Numerical Modeling of D-Mapping with Applications to Chemical Kinetics

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Abstract. Numerical modeling of D-mappings has been studied and applied to solving nonlinear stiff systems. These mappings have been locally linearized for convergence analysis, and some applications have been made to chemical kinetics.

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INTRODUCTION

A numerical method was developed by Dey (1977) for solving nonlinear systems, some applications of which were later made to stiff systems (Dey, 1982). Convergence analysis was done using nonlinear D-mappings (Dey, 1981). It is extremely difficult to represent this analysis computationally. Local linearization for such an analysis, which rendered computational modeling of D-mappings feasible, was suggested by Lomax (1983). In this article we discuss linearized modeling of D-mappings and some applications of the method.

D-MATRICES AND D-MAPPINGS

If a sequence of square matrices of the same order satisfy the following condition,

\[ A_k - I \leq Q, \]

each \( A_k \) is called a D-matrix. A D-matrix is not necessarily a convergent matrix, and conversely.

Theorem 1. A sufficient condition that \( A_k \) is a D-matrix is that

\[ \| A_k \|_q \leq \alpha < 1 \]

\( \forall k > K \) and that \( q \) is the same \( \forall k \).

Theorem 1 is easily proved. Let

\[ u^k = (u_1^k, u_2^k, \ldots, u_j^k)^T \in D_k, \]

\( k = 1, 2, \ldots \), \((u_j^k) = \) value of \( u_j \) at some kth iteration).

Let us consider a chained linear spaces \( D_k \subseteq D_{k-1} \subseteq \ldots \subseteq D \subseteq \mathbb{R}^n \). \( \mathbb{R}^n = n \)-dimensional real space. Let \( u^k, u^* \in D_k \forall k \) and

\[ G_k: D_k \times D_k \rightarrow D_k. \]

If

\[ G_k(u^{k+1}, u^k) = G_k(u^*, u^k) \]

\[ = A_k(u^{k+1} - u^*) + B_k(u^k - u^*) \]

and \( \forall k > K \), and if \((I - A_k)^{-1}B_k \) is a D-matrix, \( G_k \) is called a D-mapping (Dey, 1981).

If we now consider a nonstationary iterative scheme of the form

\[ u^{k+1} = G_k(u^{k+1}, u^k) \]

and if \( G_k: D_k \times D_k \rightarrow D_k \) is a D-mapping, then

\[ \lim_{k \to \infty} u^k = u^* \]

where \( u^* = G_k(u^*, u^*) \forall k \) (Dey, 1981).

LOCALLY LINEARIZED D-MAPPING

Let us linearize (4) on \( D_k \times D_k \), using first-order approximation of \( G_k(u^{k+1}, u^k) \) near \((u^k, u^k)\). Then,

\[ u^{k+1} = G_k(u^k, u^k) + G_k'(u^{k+1} - u^k) \]

where \( G_k' \) is the Fréchet derivative of \( G_k \) on \( D_k \times D_k \). Equation (6) may be expressed as

\[ u^{k+1} = A_k u^k + b_k \]

where \( A_k = -(I - G_k')^{-1}G_k' \),

\[ b_k = (I - G_k')^{-1}G_k(u^k, u^k). \]

We have assumed that \((I - G_k')\) is invertible. Now we may prove a second theorem.
Theorem 2. If \(|A_j - A*| < E\), where \(E\) is a matrix consisting of elements that are positive and arbitrarily small and \(|B_j - B*| < \varepsilon\), \(\varepsilon\) is a vector consisting of elements that are positive and arbitrarily small, then (5) is true (convergence) if \(A_k\) is a D-matrix (Dey, 1983a).

Theorem 3. If \(G_{kj}\) is a D-matrix, so is \(A_{kj}\) (Dey, 1983a).

This principle may now be applied computationally.

PERTURBED FUNCTIONAL ITERATION

Let a nonlinear system be expressed as

\[ u = G_0(u) \]

\[ u \in D, \quad G_0: D \rightarrow D \]

A Gauss-Seidel-type iteration for the solution may be expressed as

\[ u^{k+1} = G(u^{k+1}, u^k) \]

\[ G: D \times D \rightarrow D, \quad u^k \in D \forall k \]

A perturbed iterative scheme (Dey, 1977) may be expressed as (in the element form)

\[ u_j^{k+1} = u_j^k + G_j(u^{k+1}, u^k) \]

where

\[ u_j^{k+1} = [G_j(G_j)_{k+1}^k] - u_j^k \]

\[ \times [1 - \Delta_j]_{k+1} \]

\[ G_j(G_j)_{k+1}^k = G_j(u_1^{k+1} \ldots u_j^{k+1}, u_{j+1}^{k+1} \ldots u_J^{k+1}) \]

\[ G_j(G_j)_{k+1}^k = G_j(u_1^{k+1} \ldots u_j^{k+1}, u_{j+1}^{k+1} \ldots u_J^{k+1}) \]

\[ J = \min \left( \left[ \frac{\varepsilon}{|G_{jm}|} \right], (-1)^p \frac{(1 + \varepsilon)}{1 - G_{jj}} \right) \]

\[ J = \min \left( \left[ \frac{\varepsilon}{|G_{jm}|} \right], (-1)^p \frac{(1 + \varepsilon)}{1 - G_{jj}} \right) \]

The \(\alpha_j\) term is a perturbation parameter which accelerates the rate of convergence of (9) and stabilizes the numerical algorithm.

Following Theorems 2 and 3 we may prove that if \(G_{jm}\) is a D-matrix, then (12) is true (linearized sense). Recent results (Dey, 1983b) using local linearization indicates that

\[ \max |G_{jm}| \leq \varepsilon/J \]

where \(G_{jm} = G_{jm}/\delta u_m\) and \(0 < \varepsilon < 1\), \(G\) in (9) is a D-mapping. In order that (13) may be correct, certain input parameters for the system (e.g., mesh size and time-step) have to be chosen in special ways. If this cannot be found a convex-type operation may be defined as follows:

\[ \bar{G}(u, u) = (1 - \alpha_j)u + \alpha G_j(u, u) \]

Assuming \(G_{jj}(u, u) \neq 1\), it has been found that \(G\) is a D-mapping (locally linearized) for the following:

1. \(\alpha_j = (-1)^p(1 - G_{jj})^{-1}\) if \(G_{jm} = 0, m \neq j\) and \(p = 0\) if \(G_{jj} < 1, p = 1\) if \(G_{jj} > 1\).

2. \(\alpha_j = \min \left( \left[ \frac{\varepsilon}{|G_{jm}|} \right], (-1)^p \frac{(1 + \varepsilon)}{1 - G_{jj}} \right) \]

if \(G_{jm} \neq 0, m \neq j\) and \(p = 0\) if \(G_{jj} < 1, p = 1\) if \(G_{jj} > 1\).

The algorithm of perturbed functional iteration including a linearized convergence analysis may be briefly expressed as follows. At each iteration level, compute \(G_{jm}\), \(m = 1, 2, \ldots, J\). If (13) is satisfied, set \(\alpha_j = 1\); otherwise, compute \(\alpha_j\) using (15). If \(\alpha_j \neq 1\), replace \(G_j\) by \(G_j\), as given by (14). Compute \(u_j\) using (11a)-(11d) and compute \(u_j\) at the new iteration level by (10). If (12) is satisfied at some iteration level, convergence is found; if \(G_{jj} = 1\), the method fails.

In general, for a \(J \times J\) system the method requires (1) \(J^2 + J\) functionals to be computed for convergence analysis, (11) partial linearization along the diagonal, and (11) no Jacobians.

It has been proved analytically (Dey, 1977) that in the vicinity of the root, the method should display a superlinear rate of convergence.
A DEGENERATE IMPLICIT CODE

Let a nonlinear model be represented by
\[
du/dt = f(u), \quad u = (u_1, u_2, \ldots, u_j)^T
\]
and the analysis of its numerical solution is given in Chatterjee and others (1983). The equations and the rate constants are given in Chatterjee and Magee (1983). Stiffness was measured by Strate (1983) at \( c = 0, 0.1, 1, \) and 10. Condition numbers are, respectively, \( 10^3, 10^4, 10^5, 10^6 \) (approximately). This may be seen to be true in Fig. 1. This pattern of solution was analyzed by Chatterjee and Magee and was found to be valid. Here, difference equations were formed by approximating the derivatives by using the two-point trapezoidal rule. D-mappings were introduced, and time-accurate solutions were computed with \( \Delta t = 10^{-5}, 10^{-6} \).

CONCLUSION

Numerical solutions of stiff systems are generally obtained by using multistep implicit codes (Miranker, 1981) which require inversion of matrices obtained by computing Jacobians. This has been avoided in the technique explained here. However, the code is dependent on the Jacobians for its convergence analysis. Such a linearized analysis seems to be quite effective, and, in contrast with its nonlinear counterpart, the complete analysis can be done computationally. More applications are under consideration.

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REFERENCES


Table 1: Differential Equations for Transient Species and Radiation Products in Irradiated Neutral Water

\[
\frac{d(H)}{dt} = -2k_1(H)^2 - k_2(e^\rightarrow Aq)(H) - k_5(H)(OH) + k_7(H_2O^\rightarrow)(e^-) - k_4(H)(H_2O)
+ k_{12}(OH)(H) - k_{13}(H_2O)(H) - k_{17}(H)(O_2)
\]

\[
\frac{d(e^- Aq)}{dt} = -k_2(e^- Aq)(H) - 2k_3(e^-)^2 - k_4(e^- Aq)(OH) - k_7(H_2O^\rightarrow)(e^-)
- k_{10}(e^- Aq)(H_2O) - k_{18}(e^- Aq)(O_2)
\]

\[
\frac{d(OH)}{dt} = -k_4(e^- Aq)(OH) - k_5(H)(OH) - 2k_6(OH)^2 + k_9(H)(H_2O_2) + k_{16}(e^- Aq)(H_2O)
- k_{11}(OH)(H_2O) - k_{12}(OH)(H_2) - k_{15}(HO_2)(OH)
\]

\[
\frac{d(H_2O)}{dt} = -k_7(H_2O^\rightarrow)(e^- Aq) - k_8(H_2O^\rightarrow)(OH^-) - k_{18}(H_2O^\rightarrow)(O_2^-) + k_{15}(H_2O) + k_{19}(H_2O)
\]

\[
\frac{d(H_2)}{dt} = k_1(H)^2 + k_2(e^- Aq)(H) + k_3(H)^2 - k_{12}(OH)(H_2)
\]

\[
\frac{d(H_2O_2)}{dt} = k_4(OH)^2 - k_5(H)(H_2O_2) - k_{10}(e^- Aq)(H_2O_2) - k_{11}(OH)(H_2O_2) + k_{13}(HO_2)(H)
+ k_{16}(HO_2)^2
\]

\[
\frac{d(OH^-)}{dt} = k_2(e^- Aq)(H) + 2k_3(e^-)^2 + k_4(e^- Aq)(OH) - k_6(H_2O^\rightarrow)(OH^-)
+ k_{19}(e^- Aq)(H_2O) + k_{19}(H_2O)
\]

\[
\frac{d(HO_2)}{dt} = k_{11}(OH)(H_2O) - k_{14}(HO_2)(H) - k_{15}(HO_2)(OH) - 2k_{16}(HO_2)^2 + k_{17}(H)(O_2)
+ k_{18}(H_2O^\rightarrow)(O_2^-) - k_{22}(HO_2)
\]

\[
\frac{d(O_2^-)}{dt} = -k_{14}(e^- Aq)(O_2^-) + k_{15}(HO_2)(OH) + k_{16}(HO_2)^2 - k_{17}(H)(O_2)
\]

\[
\frac{d(O_2)}{dt} = k_{14}(e^- Aq)(O_2) - k_{16}(H_2O^\rightarrow)(O_2^-) + k_{20}(HO_2)
\]

\[
\begin{align*}
\text{where} & \\
k_1 & = 10^{10} & k_2 & = 2.5 \times 10^{10} & k_3 & = 6 \times 10^9 & k_4 & = 3 \times 10^{10} \\
k_5 & = 2.4 \times 10^{10} & k_6 & = 4 \times 10^9 & k_7 & = 2.3 \times 10^{10} & k_9 & = 3 \times 10^{10} \\
k_8 & = 10^9 & k_9 & = 1.2 \times 10^9 & k_{11} & = 5 \times 10^9 & k_{12} & = 6 \times 10^7 \\
k_{13} & = 10^9 & k_{14} & = 1.9 \times 10^9 & k_{15} & = 10^5 & k_{16} & = 2 \times 10^6 \\
k_{17} & = 10^{10} & k_{18} & = 3 \times 10^{10} & k_{19} & = 5 \times 10^{-5} & k_{20} & = 10^5 \\
k_{21} & = 2.5 \times 10^{10} & k_{22} & = 4 \times 10^9 & k_{23} & = 2.3 \times 10^{10} & k_{24} & = 3 \times 10^{10} \\
k_{25} & = 10^9 & k_{26} & = 1.2 \times 10^9 & k_{27} & = 5 \times 10^9 & k_{28} & = 6 \times 10^7 \\
k_{29} & = 10^9 & k_{30} & = 1.9 \times 10^9 & k_{31} & = 10^5 & k_{32} & = 2 \times 10^6 \\
k_{33} & = 10^{10} & k_{34} & = 3 \times 10^{10} & k_{35} & = 5 \times 10^{-5} & k_{36} & = 10^5
\end{align*}
\]
Fig. 1 Concentrations of species (Ex 2) vs. time for $I = 6.667 \times 10^{-7}$ in the logarithmic scale up to $t = 30$ sec. (Here steady state is reached for all the species.)
**Abstract**

Numerical modeling of D-mappings has been studied and applied to solving nonlinear stiff systems. These mappings have been locally linearized for convergence analysis, and some applications have been made to chemical kinetics.