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BOUNDPAX

A Package for Solving Boundary Value Problems
User's Manual
Chapter III
Multipoint Boundary Value Problems

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CHAPTER III  MULTIPOINT BOUNDARY VALUE PROBLEM

§ 1. Introduction

In this section we first describe the problem briefly. Consider the ODE:

\[ \frac{dx}{dt} = L(t)x(t) + r(t), \quad \alpha < t < \beta, \]

where \( L(t) \) is an \((n \times n)\)-matrix function and \( x(t) \) and \( r(t) \) are \( n \)-vector functions. Let for \( x \) the boundary condition (BC) be given:

\[ M_1 x(\alpha_1) + M_2 x(\alpha_2) + \ldots + M_{m+1} x(\alpha_{m+1}) = b, \]

where \( M_1, \ldots, M_{m+1} \) are \((n \times n)\)-matrices, \( b \) is an \( n \)-vector, the points \( \alpha_1, \ldots, \alpha_{m+1} \), with \( \alpha = \alpha_1 < \alpha_2 < \ldots < \alpha_{m+1} = \beta \), are the so-called switching points.

Because of the linearity of (1.1a) we may write the solution \( x(t) \) as:

\[ x(t) = F(\alpha_i, t)c_i + w(\alpha_i, t), \quad \alpha_i < t < \alpha_{i+1}, \]

where \( F(\alpha_i, t) \) is a fundamental solution on \([\alpha_i, \alpha_{i+1}]\) and \( w(\alpha_i, t) \) a particular solution of (1.1a) on \([\alpha_i, \alpha_{i+1}]\). In principle we may identify \( F(\alpha_i, t) \) with \( F(\alpha_j, t) \) for \( i \neq j \), thus reducing (1.2) to the well-known superposition of solutions. However, as was shown in \([1]\) the dichotomy character might be different on each subinterval (that is the dimension of the non-decreasing mode subspace may become smaller after such a point \( \alpha_i \)). Hence it makes sense to consider the \( F(\alpha_i, t) \) separately, at least computationally, cf. \([2]\). Matching in the usual way gives us the relation for the \( c_i \). We obtain:

\[ F(\alpha_i, \alpha_{i+1})c_i = F(\alpha_{i+1}, \alpha_{i+1})c_{i+1} + w(\alpha_i, \alpha_{i+1})w(\alpha_{i+1}, \alpha_{i+1}) \]

and the BC

\[ M_1 F(\alpha_1, \alpha_1)c_1 + \ldots + [M_m F(\alpha_m, \alpha_m) + M_{m+1} F(\alpha_m, \alpha_m)]c_m = b, \]

\[ b := b - M_1 w(\alpha_1, \alpha_1) - \ldots - M_m w(\alpha_m, \alpha_m) - M_{m+1} w(\alpha_m, \alpha_{m+1}). \]

The algorithm on which MUTSM is based now uses multiple shooting on each interval \([\alpha_i, \alpha_{i+1}]\). In this way we obtain a discrete analogue of (1.3) and (1.4) which constitutes a linear system \( A \) of order \( m \times n \). The conditioning of the problem can be measured by \( ||A^{-1}|| \) as well as by monitoring the growth behaviour of the fundamental solutions. These quantities are actually accounted for by the routine, see §4.
Remark 1.5.

If on consecutive intervals \([a_{i+1}, a_{i+1}], \ldots, [a_{i+k}, a_{i+k+1}]\) say, the dichotomy does not change, the fundamental solutions \(F(a_{i+1}, t) \mid t = 1, \ldots, k\) can be identified with \(F(a_i, t)\), the particular solutions \(w(a_{i+1}, t) \mid t = 1, \ldots, k\) with \(w(a_i, t)\) and the \(c_{i+1, l} \mid l = 1, \ldots, k\) with \(c_i\). As a consequence (1.3) and (1.4) change into

\[(1.6a) \quad F(a_i, a_{i+1}) c_{j} = F(a_{j+1}, a_{j+1}) c_{j+1} + w(a_{j+1}, a_{j+1}) - w(a_j, a_{j+1}) \quad j=1, \ldots, i-1 \text{ and } j=i+k+1, \ldots, m \]

\[(1.6b) \quad F(a_i, a_{i+k+1}) c_i = F(a_{i+k+1}, a_{i+k+1}) c_{i+k+1} + w(a_{i+k+1}, a_{i+k+1}) \]

\[- w(a_i, a_{i+k+1}). \]

\[(1.7) \quad M_i F(a_i, a_1) c_1 + \ldots + \left[ \sum_{l=1}^{i+k} M_l F(a_i, a_1) \right] c_i + M_{i+k+1} F(a_{i+k+1}, a_{i+k+1}) + \]
\[\ldots + \left[ \sum_{l=m}^{m+1} M_l F(a_m, a_1) \right] c_m = \hat{b}, \]

\[\hat{b} = b - M_i w_i(a_i, a_1) - \ldots - \sum_{l=i}^{i+k} M_l w(a_i, a_1) - \ldots - \sum_{l=m}^{m+1} M_l w(a_m, a_1). \]

This gives a linear system of order \((m-k) \times n\).
§ 2. Global description of the algorithm

In this section we outline the actual computations performed.

As mentioned in § 1, multiple shooting is used on each interval \([a_i, a_{i+1}]\) to compute a fundamental solution and a particular solution. Each interval \([a_i, a_{i+1}]\) is divided into say \(N_i-1\) subintervals. To simplify the notation we will use a local index \(j\) to describe them, i.e. let the interval \([a_i, a_{i+1}]\) be split up into subintervals \([t_{j-1}, t_j]\), \(j=2, \ldots, N_i\), \(t_1=a_i\) and \(t_{N_i}=a_{i+1}\).

Like in the algorithm described in [3] for two-point BVP, fundamental solutions \(F_j(a_i,\cdot)\) and particular solutions \(w_j(a_i,\cdot)\) are computed such that:

\[
F_j(a_i, t_{j+1}) = F_{j+1}(a_i, t_{j+1})U_{j+1}(i) = Q_{j+1}(i)U_{j+1}(i), \quad j = 1, \ldots, N_i-1,
\]

where the \(Q_j(i)\) are orthogonal and the \(U_j(i)\) upper triangular.

For the solution \(x(t)\) we have:

\[
x(t) = F_j(a_i, t)a_j(i) + w_j(a_i, t),
\]

from which the following upper triangular recursion for the \(a_j(i)\) is obtained:

\[
a_{j+1}(i) = U_{j+1}(i)a_j(i) + d_{j+1}(i), \quad j = 1, \ldots, N_i-1,
\]

where

\[
d_{j+1}(i) = Q_{j+1}(i)^{-1}[w_j(a_i, t_{j+1}) - w_{j+1}(a_i, t_{j+1})].
\]

Now assume that \(\{\Phi_j(i)\}_{j=1}^{N_i}\) is a fundamental solution of (2.3) (cf. [3, (3.4)]) and \(\{z_j(i)\}_{j=1}^{N_i}\) some particular solution. Then for some vector \(c_i\) we should have:

\[
a_j(i) = \Phi_j(i)c_i + z_j(i), \quad j = 1, \ldots, N_i
\]

By matching at the points \(a_i\) we obtain a recursion for the \(\{c_i\}\) in the usual way. So for the solution of the BVP at the switching points \(a_1, a_2, \ldots, a_{m+1}\) we have:

\[
x(a_1^i) = w_1(a_1^i, a_1^i) + Q_1(i)[z_1(i) + \Phi_1(i)c_1] \quad ,i=1, \ldots, m
\]

and
Substituting (2.6) in the BC gives a BC for the sequence \( \{c_i\}_{i=1}^m \) (cf. (1.4)) viz.

\[
M_1 Q_1(i) \Phi_1(i) c_i + \ldots + [M_m Q_m(m) \Phi_m(m) + M_{m+1} Q_{N_m}N_m(m)] c_m = \vec{\alpha},
\]

\[
\vec{\alpha} = b - \sum_{i=1}^{m} M_1 Q_1(i) z_1(i) - M_{m+1} Q_{N_m}N_m(m)
\]

\[
- \sum_{i=1}^{m} M_i w_1(\alpha_i, \alpha_i) - M_{m+1} w_1(\alpha_m, \alpha_{m+1}).
\]

Denoting:

\[
\begin{align*}
\vec{\eta}_i &= M_1 Q_1(i) \Phi_1(i) \quad i=1, \ldots, m-1, \\
\vec{\eta}_m &= M_m Q_m(m) \Phi_m(m) - M_{m+1} Q_{N_m}N_m(m), \\
\psi_i &= \Phi_{N_i}(i), \quad i=1, \ldots, m-1, \\
Q_{i+1} &= Q_{N_i}^{-1}(i) Q_1(i+1) \Phi_1(i+1), \quad i=1, \ldots, m-1, \\
q_i &= Q_{N_i}^{-1}(i) [w(\alpha_{i+1}, \alpha_{i+1}) - w_{N_i}(\alpha_{i}, \alpha_{i+1})] + \\
&\quad Q_{N_i}^{-1}(i) Q_1(i+1) z_1(i+1) - z_{N_i}(i), \quad i=1, \ldots, m-1.
\end{align*}
\]

then we obtain the linear system:

\[
(2.9a) \quad \mathbf{A} \mathbf{c} = \mathbf{q},
\]

where

\[
\mathbf{A} = \begin{bmatrix}
\psi_1 & -Q_2 & & \\
& \ddots & \ddots & \\
& & \psi_{m-1} & -Q_m \\
\vec{\eta}_1 & \vec{\eta}_2 & \ldots & \vec{\eta}_m
\end{bmatrix}, \quad \mathbf{c} = \begin{bmatrix} c_1 \\
\vdots \\
\vdots \\
c_m \end{bmatrix}, \quad \mathbf{q} = \begin{bmatrix} q_1 \\
\vdots \\
\vdots \\
q_m \end{bmatrix}.
\]
Remark 2.10

In the case that the ODE (1.1a) is homogeneous, i.e. \( r(t) = 0, \ t \in [\alpha, \beta] \), the computation of particular solutions is skipped. Then (2.2), (2.3), (2.5), (2.6) have to be replaced by:

\[
(2.2)' \quad x(t_{j+1}) = F_j(\alpha, t_{j+1})a_j(i) = F_{j+1}(\alpha, t_{j+1})a_{j+1}(i),
\]
\[
(2.3)' \quad a_{j+1}(i) = U_{j+1}(i)a_j(i),
\]
\[
(2.5)' \quad a_j(i) = \Phi_j(i)c_i, \ j = 1, \ldots, N_i,
\]
\[
(2.6a)' \quad x(\alpha) = Q_1(i)\Phi(i)c_1, \ i = 1, \ldots, m,
\]
\[
(2.6b)' \quad x(\alpha_{m+1}) = Q_{Nm}(m)\Phi_n(m)c_m,
\]
respectively.

Moreover, the vector \( b \) in (2.7) equals \( b \) and the vector \( q \) in (2.9a) becomes:

\[
q = \begin{bmatrix} 0 \\ \vdots \\ 0 \end{bmatrix}.
\]
§ 3. Special features of the method

The actual computation of the solutions \( P(\alpha_i, \cdot) \) and \( w(\alpha_i, \cdot) \) on each interval is basically the same as described in [3, §§3.1, 3.2], i.e. the algorithm uses the adaptivity feature for the integration for the particular mode only. Also it uses the decoupled form of the recursion (2.3) for the computation of \( \Phi_j(i) \) and \( z_j(i) \). Below we summarize some more aspects.

§ 3.1 Computation of the \( \Phi_j(i) \)

As was shown in [1] a well conditioned multipoint boundary value problem is dichotomic on each interval \([\alpha_i, \alpha_{i+1}]\). As a consequence we basically should reckon with a different partitioning integer \( k_p \) (cf. [§I.3.2]), indicating the dimension of the increasing solutionspace, on each such interval. If we denote this integer at the \( i^{th} \) interval by \( k(i) \), we then know from [1] that for well conditioned multipoint boundary value problems, \( k(i) \) is a non-increasing set, i.e. \( k(1) > k(2) > \ldots > k(m) \). The fundamental solution \( \{ \Phi_j(i) \}_{j=1}^{N_1} \) cf. (2.3) on the \( i^{th} \) interval is then computed using the BC:

\[
\Phi_j^{2}(i) = [\emptyset | I_{n-k(i)}] \quad ; \quad \Phi_j^{1}(i) = [I_{k(i)} | \emptyset]
\]

where the superscript refers to an obvious local partitioning involving the integer \( k(i) \).

§ 3.2 Choosing \( P(\alpha_i, \alpha_i) \) and \( w(\alpha_i, \alpha_i) \)

Like in the two point case there is, in general, no information available for choosing the particular solution \( w_j(\alpha_i, t) \) in a special way. Hence \( w_j(\alpha_i, t_j) = 0 \) is a good one, simplifying the formulae in (2.4)-(2.9) substantially.

At \( t = a_1 \) the algorithm initially chooses \( Q_i(1) = P(\alpha_i, a_1) = I \) and checks the ordering of the diagonal elements of the first upper triangular matrices \( U_j(i) \), computed after reaching the endpoint of a minor shooting interval. If this ordering is found to be improper it performs permutation of columns like in [§I.3.3]. Arriving at \( t = a_2 \) we have a complete freedom to choose \( P(\alpha_2, a_2) \).

A very useful choice is:

\[
P(\alpha_2, a_2) = Q_{N_1}^{-1}(1).
\]

Indeed, if the dichotomy is invariant on \([\alpha_1, \alpha_3]\) then we may proceed on \([\alpha_2, \alpha_3]\) like we did on the previous interval, thus computing an upper triangular recursion for the superposition vectors \( a_j(1) \) and \( a_j(2) \) combined. By formally writing
we may extend the recursion (2.3) for \( i = 1 \) over the index range \( j = 1, \ldots, N_1 + N_2 - 1 \).

If \( Q_{N_1}^{-1}(1) \) is found not to be a good starting value on the interval \([a_2, a_3]\), for similar reasons as the identity might be an improper starting matrix on \([a_1, a_2]\), a permutation of its columns is carried out until some satisfactory ordering on the diagonal of the upper triangular matrices \( U_j \) has been found. Since for well conditioned multipoint BVP, \( [k(i)]_{i=1}^{m} \) is a non-increasing set, a permutation is carried out on the first \( k(i) \) columns of \( Q_{N_1}^{-1}(1) \) only.

§ 3.3 Reduction of the system (2.9)

If the choice (3.2) is a proper one then we can identify \( c_1 \) and \( c_2 \) in (2.5), so the system (2.9a) is of order \((m-1) \times n \) only, being of the form:

\[
\begin{align*}
(3.4a) & \quad \hat{A} \hat{c} = \hat{q} \\
& \quad \text{where} \\
(3.4b) & \quad \hat{A} = \begin{bmatrix}
\hat{\Psi}_1 & -\hat{\Psi}_3 \\
\hat{\Psi}_3 & -\hat{Q}_4 \\
\hat{M}_1 & \hat{M}_3 & \hat{M}_4 & \cdots & \hat{M}_m
\end{bmatrix}, \quad \hat{c} = \begin{bmatrix}
c_1 \\
c_3 \\
\vdots \\
c_m
\end{bmatrix}, \quad \hat{q} = \begin{bmatrix}
q_1 \\
q_3 \\
\vdots \\
q_{m-1} \\
b
\end{bmatrix}
\end{align*}
\]

and where we have denoted for short \((L=N_1+N_2-1)\):

\[
\begin{align*}
(3.4c) & \quad \Psi_1 = \Psi_L(1); \quad \Psi_3 = \Psi_L^{-1}\Psi_1(3)\Psi_1(3), \\
(3.4d) & \quad \hat{M}_1 = M_1\Psi_1(1)\Psi_1(1) + M_2Q_{N_1}(1)\Psi_{N_1}(1), \\
(3.4e) & \quad \hat{Q}_1 = \Psi_L^{-1}(1)[\nu(\alpha_3, \alpha_3) - \nu_L(\alpha_1, \alpha_3)] + \Psi_L^{-1}(1)Q_1(3)z_1(3) - z_L(1).
\end{align*}
\]

Hopefully it will be clear how further reductions can be carried out now. Such a further reduction may arise either from an even longer interval \([a_1, a_3]\) where the dichotomy is invariant or from an invariance on other consecutive intervals. In particular it may happen that the order of the thus obtained matrix \( \hat{A} \) is just \( n \); in such a situation we virtually have reduced the procedure to that of the two-point case.
§ 3.4 Special solution of the algebraic system (2.9)

Instead of solving the system (2.9) (or its condensed variant (3.4)) by LU-decomposition, we do the following: Rewrite the matrix $A$ for simplicity as:

\[
A = \begin{bmatrix}
S_1 & -R_2 & & \\
& S_2 & -R_3 & \\
& & \ddots & \ddots \\
& & & S_{N-1} & -R_N \\
T_1 & T_2 & T_3 & \cdots & T_{N-1} & T_N
\end{bmatrix}, \quad q = \begin{bmatrix}
q_1 \\
q_2 \\
\vdots \\
q_N
\end{bmatrix}
\]

At the $i$th switching point interval, let $k_i$ be the partitioning integer, i.e. there are $k_i$ increasing solutions at that interval. From [1] we know that \{k_i\} is a non-increasing set, i.e. we expect

\[
k_1 > k_2 > \cdots > k_{N-1} > k_N.
\]

In the recursion (cf. (2.9) and (3.5))

\[
R_{i+1}c_{i+1} = S_ic_i - q_i,
\]

we have

\[
R_{i+1} = \begin{bmatrix}
R_{i+1}^{11} & R_{i+1}^{12} \\
0 & I
\end{bmatrix},
\]

where $R_{i+1}^{11}$ is $k_i \times k_i$ and the identity matrix is of order $n - k_{i+1}$, and

\[
S_i = \begin{bmatrix}
I & 0 \\
0 & S_{22}
\end{bmatrix},
\]

where $S_i$ is $(n-k_i) \times (n-k_i)$ and the identity matrix is of order $k_i$.

We now like to solve (3.7) plus BC again by superposition. Since we do not have a uniform dichotomy on $[a, \beta]$ we use a more refined fundamental solution $\{W_i\}_{i=1}^N$ (cf. § 3.1). By assumption we let the partitioning depend on the index.
At \( i = 1 \) we define:

\[
\psi_i = \begin{bmatrix} \psi_{11} & \psi_{12} \\ \phi & \psi_{22} \end{bmatrix}, \psi_{11} \text{ of order } k_1.
\]

and compute

\[
\psi_{22} = S_{11} \psi_{12},
\]

(For \( S_{11} \), the right lower block of \( S_1 \), see (3.8b)), where \( \psi_{22} \) has the same order as \( S_{11} \) and \( \psi_{12} \).

Now compute \( \psi_{22} \) as follows:

\[
\psi_{22} = \begin{bmatrix} k_{1-k_2} & \phi \\ \phi & \psi_{22} \end{bmatrix}, \text{ if } k_1 > k_2 \text{ and } \psi_{22} = \psi_{22} \text{ otherwise.}
\]

and from this \( \psi_{22} \) etc.. In general we have

\[
\psi_{i+1} = \begin{bmatrix} k_{1-k_{i+1}} & \phi \\ \phi & \psi_{i+1} \end{bmatrix}, \text{ if } k_i > k_{i+1} \text{ and } \psi_{i+1} = \psi_{i+1} \text{ otherwise.}
\]

At \( i = N \) we set

\[
[\psi_{11} | \psi_{12}] = [I_{k_N} | \emptyset].
\]

Then we have

\[
\psi_N = \begin{bmatrix} \psi_{11} & \emptyset \\ \emptyset & \psi_{22} \end{bmatrix} = \begin{bmatrix} \psi_{11} & \psi_{12} \\ \phi & \psi_{22} \end{bmatrix},
\]

where \( \psi_{11} \) is of order \( k_{N-1} \), \( \psi_{12} k_{N-1} \times (n-k_{N-1}) \) and \( \psi_{22} \) is of order \( n-k_{N-1} \) (the latter already being computed in the forward sweep). Next we have

\[
\psi_{i+1} = R_{N-1} \psi_{i+2} + R_{N} \psi_{22},
\]

\[
\psi_{N-1} = R_{N} \psi_{i+2}.
\]

And in general:
where \( \psi_{i}^{11} \) is of order \( k_{i} \) and \( \psi_{i}^{11} \) is of order \( k_{i-1} \).

Then:

\[
(3.16a) \quad \psi_{i}^{12} = n! \psi_{i}^{12} + n \psi_{i}^{22} ,
\]

\[
(3.16b) \quad \psi_{i-1}^{11} = R_{i}^{11} \psi_{i}^{11} ,
\]

Note that this scheme to compute \( \{ \psi_{i} \} \) is a generalization of the dichotomic case dealt with in Ch. I.

Finally we compute a particular solution \( \{ p_{i} \} \), which is done in a similar way as the computation of the fundamental solution. We start with

\[
(3.18a) \quad P_{i}^{2} = 0 , \quad P_{N}^{1} = 0
\]

(again the partitioning here and below is local!). At each of the switching points where \( k_{i+1} < k_{i} \) we add sufficient zeros to obtain a larger second component vector, so for \( i = 1, \ldots, N \)

\[
(3.18b) \quad p_{i+1}^{2} := s_{i}^{2} P_{i}^{2} - q_{i}^{2} ;
\]

\[
(3.18c) \quad p_{i+1}^{2} = \tilde{p}_{i+1}^{2} , \quad \text{if } k_{i} = k_{i+1} ,
\]

\[
= \left[ \begin{array}{c} b \\ \tilde{p}_{i+1}^{2} \end{array} \right] , \quad \text{if } k_{i} > k_{i+1} ,
\]

i.e. the first \( k_{i} - k_{i+1} \) elements of \( p_{i+1}^{2} \) are 0.

At the backward sweep we typically compute

\[
(3.18d) \quad P_{i} = \begin{bmatrix} P_{i}^{1} \\ P_{i}^{2} \end{bmatrix} = \begin{bmatrix} P_{1}^{1} \\ P_{1}^{2} \end{bmatrix} ,
\]

where \( \tilde{p}_{i}^{1} \) is a vector of order \( k_{i-1} \).

\[
(3.18e) \quad p_{i-1}^{1} = R_{i}^{11} \tilde{p}_{i}^{1} + R_{i}^{12} \tilde{p}_{i}^{2} + q_{i-1}^{1} ,
\]

where \( q_{i-1}^{1} \) represents the first \( k_{i-1} \) elements of \( q_{i-1} \).

The solution \( \{ c_{i} \} \) of (2.9) is then given by:

\[
(3.19) \quad c_{i} = \psi_{i} v + p_{i} ,
\]
where the vector \( v \) can be found from:

\[
(3.20) \quad \left[ N \sum_{j=1}^{N} T_j \varphi_j \right] v = \hat{b} - \sum_{j=1}^{N} T_j p_i
\]

§ 3.5 Conditioning and stability

Since multipoint problems are essentially more complicated than two point ones, the algorithm outlined before and - as a consequence - also its stability analysis is more difficult. As we already indicated, the homogeneous solution space is polychomic, that is dichotomic on each interval \([\alpha_i, \alpha_{i+1}]\) and moreover such that non decreasing basis solutions may become non increasing at one of the switching points at most. Since the algorithm is tuned to monitor the particular dichotomy on each interval, it follows from arguments in Ch. I, §3.2 that the recursions are used in stable directions only (that is if we assume well-conditioning, so polychotomy cf. [1]). The only remaining problem then is the conditioning of the system in (3.20), that is of the matrix \( W \) defined by

\[
(3.21) \quad W := \sum_{j=1}^{m} M_{i-j} \varphi_j
\]

One can show that in general

\[
(3.22) \quad \| W^{-1} \| < (m+1)CN,
\]

where

\[
(3.23) \quad CN := \max_{t \in [\alpha, \beta]} \left\| \sum_{j=1}^{m+1} M_j F(\alpha_j)^{-1} \right\|,
\]

where \( F \) is any fundamental solution. Note that (3.23) is a straightforward generalization of I.(3.12) and is a measure for amplifications of perturbation in the BC. For stability with respect to perturbations in the ODE as such we may monitor appropriate blocks of the upper triangular matrices.
§ 4. Computational aspects

The routine MUTSM basically uses the same strategy for computing the upper triangular recursion on the intervals \([\alpha_i, \alpha_{i+1}]\), \(i=1, \ldots, m\) as the routine MUTSG for two-point BVP (see Ch.1). Only the choice of the \(Q_i(i)\), \(i=2, \ldots, m\) (that is the orthogonal value for \(P(\alpha_i, \alpha_{i+1})\)) and the computation of the k-partitionings are different (see next section).

The computations of the \(\{c_i\}_{i=1}^m\) is described in § 3. Once knowing the \(c_i\), the computation of the solution at the \(i\)th interval \([\alpha_i, \alpha_{i+1}]\) is the same as in the two-point case (see Ch.1).

§ 4.1 The computation of \(Q_i(i)\)

On the first interval \([\alpha_1, \alpha_2]\) we do the same as in the two-point case, i.e. \(Q_i(1)=I\) and if this is not a satisfactory choice, the columns of \(Q_i(1)\) are permuted such that diagonal(\(H U_i(1)\)) is ordered.

As a first choice for \(Q_i(1), i=2, \ldots, m\) we take (see §3.2)

\[
(4.1) \quad Q_i(1) = Q_{N_i}^{(i-1)}.
\]

Since the dichotomic character of the solution space may change at each switching point, it may be necessary to carry out a permutation of columns of \(Q_i(1)\). Anticipating that the problem is well-conditioned (i.e. the partitioning parameters satisfies \(k_{i-1} > k_i\)) no column interchanges are necessary for the last \(n-k_i-1\) columns. So an initial choice of \(Q_i(i)\) is accepted if the first \(k_i-1\) elements of diagonal(\(H U_i(i)\)) are ordered, otherwise a permutation of the first \(k_i-1\) columns of \(Q_i(i)\) is carried out. At this stage the partitioning parameter \(k_i\) is computed as the number of elements of the first \(k_i-1\) elements of diagonal(\(H U_j(i)\)) which are greater than 1. If no permutations are needed and \(k_{i-1}=k_i\) then the two successive intervals \([\alpha_{i-1}, \alpha_i]\) and \([\alpha_i, \alpha_{i+1}]\) are assembled (see §3.2).

However, it is possible that due to discretization errors, the computed \(k_i\) does not correspond to the proper partitioning. Therefore, after the above described procedure, globally correct partitioning parameters are determined.

§ 4.2 Finding a globally correct partitioning

Although the algorithm tries to determine a correct partitioning parameter \(k_i\) on each interval \([\alpha_i, \alpha_{i+1}]\), its resolution of the growth behaviour of the various modes may be fairly small (e.g. if \(\alpha_{i+1}-\alpha_i\) is small) and/or it may be
mised by non growing- non decreasing modes. Since a normal (that is a wellconditioned) situation implies the existence of a non increasing sequence \( \{ k_i \} \), we need a check on this and - if this does not turn out to be monotonic - an update. This is done by the following procedure:

step 1: Compute on each interval \([\alpha_i, \alpha_{i+1}]\), \(i=1,\ldots,m\), a partitioning parameter \( k_i \), where \( k_i \) is the number of elements of \( N_i \) diagonal( \( \Pi U_j(i) \) ), which are greater than 1.

step 2: Determine the lowest index \( i \), where \( k_i > k_{i-1} \). If no such index exists, goto step 8.

step 3: Determine the lowest index \( j < i \), where \( k_j < k_1 \).

step 4: Determine the index \( p > i \), where \( k_i = k_{i+1} = \ldots = k_p = k_{p+1} \).

step 5: Compute a global partitioning parameter \( \tilde{k}_1 \) say, for the interval \([\alpha_j, \alpha_{p+1}]\) by checking the increments over \([\alpha_j, \alpha_{p+1}]\) in an obvious way, taking into account the various permutations at the switching points.

step 6: The new updated sequence \( \{ k_i \}^m_{i=1} \) is defined as

\[
\begin{bmatrix}
  k_i \\
  k_1 \\
\end{bmatrix}
\begin{bmatrix}
  \max(k_i, \tilde{k}_1) \\
  \tilde{k}_1 \\
\end{bmatrix}
\begin{bmatrix}
  i=1,\ldots,j-1,p+1,\ldots,m \\
  i=j,\ldots,l-1 \\
  i=1,\ldots,p \\
\end{bmatrix}
\]

step 7: Go back to step 2.

step 8: The current sequence \( \{ k_i \}^m_{i=1} \) is correct.

With this procedure we get, at least theoretically, a good choice for the sequence of the \( k_i \). However, if the problem is not polychotomic also this procedure may not be satisfactory, naturally, and a large amplification factor may result (as is to be expected of course).

§ 4.3 The computation of stability constants

Since the algorithm computes fundamental solutions at (possibly "enlarged") switching intervals, it does some bookkeeping of stability constants. The computations of the stability constant \( C_\infty \) (see §3.5) is a straightforward matter and its value can be found in ER(4).

Concerning the "amplification factor", which is an estimate for the Green's functions, the algorithm computes an estimate for this on each interval. Therefore the output value in ER(5) is the maximum of such factors over the entire region.
Remark 4.4

If the partitioning is incorrect, we may expect at least ER(5) to be "large". On the other hand, due to the special way the algorithm tries to seek the appropriate partitionings, it should be expected that a large value of ER(5) has to be attributed to the problem.
References


DMUTSM

***************
SPECIFICATION (FORTRAN IV)
***************

SUBROUTINE DMUTSM(FLIN,FDIF,N,IHOM,TSP,NSP,BCM,BCV,AMP,ER,NRTI,TI,
1 NTI,X,NU,Q,D,KPART,PHIREC,W,LW,LIW,LIW,IERROR)
C INTEGER N,IHOM,NSP,NRTI(NSP),NU,KPART(NSP),LW,LIW,LIW,IERROR
C DOUBLE PRECISION TSP(NSP),BCM(N,N,NSP),BCV(N),AMP,ER(5),TI(NTI),
C 1 X(N,NTI),U(NU,NTI),Q(N,N,NTI),D(N,NTI),
C 2 PHIREC(NU,NTI),W(LW)
C EXTERNAL FLIN,FDIF

***************
Purpose
***************

DMUTSM solves the multi-point BVP:
\[ \frac{dy(t)}{dt} = L(t)y(t) + r(t), \]
with BC:
\[ M_{A_1} y(A_1) + M_{A_2} y(A_2) + \cdots + M_{A_k} y(A_k) = BCV, \]
where \( M_{A_j} \), \( j = 1, \ldots, k \) are the NxN BC matrices, \( BCV \) an N BC vector and
\( A_1 < A_2 < \ldots < A_k \) or \( A_1 > A_2 > \ldots > A_k \) the switching points.

***************
Parameters
***************

FLIN SUBROUTINE, supplied by the user with specification:

SUBROUTINE FLIN(T,Y,F)
DOUBLE PRECISION T,Y(N),F(N)
where \( N \) is the order of the system. FLIN must evaluate the homogeneous part of the differential equation, \( L(t)y(t) \), for \( t=T \) and \( y(t)=Y \) and place the result in \( F(1), F(2), \ldots, F(N) \).

FLIN must be declared as EXTERNAL in the (sub)program from which
DMUTSM is called.

FDIF SUBROUTINE, supplied by the user, with specification:

SUBROUTINE FDIF(T,Y,F)
DOUBLE PRECISION T,Y(N),F(N)
where \( N \) is the order of the system. FDIF must evaluate the righthand-side of the inhomogeneous differential equation, \( L(t)y(t) + r(t) \), for \( t=T \) and \( y(t)=Y \) and place the result in \( F(1), F(2), \ldots, F(N) \).

FDIF must be declared as EXTERNAL in the (sub)program from which
DMUTSM is called.

-- 16 --
In the case that the system is homogeneous FDIF is the same as FLIN.

N INTEGER, the order of the system.
Unchanged on exit.

IHOM INTEGER. IHOM indicates whether the system is homogeneous or inhomogeneous.
IHOM = 0 : the system is homogeneous,
IHOM = 1 : the system is inhomogeneous.
Unchanged on exit.

TSP DOUBLE PRECISION array of dimension (m), m > NSP.
On entry TSP must contain the switching points \( A_j, j=1,\ldots,\text{NSP} \) in monotone order, i.e. \( TSP(j) = A_j, j=1,\ldots,\text{NSP} \).
Unchanged on exit.

NSP INTEGER. NSP is the number of switching points.
Unchanged on exit.

BCM DOUBLE PRECISION array of dimension \((N,N,m), m > \text{NSP}\).
On entry: BCM(\(.,.,j\)) must contain the BC matrix \( MA_j, j=1,\ldots,\text{NSP} \).
Unchanged on exit.

BCV DOUBLE PRECISION array of dimension \((N)\).
On entry BCV must contain the BC vector.
Unchanged on exit.

AMP DOUBLE PRECISION.
On entry AMP must contain the allowed incremental factor of the homogeneous solutions.
AMP should be greater than 1, if not the subroutine will change AMP into \( \max(\text{ER}(1),\text{ER}(2)) / \text{ER}(3) \).
If \( \text{NRTI}(1) > 0 \), AMP is a dummy parameter.

ER DOUBLE PRECISION array of dimension \((5)\).
On entry ER(1) must contain a relative tolerance for solving the differential equation. If the relative tolerance is smaller than \( 1.0 \times 10^{-12} \) the subroutine will change ER(1) into \( 1.0 \times 10^{-12} + 2 \times \text{ER}(3) \).
On entry ER(2) must contain an absolute tolerance for solving the differential equation.
On entry ER(3) must contain the machine constant.
On exit ER(2) and ER(3) are unchanged.
On exit ER(4) contains an estimation of the condition number of the BVP.
On exit ER(5) contains an estimated error amplification factor.

NRTI INTEGER array of dimension \((m), m > \text{NSP}\).
On entry: NRTI(1) = 0, in this case the subroutine determine automatically the output-points using AMP.
NRTI(1) = 1, in this case the output-points are supplied by the user in the array TI. The output-points must be given in strict monotone order and must include the switching points.
NRTI(1) > 1, in this case the NRTI(j), j=2,\ldots,\text{NSP} must contain the number of output-points - 1, which are required on the interval \([TSP(j-1),TSP(j)], j=2,\ldots,\text{NSP}\). The output-points are then computed by:
\[ \text{TI}(1) = \text{TSP}(1), \]
\[ \text{TI}((j-1) \times \text{NRTI}(j+1)+1+m) = \text{TSP}(j)+m \times (\text{TSP}(j+1)-\text{TSP}(j))/\text{NRTI}(j+1), \]
\[ m = 1, \ldots, \text{NRTI}(j+1). \]

If \( \text{NRTI}(i) < 2, i = 2, \ldots, \text{NSP}, \) \( \text{NRTI}(i) = 1 \) is used in the above formular.

Note that the switching points will always be output-points.

On exit \( \text{NRTI}(1) \) contains the total number of output-points.

\textbf{TI} DOUBLE PRECISION array of dimension (\text{NTI}).

On entry; if \( \text{NRTI}(1) = 1, \) \text{TI} must contain the required output-points in strict monotone order: \( A_1 = \text{TI}(1) < \cdots < \text{TI}(l) = A_k \) or \( A_1 = \text{TI}(1) > \cdots > \text{TI}(l) = A_k \) (1 denotes the total number of required output-points). The output-points must include all switching points \( A_j, j = 1, \ldots, k. \)

On exit: \( \text{TI}(1), i = 1, 2, \ldots, \text{NRTI}(1), \) contains the output-points.

\textbf{NTI} INTEGER.

\( \text{NTI} \) is the dimension of \text{TI} and one of the dimensions of the arrays \text{X, U, Q, D, PHIREC}. \( \text{NTI} \) must be greater then the total number of output-points + 4.

Unchanged on exit.

\textbf{X} DOUBLE PRECISION array of dimension (\text{N,NTI}).

On exit \( \text{X}(i,k), i = 1, 2, \ldots, \text{N} \) contains the solution of the BVP at the output-point \( \text{TI}(k), k = 1, \ldots, \text{NRTI}(1). \)

\textbf{U} DOUBLE PRECISION array of dimension (\text{NU,NTI}).

On exit \( \text{U}(i,k), i = 1, 2, \ldots, \text{NU} \) contains the relevant elements of the uppertriangular matrix \( \text{U}_k, k = 2, \ldots, \text{NRTI}(1). \) The elements are stored column wise, the \( j \)th column of \( \text{U}_k \) is stored in \( \text{U}(nj+1,k), \text{U}(nj+2,k), \ldots, \text{U}(nj+j,k), \) where \( nj = (j-1) \times j/2. \)

\textbf{NU} INTEGER.

\( \text{NU} \) is one of the dimensions of \text{U} and \text{PHIREC}. \( \text{NU} \) must be at least equal to \( \text{N} \times (\text{N}+1) / 2. \)

Unchanged on exit.

\textbf{Q} DOUBLE PRECISION array of dimension (\text{N,N,NTI}).

On exit \( \text{Q}(i,j,k), i = 1, 2, \ldots, \text{N}, j = 1, 2, \ldots, \text{N} \) contains the \( N \) columns of the orthogonal matrix \( \text{Q}_k, k = 1, \ldots, \text{NRTI}(1). \)

\textbf{D} DOUBLE PRECISION array of dimension (\text{N,NTI}).

If \( \text{IHOM} = 0 \) the array \text{D} has no real use and the user is recommanded to use the same array for the \text{X} and the \text{D}.

If \( \text{IHOM} = 1 ; \) on exit \( \text{D}(i,k), i = 1, 2, \ldots, \text{N} \) contains the inhomogeneous term \( d_k, k = 1, 2, \ldots, \text{NRTI}(1) \), of the multiple shooting recursion.

\textbf{KPART} INTEGER array of dimension (\text{m}), \text{m} \geq \text{NSP}.

On exit \text{KPART}(j) contains the global partitioning parameter of the interval \( [\text{TSP}(j-1),\text{TSP}(j)] \), \( j = 2, \ldots, \text{NSP}. \)

\textbf{PHIREC} DOUBLE PRECISION array of dimension (\text{NU,NTI}).

On exit \text{PHIREC} contains a fundamental solution of the multiple shooting recursion. The fundamental solution is uppertriangular and is stored in the same way as the \( \text{U}_k. \)
DMUTSM

\text{CH. III,3}

\begin{itemize}
\item **W**: DOUBLE PRECISION array of dimension (LW).
  Used as work space.

\item **LW**: INTEGER.
  LW is the dimension of the work array W.
  \( NW > 3N^2N + 8N + NSP(1.5N^2N + 2.5N) \)

\item **IW**: INTEGER array of dimension (NIW)
  Used as work space.

\item **NIW**: INTEGER.
  NIW is the dimension of the INTEGER array IW.
  \( NIW > 3N + (N+1)\ast NSP. \)

\item **IERROR**: INTEGER.
  Error indicator; IERROR = 0 then there are no errors detected.
\end{itemize}

****************
Error indicators
****************

Errors detected by the subroutine

\begin{itemize}
\item **IERROR = 0**: No errors detected.

\item **IERROR = 100**: INPUT ERROR: either \( N < 2 \) or \( IHOM < 0 \) or \( NSP < 2 \) or \( NRTI(1) < 0 \) or \( NTI < NSP + 4 \) or \(NU < N\ast(N+1)/2.\)
  TERMINAL ERROR.

\item **IERROR = 101**: INPUT ERROR: either \( ER(1) \) or \( ER(2) \) or \( ER(3) \) is negative.
  TERMINAL ERROR.

\item **IERROR = 103**: INPUT ERROR: either \( LW < 3N^2N + 8N + NSP(1.5N^2N + 2.5) \) or \( LIW < 3N + NSP(N+1) \).
  TERMINAL ERROR.

\item **IERROR = 120**: INPUT ERROR: the routine was called with \( NRTI = 1 \), but the given output-points in the array TI are not in strict monotone order.
  TERMINAL ERROR.

\item **IERROR = 121**: INPUT ERROR: the routine was called with \( NRTI = 1 \), but the first given output-point or the last output-point is not equal to \( A \) or \( B \).
  TERMINAL ERROR.

\item **IERROR = 122**: INPUT ERROR: the value of \( NTI \) is too small; the number of output-points is greater than \( NTI - 4 \).
  TERMINAL ERROR.

\item **IERROR = 130**: INPUT ERROR: the switching points are not given in strict monotone order.
  TERMINAL ERROR.

\item **IERROR = 131**: INPUT ERROR: the routine was called with \( NRTI(1) = 1 \), but the given output-points in the array TI do not include all switching points.
\end{itemize}
TERMINAL ERROR.

IERROR = 200  This indicates that there is a minor shooting interval on which the incremental growth is greater than the AMP. The cause of this error lies in the used method for computing the fundamental solution.
WARNING ERROR.

IERROR = 213  This indicates that the relative tolerance was too small. The subroutine has changed it into a suitable value.
WARNING ERROR.

IERROR = 215  This indicates that during integration the particular solution or a homogeneous solution has vanished, making a pure relative error test impossible. Must use non-zero absolute tolerance to continue.
TERMINAL ERROR.

IERROR = 216  This indicates that during integration the requested accuracy could not be achieved. User must increase error tolerance.
TERMINAL ERROR.

IERROR = 218  This indicates that the input parameter N <= 0, or that either the relative tolerance or the absolute tolerance is negative.
TERMINAL ERROR.

IERROR = 240  This indicates that the global error is probably larger than the error tolerance due to instabilities in the system. Most likely the problem is ill-conditioned. Output value is the estimated error amplification factor.
WARNING ERROR.

IERROR = 250  This indicates that one of the $U_k$ is singular.
TERMINAL ERROR.

IERROR = 260  This indicates that the problem is probably too ill-conditioned with respect to the BC.
TERMINAL ERROR.

***************
Auxiliary Routines
***************

This routine calls the BOUNDPAK library routines DMTSMP.

***************
Remarks
***************

DMUTSM is written by G.W.M. Staarink and R.M.M. Mattheij.
Last update: 01-04-1986.

***************
Method
***************
Example of the use of DMUTSM

Consider the ordinary differential equation

$$\frac{dx(t)}{dt} = L(t) x(t) + r(t), \quad -1 < t < 1$$

and a BC

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} x(-1) + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} x(0) + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} e \\ 1 + e^{-1} \end{bmatrix},$$

where

$$L(t) = \begin{bmatrix} -t + \frac{1}{2} (t+\frac{1}{2}) \cos 2t & 1 + (t+\frac{1}{2}) \sin 2t \\ -1 + (t+\frac{1}{2}) \sin 2t & -t + \frac{1}{2} (t+\frac{1}{2}) \cos 2t \end{bmatrix},$$

$$r(t) = \begin{bmatrix} (-3 + \sin t (\sin t - \cos t) (2t+1)) e^{-t} \\ (-1 + \sin (\sin t - \cos t) (2t+1)) e^{-t} \end{bmatrix}.$$

The solution of this problem is $x = (e^{-1}, e^{-t})^T$. The ODE has fundamental solutions growing like $\exp(-t^2)$ and $\exp(t)$, so there is a change of dichotomy at $t=0$.

In the next program the solution is computed and compared to the exact solution.

This program has been run on a AS9000 VM/CMS computer.

```c
DOUBLE PRECISION TSP(3),BCM(2,2,3),BCV(2),AMP,ER(5),TI(16),
1 X(2,16),U(3,16),Q(2,2,16),D(2,16),PHIREC(3,16),W(61),XBX,AE
INTEGER KPART(3),NRTI(3),IW(15)
EXTERNAL FLIN,FDIF

C SETTING OF THE INPUT PARAMETERS

C

N = 2
IHOM = 1
NSP = 3
NTI = 16
NU = 3
LW = 61
LIW = 15
TSP(1) = -1.DO
TSP(2) = 0.DO
TSP(3) = 1.DO
ER(1) = 1.D-12
ER(2) = 1.D-6
ER(3) = 1.D-15
NRTI(1) = 2
```

-- 21 --
NRTI(2) = 4
NRTI(3) = 4
DO 1100 I = 1 , NSP
DO 1100 J = 1 , N
DO 1100 L = 1 , N
   BCM(J,L,I) = 0.DO
1100 CONTINUE
   BCM(1,1,1) = 1.DO
   BCM(2,1,2) = 1.DO
   BCM(2,2,3) = 1.DO
   BCV(1) = DEXP(1.DO)
   BCV(2) = 1.DO + DEXP(-1.DO)
C CALL DMUTSP
C CALL DMUTSM(FLIN,FDIF,N,IHOM,TSP,NSP,BCM,BCV,AMP,ER,NRTI,TI,NTI,
   X,U,NU,Q,D,KPART,PHIREC,W,LW,IW,LIW,IERERROR)
C PRINTING OF THE SWITCHING POINTS, CONDITION NUMBER AND
C AMPLIFICATION FACTOR
WRITE(*,100) (TSP(I),I=1 ,NSP)
WRITE(*,110) ER(4),ER(5)
C COMPUTATION OF THE ABSOLUTE ERROR IN THE SOLUTION AND WRITING OF
C THE SOLUTION AT THE OUTPUT POINTS
WRITE(*,120)
DO 1200 I = 1 , NRTI(1)
   XEX = DEXP(-TI(I))
   AE = XEX - X(1,I)
   WRITE(*,130) I,TI(I),X(1,I),XEX,AE
1200 CONTINUE
STOP
100 FORMAT(' SWITCHING POINTS: ',3(F5.2,3X),/)
110 FORMAT(' CONDITION NUMBER = ',D12.5,/,1 'AMPLIFICATION FACTOR = ',D12.5,/
1 'ABS. ERROR',/)
120 FORMAT( ' I',6X,'T',8X,'APPROX. SOL.',7X,'EXACT SOL.',9X,
1 'ABS. ERROR',/)
130 FORMAT( ' ',I3,3X,F7.3,3(3X,D16.9))
140 FORMAT( ' ',13X,3(3X,D16.9))
END
SUBROUTINE FLIN(T,Y,F)
DOUBLE PRECISION T,Y(2),F(2),TI,SI,CO
   TI = 2.DO * T
   SI = DSIN(TI) * (T + 0.5DO)
   CO = DCOS(TI) * (T + 0.5DO)
   TI = 0.500 - T
   F(1) = (-CO + TI) * Y(1) + (1.DO + SI) * Y(2)
   F(2) = (-1.DO + SI) * Y(1) + (CO + TI) * Y(2)
RETURN
END
SUBROUTINE FDIF(T,Y,F)
```
DOUBLE PRECISION T,Y(2),F(2),TI,SI,CO

CALL FLIN(T,Y,F)
TI = 2.0D0 * T + 1.0D0
SI = DSIN(T)
CO = DCOS(T)
F(1) = F(1) + (CO * (CO - SI) * TI - 3.0D0) * DEXP(-T)
F(2) = F(2) + (SI * (SI - CO) * TI - 1.0D0) * DEXP(-T)
RETURN
END

SWITCHING POINTS: -1.00  0.00  1.00

CONDITION NUMBER = 0.61297D+01
AMPLIFICATION FACTOR = 0.43276D+01

<table>
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<tr>
<th>I</th>
<th>T</th>
<th>APPROX. SOL.</th>
<th>EXACT SOL.</th>
<th>ABS. ERROR</th>
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