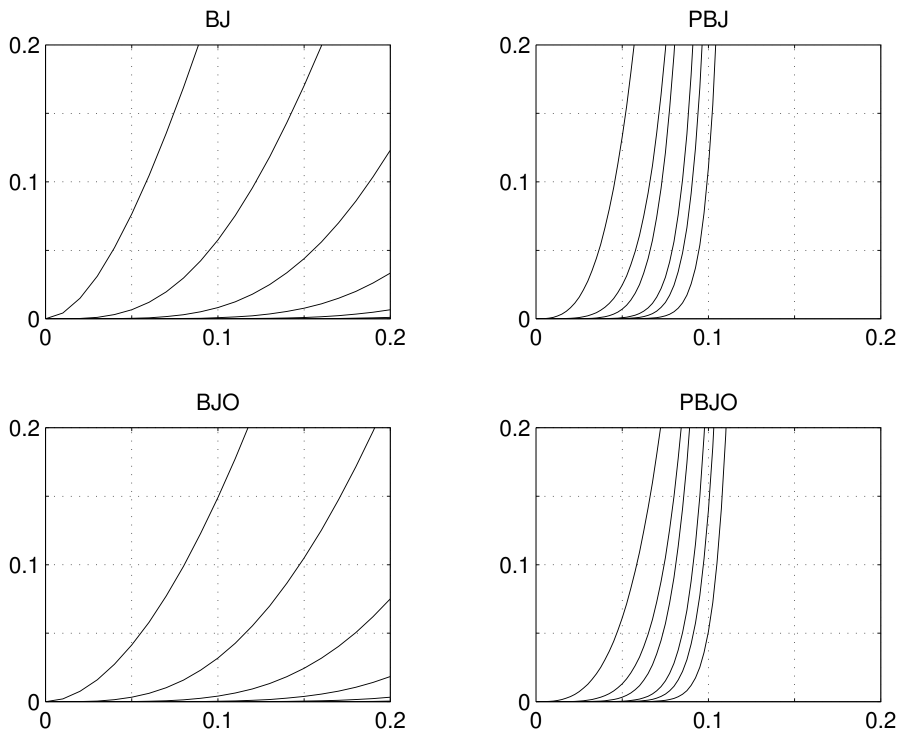

Figure 2: Error function of first 6 iterates for the four modes

We can see that the convergence of BJ and BJO modes is quite fast in the window $[0, 0.2]$ and that the window of rapid convergence of PBJ and PBJO iterations is much smaller and approximately equal to $[0, 0.05]$. These modes still converge at $T = 0.1$ but the errors grow rapidly as $T \to 0.2$. We can also observe that overlapping improves somewhat the rate of convergence of the resulting iterations. However, this improvement is not as dramatic as for the linear system with normal matrix Q considered in [2] which approximates the heat equation in one space dimension.

The behaviour of the dynamic iterations displayed in Figure 2 is clearly reflected in the corresponding pseudospectra. These pseudospectra, computed for all four modes at $T = 0.1$ and $T = 0.2$ for $\epsilon = 0.01$, are plotted in Figure 3 and Figure 4. We see in Figure 3 that the pseudospectra of all four modes are contained within a disk centered at the origin and with a radius of approximately 0.4. We see that while the BJ and BJO modes experience only a modest change in pseudospectra, the effect on the PBJ and PBJO modes is dramatic. By using the resolvent condition (4.1) we found that the pseudospectral radii for PBJ and PBJO exceed unity and we might expect that the error will grow rapidly in the first few iterations.

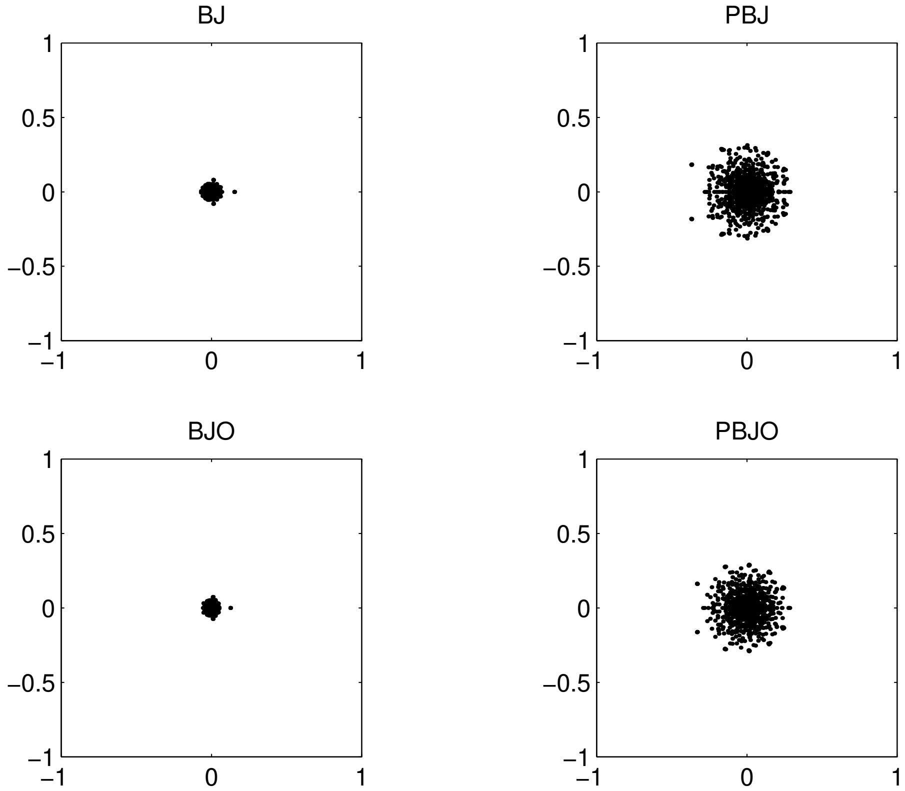

Figure 3: Pseudospectra for the four modes at $T = 0.1$

We have plotted in Figure 5 the ϵ-pseudospectral radii for $\epsilon = 0.01$ for the BJ and PBJ modes versus T. The top two curves correspond to the parameter $a = 1$, the two curves in the middle to $a = \frac{1}{2}$ and the bottom ones to $a = \frac{1}{4}$. These graphs indicate that for $a = 1$ the BJ mode should converge faster than the PBJ mode for any T. For $a = \frac{1}{2}$ and $a = \frac{1}{4}$ the PBJ mode should converge faster on windows $[0, T]$ where $T \leq 0.05$ and $T \leq 0.11$, respectively.

We conclude this section by analyzing pseudospectra of the iteration matrices $H_{BJ} = M^{-1}N$ and $H_{BJO} = \tilde{M}^{-1}\tilde{N}$ which correspond to the BJ and BJO modes as well as

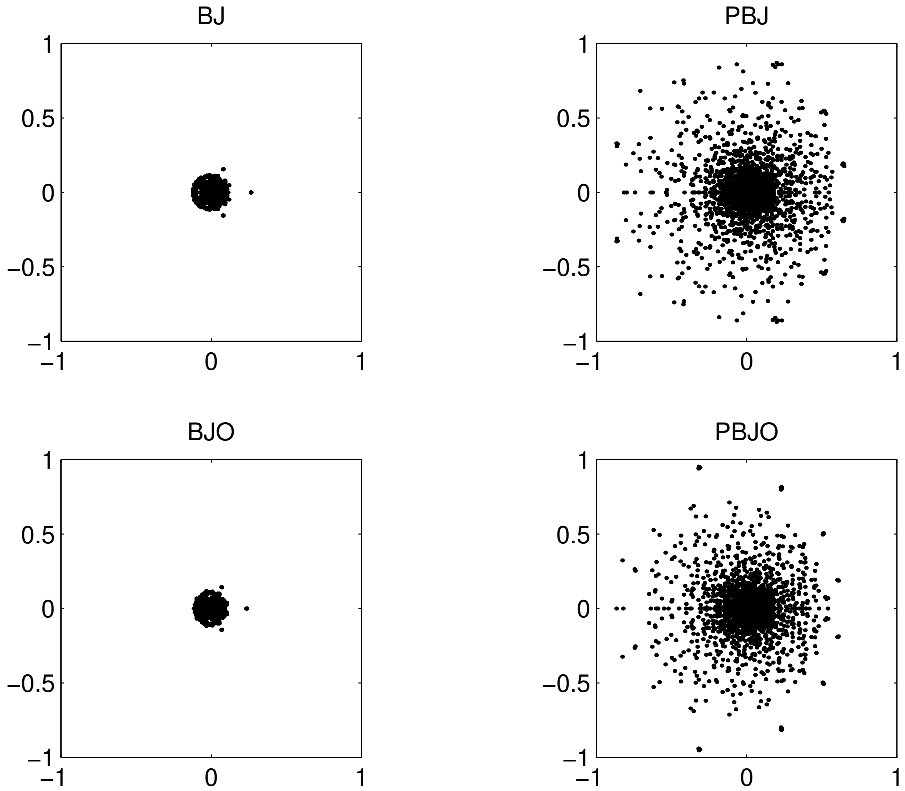

Figure 4: Pseudospectra for the four modes at $T = 0.2$

$H_{PBJ}(t) = M^{-1}N(t)$ and $H_{PBJO}(t) = \tilde{M}^{-1}\tilde{N}(t)$ which correspond to the PBJ and PBJO modes. The spectral radii of these matrices are given by

$$
\begin{array}{llll}
\rho(H_{BJ}) & = 0.0997, & \rho(H_{BJO}) & = 0.0073, \\
\rho(H_{PBJ}(0.05)) & = 0.0192, & \rho(H_{PBJO}(0.05)) & = 0.0083, \\
\rho(H_{PBJ}(0.1)) & = 0.0385, & \rho(H_{PBJO}(0.1)) & = 0.0166, \\
\rho(H_{PBJ}(0.2)) & = 0.0790, & \rho(H_{PBJO}(0.2)) & = 0.0334.
\end{array}
$$

If Q were normal these spectral radii would represent rates of convergence of the corresponding dynamic iterations at infinity (compare [10]). However, in our case the matrix Q is highly non-normal and more accurate information on the rate of convergence of the corresponding iterations is revealed by analyzing pseudospectra. Non-normality of H is usually measured by the condition number of the matrix V whose columns are eigenvectors of H and these condition numbers are listed below for the four waveform relaxation modes.

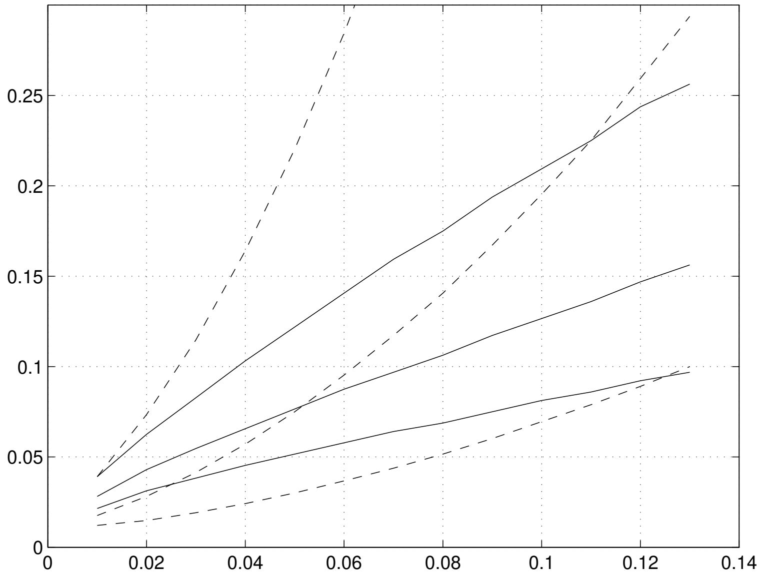

Figure 5: Pseudospectral radii in terms of T. The BJ modes are displayed as solid lines and PBJ modes as dashed lines.

$$\begin{array}{llll}
\mathrm{cond}(V_{BJ}) & = 1.72 \cdot 10^{17}, & \mathrm{cond}(V_{BJO}) & = 1.49 \cdot 10^{17}, \\
\mathrm{cond}(V_{PBJ}(0.05)) & = 8.87 \cdot 10^{19}, & \mathrm{cond}(V_{PBJO}(0.05)) & = 9.17 \cdot 10^{20}, \\
\mathrm{cond}(V_{PBJ}(0.1)) & = 1.13 \cdot 10^{20}, & \mathrm{cond}(V_{PBJO}(0.1)) & = 3.44 \cdot 10^{21}, \\
\mathrm{cond}(V_{PBJ}(0.2)) & = 2.46 \cdot 10^{20}, & \mathrm{cond}(V_{PBJO}(0.2)) & = 4.37 \cdot 10^{20}.
\end{array}$$

We have plotted in Figure 6 the pseudospectra for $\epsilon = 10^{-3}$ of the matrices H_{BJ} and H_{BJO} as well as $H_{PBJ}(T)$ and $H_{PBJO}(T)$ for $T = 0.05$, $T = 0.1$, and $T = 0.2$. These graphs were obtained as contourplots of the function

$$f(z) = \|(zI - H)^{-1}\|,$$

where H is the appropriate iteration matrix. Analyzing these plots we can see again that pseudospectra provide much more accurate information about the behaviour of dynamic iteration than spectral radii. In fact, the analysis of the spectral radii alone may lead to the wrong conclusions about the respective convergence rates.

6 Concluding remarks

By discretizing the continuous waveform relaxation operator, we have used pseudospectra for analyzing the convergence rate in the first few iterations. This approach offers more precise information than other techniques that have been suggested, for instance Laplace transformation techniques considered in [2].

There are two difficulties that have to be addressed when pseudospectra analysis is to be used. One is the choice of the parameter ϵ. The "most relevant ϵ" depends on the k for

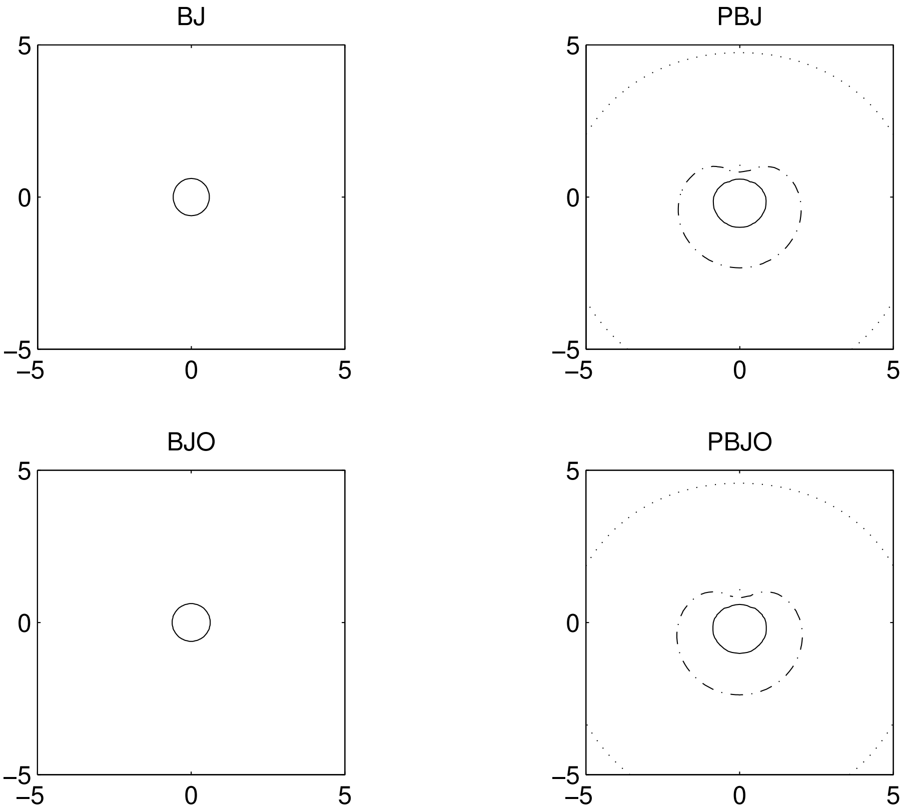

Figure 6: Contour plots for pseudospectra of the static iteration matrices

which one wishes to study the convergence rate, that is

$$\frac{\|\mathcal{K}_q^k\|}{\|\mathcal{K}_q^{k-1}\|}.$$

By making comparisons between the above ratios and $\rho_\epsilon(\mathcal{K}_q)$ for various values of ϵ, we have found experimentally that $\epsilon = 0.01$ gives a good approximation to this ratio in the first few iterations (Compare Figure 1).

Another difficulty is to compute the ϵ-pseuospectral radii. As q, the number of points in the trapezoidal approximation increases, our algorithms quickly reach the bound for which it is possible to compute the relevant quantities with the hardware and software available to us. We believe that the success of our approach depends on the future development of faster algorithms for computing pseudospectra. There is some hope for this, since the matrices we consider have a special block structure. One should look for algorithms whose complexity is practically independent of q. We have shown that such estimates can be obtained in the case where $\mathcal{K}_q$ is of block Toeplitz type, but the estimates only seemed to work well in the case where the blocks $K(t_i, t_j)$ where normal matrices. Moreover, when preconditioning was used, the block Toeplitz structure was lost which further complicates the situation.

Numerical experiments were performed for three different modes of waveform relaxation, BJ, PBJ, BJO and PBJO, the P signifying preconditioning and O overlapping. As the model for our experiments, we have chosen an advection-diffusion equation in one space dimension with discretized space variable. We were particularly interested in studying the case where the advection term is dominating since this leads to a linear system of ODEs with a coefficient matrix which is highly non-normal. In [2] the numerical tests were performed on a semidiscretised version of the heat equation, and it was found that preconditioning improved the convergence on small time windows. We found that in the non-normal case, extremely small time windows must be used if preconditioning is to be effective. Overlapping helps, but probably not enough to justify the enlarged dimension of the ODE system to be integrated in each iteration.

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