

Applications of the Simplified Topological ε -algorithms

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Shanks transformation and the ε -algorithm

Shanks transformation (1955) is a well-known sequence transformation for accelerating the convergence of sequences of numbers. It can be recursively implemented by the **scalar ε -algorithm** of **Wynn** (1956).

They were both extended to sequences of elements of a vector space by **Brezinski** (1975).

The idea is as follows.

Let (\mathbf{S}_n) be a sequence of elements of a vector space E converging to \mathbf{S} , and assume that it satisfies, for a fixed value of k , the difference equation

$$a_0(\mathbf{S}_n - \mathbf{S}) + \cdots + a_k(\mathbf{S}_{n+k} - \mathbf{S}) = \mathbf{0} \in E, \quad n = 0, 1, \dots$$

with $a_0 a_k \neq 0$ and $a_0 + \cdots + a_k \neq 0$.

We want to transform (\mathbf{S}_n) into a new sequence $(\mathbf{e}_k(\mathbf{S}_n))$ such that

$$\mathbf{e}_k(\mathbf{S}_n) = \mathbf{S}, \quad \text{for all } n.$$

If (\mathbf{S}_n) satisfies the difference equation above then \mathbf{S} is given by

$$\mathbf{S} = (a_0 \mathbf{S}_n + \cdots + a_k \mathbf{S}_{n+k}) / (a_0 + \cdots + a_k), \quad \forall n.$$

This linear combination can be computed even if (\mathbf{S}_n) does not satisfy the difference equation, thus defining a sequence transformation.

We now have to compute the coefficients a_0, \dots, a_k (now depending on k and n).

It holds, $\forall n$,

$$a_0 \Delta \mathbf{S}_n + \dots + a_k \Delta \mathbf{S}_{n+k} = \mathbf{0}.$$

We need to transform this relation in E into a system of scalar relations.

Let \mathbf{y} be an element of the dual space E^* of E (which means that it is a linear functional).

Taking the duality product of this relation with \mathbf{y} , we have, $\forall n$,

$$a_0 \langle \mathbf{y}, \Delta \mathbf{S}_n \rangle + \cdots + a_k \langle \mathbf{y}, \Delta \mathbf{S}_{n+k} \rangle = 0.$$

Writing this relation for the indices $n, \dots, n+k-1$ and adding that $a_0 + \cdots + a_k = 1$ (which does not restrict the generality), leads to the system

$$\begin{cases} a_0 + \cdots + a_k = 1 \\ a_0 \langle \mathbf{y}, \Delta \mathbf{S}_{n+i} \rangle + \cdots + a_k \langle \mathbf{y}, \Delta \mathbf{S}_{n+k+i} \rangle = 0, \quad i = 0, \dots, n+k-1, \end{cases}$$

where the unknowns depend on n (and k) if (\mathbf{S}_n) does not satisfy the difference equation.

The **first topological Shanks transformation** is then defined by

$$\mathbf{e}_k(\mathbf{S}_n) = a_0\mathbf{S}_n + \cdots + a_k\mathbf{S}_{n+k},$$

and the **second topological Shanks transformation** by

$$\tilde{\mathbf{e}}_k(\mathbf{S}_n) = a_0\mathbf{S}_{n+k} + \cdots + a_k\mathbf{S}_{n+2k}.$$

By construction, $\forall n, \mathbf{e}_k(\mathbf{S}_n) = \tilde{\mathbf{e}}_k(\mathbf{S}_n) = \mathbf{S}$ if

$$\forall n, a_0(\mathbf{S}_n - \mathbf{S}) + \cdots + a_k(\mathbf{S}_{n+k} - \mathbf{S}) = \mathbf{0}.$$

Each of these transformations can be implemented by a recursive algorithm which generalizes the scalar ε -algorithm of Wynn (Brezinski, 1975). They are named the **Topological ε -algorithms (TEA)**.

However, these algorithms are quite complicated:

- they possess two rules,
- they require the storage of elements of E and of E^* ,
- the duality product with \mathbf{y} is recursively used in their rules.

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- they possess two rules,
- they require the storage of elements of E and of E^* ,
- the duality product with \mathbf{y} is recursively used in their rules.

Recently, simplified versions of these algorithms were obtained (Brezinski and R.-Z., 2014), and called the **Simplified Topological ε -algorithms (STEA)**.

- only one recursive rule,
- they require less storage than the initial algorithms and only elements of E ,
- the elements of the dual vector space E^* no longer have to be used in the recursive rules (only in their initializations),
- numerical stability is improved (thanks to particular rules of Wynn).

The rule of the **First Simplified Topological ε -algorithm**, denoted by **STE1**, is

$$\varepsilon_{2k+2}^{(n)} = \varepsilon_{2k}^{(n+1)} + \frac{\varepsilon_{2k+2}^{(n)} - \varepsilon_{2k}^{(n+1)}}{\varepsilon_{2k}^{(n+1)} - \varepsilon_{2k}^{(n)}} (\varepsilon_{2k}^{(n+1)} - \varepsilon_{2k}^{(n)}), \quad k, n = 0, 1, \dots,$$

with $\varepsilon_0^{(n)} = \mathbf{S}_n \in E$, $n = 0, 1, \dots$

The scalars $\varepsilon_{2k}^{(n)}$ are computed by the **scalar ε -algorithm** of Wynn whose rule is

$$\begin{cases} \varepsilon_{-1}^{(n)} &= 0, \quad n = 0, 1, \dots, \\ \varepsilon_0^{(n)} &= \langle \mathbf{y}, \mathbf{S}_n \rangle, \quad n = 0, 1, \dots, \\ \varepsilon_{k+1}^{(n)} &= \varepsilon_{k-1}^{(n+1)} + (\varepsilon_k^{(n+1)} - \varepsilon_k^{(n)})^{-1}, \quad k, n = 0, 1, \dots \end{cases}$$

The rule of the **Second Simplified Topological ε -algorithm**, denoted by **STE A2**, is

$$\tilde{\varepsilon}_{2k+2}^{(n)} = \tilde{\varepsilon}_{2k}^{(n+1)} + \frac{\varepsilon_{2k+2}^{(n)} - \varepsilon_{2k}^{(n+1)}}{\varepsilon_{2k}^{(n+2)} - \varepsilon_{2k}^{(n+1)}} (\tilde{\varepsilon}_{2k}^{(n+2)} - \tilde{\varepsilon}_{2k}^{(n+1)}), \quad k, n = 0, 1, \dots,$$

with $\tilde{\varepsilon}_0^{(n)} = \mathbf{S}_n \in E$, $n = 0, 1, \dots$, and the numbers $\varepsilon_{2k}^{(n)}$ are the same as above.

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with $\tilde{\varepsilon}_0^{(n)} = \mathbf{S}_n \in E$, $n = 0, 1, \dots$, and the numbers $\varepsilon_{2k}^{(n)}$ are the same as above.

These algorithms are related to the topological Shanks transformation by

$$\varepsilon_{2k}^{(n)} = \mathbf{e}_k(\mathbf{S}_n) \quad \text{and} \quad \tilde{\varepsilon}_{2k}^{(n)} = \tilde{\mathbf{e}}_k(\mathbf{S}_n).$$

Remark 1: These simplified algorithms allow to prove easily convergence and acceleration results.

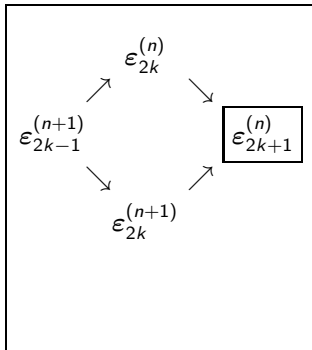
Remark 2: For STEA1 there exist **four different equivalent formulas**. The same for STEA2.

The ε -array

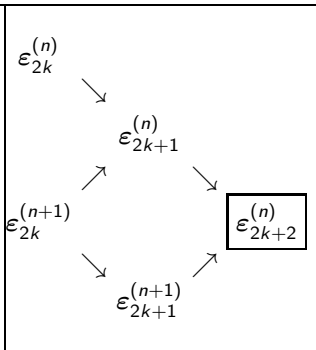
$$\begin{array}{cccccc} \varepsilon_{-1}^{(0)} = 0 & & & & & \\ & \varepsilon_0^{(0)} & & & & \\ \varepsilon_{-1}^{(1)} = 0 & & \varepsilon_1^{(0)} & & & \\ & \varepsilon_0^{(1)} & & \varepsilon_2^{(0)} & & \\ \varepsilon_{-1}^{(2)} = 0 & & \varepsilon_1^{(1)} & & \varepsilon_3^{(0)} & \\ & \varepsilon_0^{(2)} & & \varepsilon_2^{(1)} & & \varepsilon_4^{(0)} \\ \varepsilon_{-1}^{(3)} = 0 & & \varepsilon_1^{(2)} & & \varepsilon_3^{(1)} & \vdots \\ & \varepsilon_0^{(3)} & & \varepsilon_2^{(2)} & & \vdots \\ \varepsilon_{-1}^{(4)} = 0 & & \varepsilon_1^{(3)} & & \vdots & \\ & \varepsilon_0^{(4)} & & \vdots & & \\ \varepsilon_{-1}^{(5)} = 0 & & \vdots & & & \\ \vdots & & & & & \end{array}$$

TEA1 vs STEA1

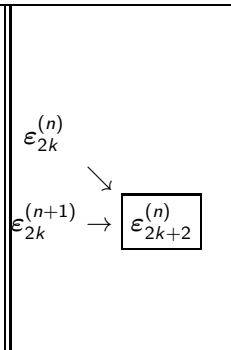
Odd rule TEA1



Even rule TEA1



STEA1



Similar for STEA2.

Exploitation of the algorithms

The algorithms will be used in two different ways

- **Acceleration method (AM)**
- **Restarted method (RM)**

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The **Acceleration Method (AM)** can be applied to the solution of systems of linear and nonlinear equations, to the computation of matrix functions,

Choose $2k$ and \mathbf{x}_0 .

For $n = 1, 2, \dots$

 Compute \mathbf{x}_n .

 Apply the STEA1 to $\mathbf{x}_0, \mathbf{x}_1, \mathbf{x}_2, \dots$ and compute the sequence of extrapolated values

$$\epsilon_0^{(0)} = \mathbf{x}_0, \epsilon_0^{(1)}, \epsilon_2^{(0)}, \epsilon_2^{(1)}, \dots, \epsilon_{2k}^{(0)}, \epsilon_{2k}^{(1)}, \epsilon_{2k}^{(2)}, \dots$$

 or similar quantities by the STEA2.

end

The **Restarted Method (RM)** is used for **fixed point problems**, that is for solving systems of linear and nonlinear equations.

Let $F : \mathbb{R}^m \mapsto \mathbb{R}^m$. We have to find the solution of equations of the form

$$\mathbf{x} = F(\mathbf{x}) \quad \text{or} \quad f(\mathbf{x}) = F(\mathbf{x}) - \mathbf{x} = \mathbf{0} \quad \text{or} \quad \mathbf{x} = \mathbf{x} + \alpha f(\mathbf{x}).$$

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Choose $2k$ and \mathbf{x}_0 .
For $i = 0, 1, \dots$ (*cycle or outer iterations*)
 Set $\mathbf{u}_0 = \mathbf{x}_i$
 For $n = 1, \dots, 2k$ (*inner iterations*)
 Compute $\mathbf{u}_n = F(\mathbf{u}_{n-1})$
 Apply the STEA to $\mathbf{u}_0, \dots, \mathbf{u}_{2k}$
 end
 Set $\mathbf{x}_{i+1} = \epsilon_{2k}^{(0)}$ or $\tilde{\epsilon}_{2k}^{(0)}$
end

Generalized Steffensen Method (GSM)

A particular case of the RM is the **Generalized Steffensen Method (GSM)** that corresponds to take in the RM $k = m$ (the dimension of the system).

In this case, under some assumptions, the sequence (\mathbf{x}_i) of the vertices of the successive ε -arrays asymptotically **converges quadratically** to the fixed point \mathbf{x} of F (Le Ferrand, 1992).

Remark: This method can also be applied when $F : \mathbb{R}^{m \times s} \mapsto \mathbb{R}^{m \times s}$ but the quadratic convergence of the GSM has not yet been proved in this case.

- C. Brezinski, M. Redivo–Zaglia, [The simplified topological \$\varepsilon\$ -algorithms for accelerating sequences in a vector space](#), SIAM J. Sci. Comput., 36 (2014) A2227–A2247.

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- C. Brezinski, M. Redivo–Zaglia, [The simplified topological \$\varepsilon\$ -algorithms: software and applications](#), submitted.

- C. Brezinski, M. Redivo–Zaglia, [The simplified topological \$\varepsilon\$ -algorithms for accelerating sequences in a vector space](#), SIAM J. Sci. Comput., 36 (2014) A2227–A2247.
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A Matlab toolbox called **EPSfun** has been submitted with the paper. It contains:

- All the STEA functions and SEAW function.
- Script for users.
- Demo scripts (producing all the examples of the paper).
- TEA and VEAW functions for comparisons.

Example 1

Let us consider the following **nonlinear system**

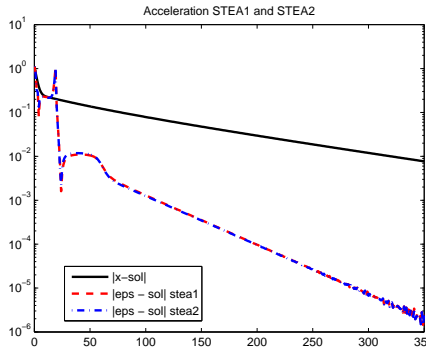
$$\begin{cases} f_i(\mathbf{x}) = x_i + \sum_{j=1}^m x_j - (m+1), & i = 1, \dots, m-1, \\ f_m(\mathbf{x}) = \prod_{j=1}^m x_j - 1, \end{cases}$$

whose solution is $\mathbf{x} = (1, \dots, 1)^T$.

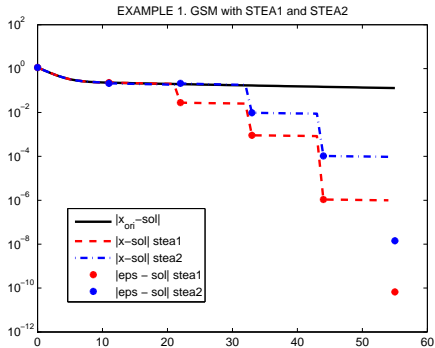
For $m = 5$, starting from $\mathbf{x}_0 = (1/2, \dots, 1/2)^T$, taking $\alpha = -0.05$, and $k = 2$ for the **AM**, we obtain the results of the next Figure.

After **350 iterations**, an error of $7.70 \cdot 10^{-3}$ is obtained by the iterative procedure while the AM goes down to $1.4 \cdot 10^{-6}$.

The **GSM** needs **5 iterations** (thus a total of 50 basic iterations) to achieve an error of $1.43 \cdot 10^{-8}$ for the STEA2 and $6.66 \cdot 10^{-11}$ for the STEA1. \mathbf{y} is the **mean value of a vector** (also in Examples 2:5).



Acceleration Method



Generalized Steffensen Method

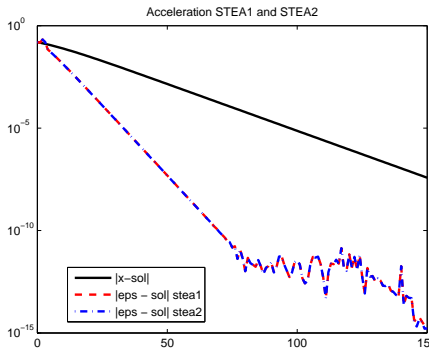
Example 2

We consider the nonlinear system

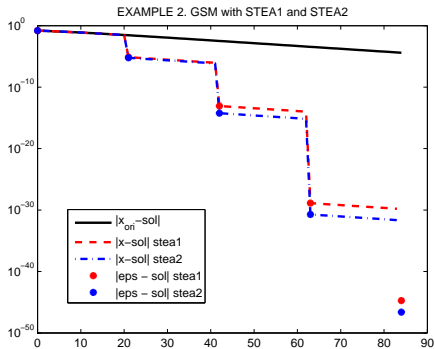
$$f_i(\mathbf{x}) = m - \sum_{j=1}^m \cos x_j + i(1 - \cos x_i) - \sin x_i, \quad i = 1, \dots, m,$$

whose solution is zero.

For $m = 10$ and $\mathbf{x}_0 = (1/(2n), \dots, 1/(2n))^T$, we obtain with $\alpha = 0.1$ and $k = 2$ for the AM, the results of the next Figure. They show that instability occurs for the AM after iteration 75 (where the error attains $1.48 \cdot 10^{-11}$), and that the GSM achieved a much better precision with a fewer number of iterations (after 2 iterations the STEA1 has an error of $8.54 \cdot 10^{-14}$, and the STEA2 an error of $5.78 \cdot 10^{-15}$).



Acceleration Method



Generalized Steffensen Method

Example 3

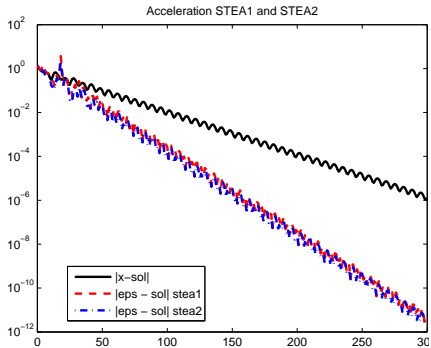
We consider the **nonlinear system**

$$\begin{cases} x_1 &= x_1 x_2^3 / 2 - 1/2 + \sin x_3 \\ x_2 &= (\exp(1 + x_1 x_2) + 1) / 2 \\ x_3 &= 1 - \cos x_3 + x_1^4 - x_2, \end{cases}$$

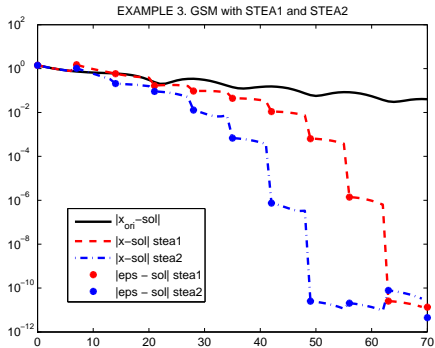
whose solution is $(-1, 1, 0)^T$.

Starting from $\mathbf{x}_0 = \mathbf{0}$, we obtain the results of the next Figure (left) for the **AM** with $\alpha = 0.2$ and $k = 4$.

For the **GSM** with $\alpha = 0.1$ and $k = 3$ the STEA2 gives better results than the STEA1 as shown on the Figure (right).



Acceleration Method



Generalized Steffensen Method

Example 4

Consider now the **non-differentiable system**

$$\begin{cases} |x_1^2 - 1| + x_2 - 1 = 0 \\ x_2^2 + x_1 - 2 = 0. \end{cases}$$

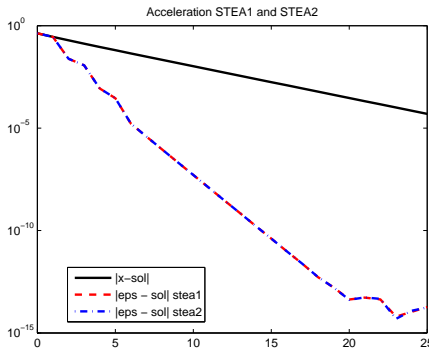
It has two solutions:

$(1, 1)^T$ for which we are starting from $\mathbf{x}_0 = (1.3, 1.3)^T$, with $\alpha = -0.1$ (First Figure - left),

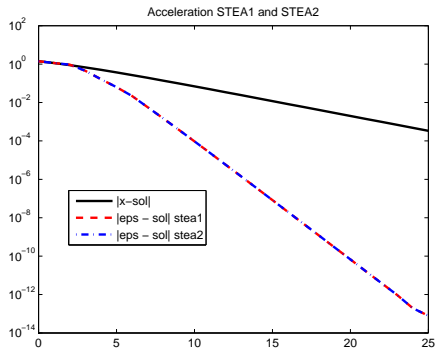
and $(-2, -2)$ for which we are starting from $\mathbf{x}_0 = (-1, -1)^T$, with $\alpha = 0.1$ (First Figure - right).

For the **AM** we took $k = 3$. We see that, for both solutions, the AM works quite well.

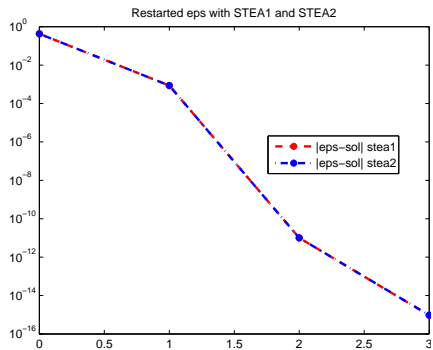
The **GSM** with $k = 2$ achieves a precision of 10^{-15} in three iterations.



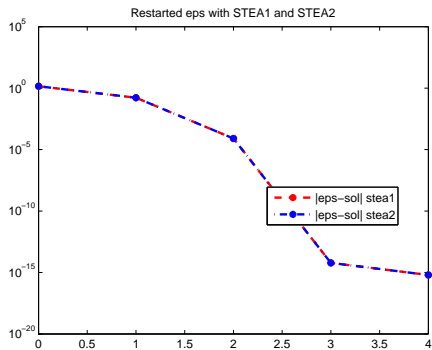
AM, first solution



AM, second solution



GSM, first solution



GSM second solution

Example 5

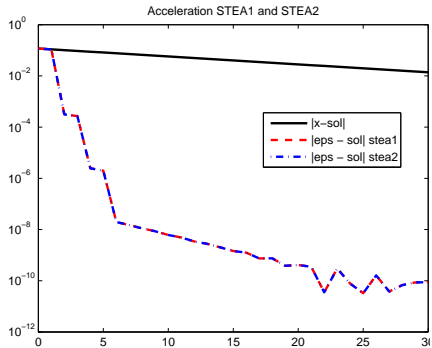
For the **nonlinear system**

$$\sum_{j=1}^7 x_j - (x_i + e^{-x_i}) = 0, \quad i = 1, \dots, 7,$$

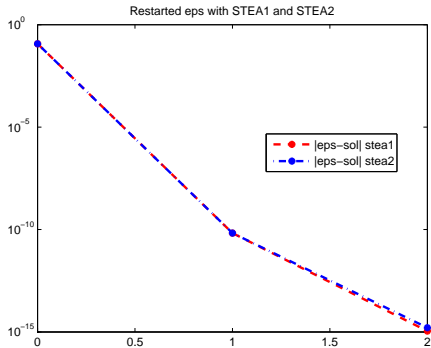
the solution is the vector with all components equal to **0.14427495072088622350**.

Starting from $\mathbf{x}_0 = (1, \dots, 1)^T / 10$, $\alpha = -0.01$ and with $k = 3$ for the **AM**, we obtain the results of the following Figure.

Notice that the with **GSM** with $k = 7$ achieves with **full precision in only two iterations**.



Acceleration Method



Generalized Steffensen Method

Example 6

We consider the linear system $AX = B$,

- A is the *parter* matrix of dimension 5 divided by 3 (its spectral radius is 0.9054 and its condition number is 2.149)
- X is formed by the first two columns of the matrix *pei*
- B is computed accordingly.

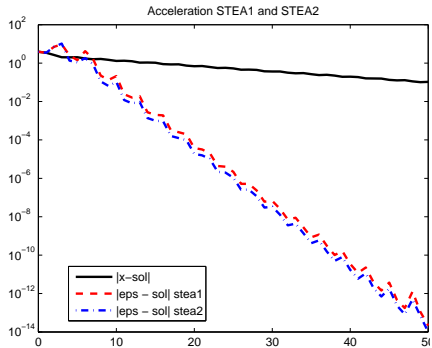
We perform the iterations

$$X_{n+1} = (I - A)X_n + B$$

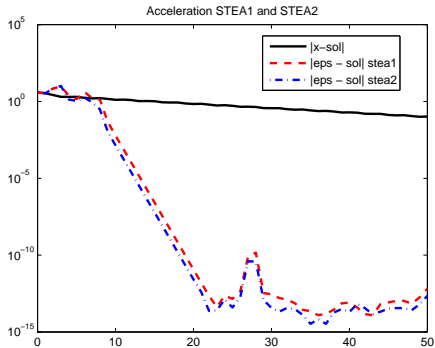
starting from $X_0 = 0$.

With y defined as the linear functional associating to a matrix the **sum of its elements**, we obtain for the **AM** the results of next Figure, with $k = 3$ (left) and $k = 4$ (right).

For $k = 5$ (that is for column 10 of the ε -array), the solution is obtained with full precision in **one iteration** by the **GSM** as stated by the theory.



AM, $k = 3$



AM, $k = 4$

Example 7

We are looking for the maximal Hermitian positive definite solution X_+ of the **matrix equation**

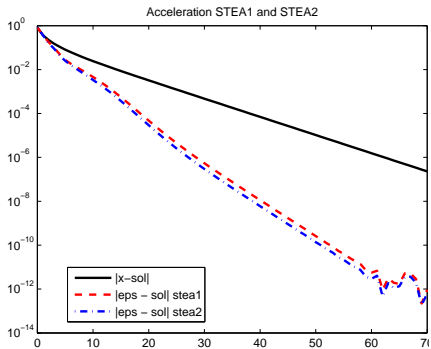
$$f(X) = X + A^*X^{-1}A - Q = 0,$$

where $A, Q \in \mathbb{C}^{m \times m}$ with Q Hermitian positive definite.

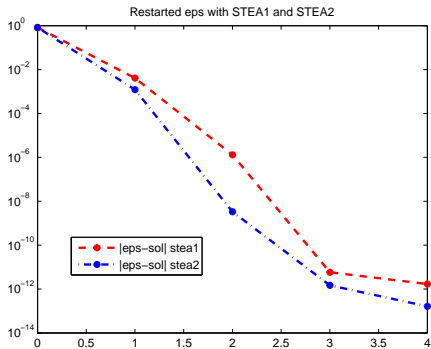
For $Q = I + A^*A$, $X_+ = I$ if and only if $\rho(A) < 1$, a result by **C.-H. Guo (2001)** which provides an easy way of constructing numerical examples by taking $A = S/r$ with $r > \rho(S)$ and S any matrix. He also proposed the following iterative method

$$\begin{aligned} X_0 &= Q, \\ X_{n+1} &= Q - A^*X_n^{-1}A, \quad n = 0, 1, \dots \end{aligned}$$

that converges slowly if the spectral radius of A is close to 1. We take as matrix S the **prolate** matrix, $m = 5$. For the **AM**, we took $k = 2$ and for the **GSM** $k = 5$. \mathbf{y} is the **trace** of a matrix.



Acceleration Method



Generalized Steffensen Method

Example 8

We now want to solve the **matrix equation**

$$X = \sum_{i=0}^{\infty} A_i X^i. \quad (1)$$

We use the algorithm of **Z.-Z. Bai (1997)** which consists, for $n = 1, 2, \dots$, in the iterations

$$\begin{aligned} Q_n &= I - \sum_{i=1}^{\infty} A_i X_{n-1}^{i-1}, \\ B_n &= 2B_{n-1} - B_{n-1} Q_n B_{n-1}, \\ X_n &= B_n A_0, \end{aligned}$$

starting from a given A_0 , $B_0 = I$ and $X_0 = B_0 A_0$. He proved that the sequence (X_n) converges to the minimal nonnegative solution of the matrix equation.

We consider the numerical example treated by **C.-H. Guo (1999)**, where

$$A_0 = \frac{4}{3}(1 - \rho) \begin{pmatrix} 0.05 & 0.1 & 0.2 & 0.3 & 0.1 \\ 0.2 & 0.05 & 0.1 & 0.1 & 0.3 \\ 0.1 & 0.2 & 0.3 & 0.05 & 0.1 \\ 0.1 & 0.05 & 0.2 & 0.1 & 0.3 \\ 0.3 & 0.1 & 0.1 & 0.2 & 0.05 \end{pmatrix},$$

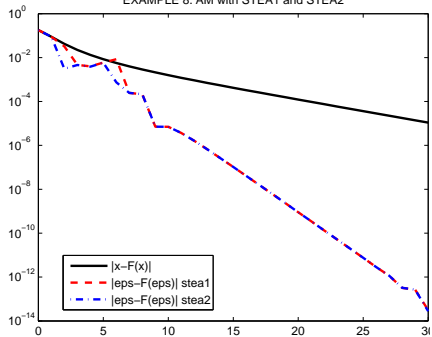
$A_i = \rho^i A_0$ for $i = 1, 2, \dots$, and $\rho = 0.49$.

The linear functional **y** used in the duality product corresponds to the **trace of the matrix** (also in all the Examples presented in the sequel).

The infinite sum in the computation of Q_n was stopped after 100 terms.

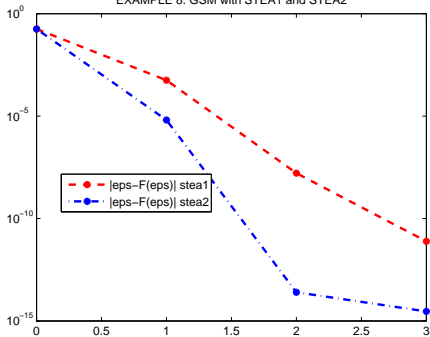
The results are given in the next Figure with $k = 3$ for the **AM**, and $k = 5$ for the **GSM**.

EXAMPLE 8. AM with STEA1 and STEA2



Acceleration Method

EXAMPLE 8. GSM with STEA1 and STEA2



Generalized Steffensen Method

Example 9

We now consider the computation of the **matrix exponential** by its series expansion

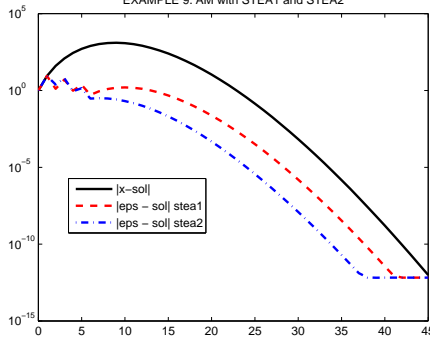
$$e^{At} = I + \frac{At}{1!} + \frac{A^2t^2}{2!} + \dots$$

In order to be able to compute the error, we take $A = UDU^{-1}$, where D is a diagonal matrix, so that $e^{At} = Ue^{Dt}U^{-1}$.

For D , we took the *frank* matrix and for U the matrix *orthog*, both of dimension 100.

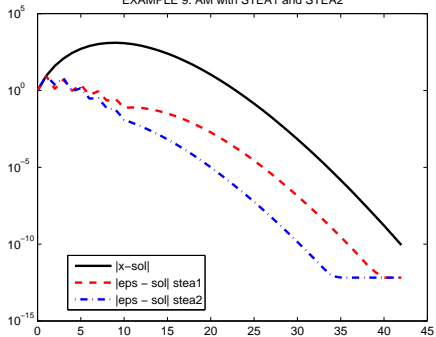
With $t = -0.099$, we obtain the results of the following Figure with $k = 3$ and $k = 5$ for the **AM**.

EXAMPLE 9. AM with STEA1 and STEA2



AM, $k = 3$

EXAMPLE 9. AM with STEA1 and STEA2



AM, $k = 5$

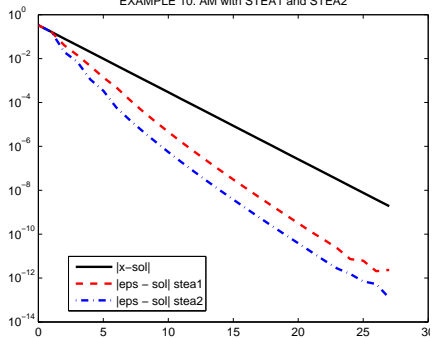
Example 10

We want now to **accelerate the series**

$$(I - At)^{-1} = 1 + (At) + (At)^2 + \dots$$

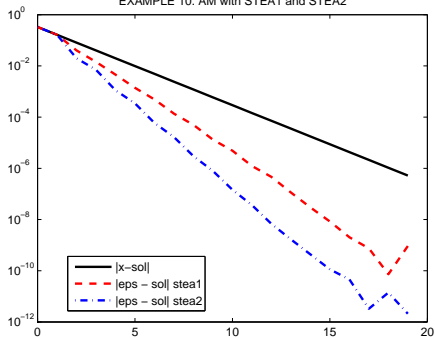
With the same matrix A as in Example 9, but of dimension **50** and with $t = -0.0099$, we obtain for the **AM** the results of the next Figure (on the left $k = 3$, and on the right $k = 6$).

EXAMPLE 10. AM with STEA1 and STEA2



AM, $k = 3$

EXAMPLE 10. AM with STEA1 and STEA2



AM, $k = 6$

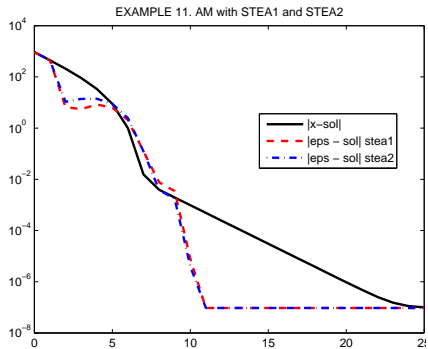
Example 11

We want now to compute the **square root of a symmetric positive definite matrix** A by the iterative method, denoted as the IN iteration by **N.J Higham (2008)**, which is a variant of Newton's method

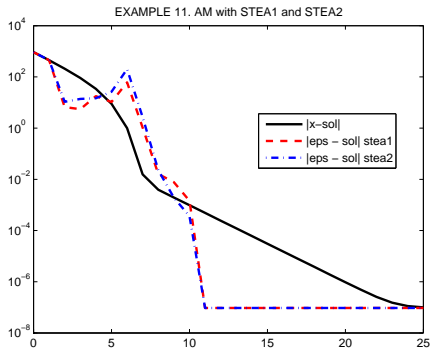
$$\begin{aligned}X_{n+1} &= X_n + E_n \\E_{n+1} &= -\frac{1}{2}E_n X_{n+1}^{-1} E_n.\end{aligned}$$

with $X_0 = A$ and $E_0 = (I - A)/2$.

With the matrix *moler* of dimension **50**, the **AM** gives the results of the next Figure with $k = 1$ on the left and $k = 2$ on the right.



AM, $k = 1$



AM, $k = 2$

Example 12

The binomial iteration for computing the AM, **square root of** $I - C$, where $\rho(C) < 1$, consists in the iterations

$$X_{n+1} = \frac{1}{2}(C + X_n^2), \quad k = 0, 1, \dots,$$

with $X_0 = 0$.

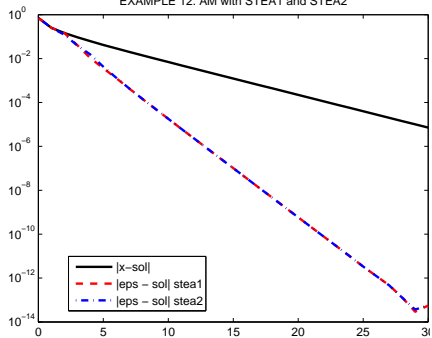
The sequence (X_n) converges linearly to $X = I - (I - C)^{1/2}$ and X_n reproduces the series

$$(I - C)^{1/2} = \sum_{i=0}^{\infty} \binom{1/2}{i} (-C)^i = I - \sum_{i=1}^{\infty} \alpha_i C_i, \quad \alpha_i > 0,$$

up to and including the term C^n .

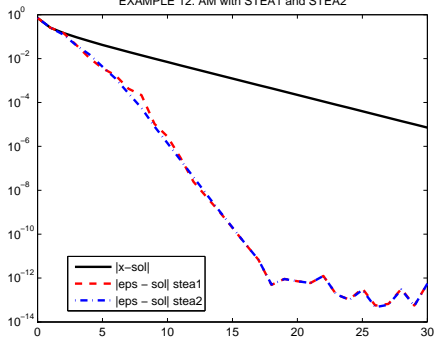
For C , we took the matrix *moler* of dimension 500 divided by $1.1 \cdot 10^5$ so that $\rho(C) = 0.9855$. The **AM** gives the results of the following Figure with $k = 2$ on the left and $k = 4$ on the right, for the acceleration of the sequence (X_n) .

EXAMPLE 12. AM with STEA1 and STEA2



AM, $k = 2$

EXAMPLE 12. AM with STEA1 and STEA2



AM, $k = 4$

THANK YOU !