A generalised multiple shooting method

Eindhoven University of Technology
Department of Mathematics and Computing Science

RANA 89-29
December 1989

A GENERALISED MULTIPLE SHOOTING METHOD

by

M.E. Kramer

Reports on Applied and Numerical Analysis
Department of Mathematics and Computing Science
Eindhoven University of Technology
P.O. Box 513
5600 MB Eindhoven
The Netherlands

A generalised multiple shooting method

by

M.E. Kramer

Abstract

The usual multiple shooting method for solving BVP's is based on solving initial value problems on suitable subintervals. Generally these IVP's will be ill-conditioned. Consequently the convergence domain of the Newton iteration on the shooting vector can become quite small and unequilibriatedly shaped.
The new approach presented in this paper is the use of well-conditioned BVP's on the local intervals with linear boundary conditions. This is likely to enlarge the convergence domain. A complication is, however, that the local problems cannot be solved with an initial value integrator. We have chosen to use a one-step finite difference scheme to approximate the solution of the local BVP's. It will be shown that alternate application of Newton's method to the 'shooting' vectors and the finite difference approximation of the solution converges locally super-linear (order approx. 1.4) if the finite difference grid is sufficiently fine.
An advantage of this method over finite differences on the entire interval is that less memory space and flops are required at each iteration step and that it is suited for parallel processing.

§1 Introduction

In this paper we will focus on solving a well–conditioned non–linear differential equation with two–point boundary conditions. Let the smooth functions $h : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ and $g : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^n$ induce the BVP

$$\begin{cases} \frac{dy}{dx} = h(x,y(x)) & a \le x \le b \qquad (1.1a) \\ g(y(a),y(b)) = 0 & \qquad (1.1b) \end{cases}$$

with $y \in C^1([a,b] \to \mathbb{R}^n)$.

1.1 Assumption

The BVP (1.1) has at least one solution $y^*(x)$ at which it is well–conditioned (see A.3).

∎

In the sequel we will only consider solutions of the type mentioned in assumption 1.1.
A generalisation of multiple shooting can be descibed as follows.

- Divide the interval [a,b] into subintervals $[x_k,x_{k+1}]$ with $a = x_1 \le x_2 \le \ldots \le x_{N+1} = b$ and define a BVP with linear boundary conditions on each subinterval.

$$\begin{cases} \dot{y} = h(x,y(x)) & x_k \le x \le x_{k+1} \qquad (1.2a) \\ A_k y(x_k) + B_k y(x_{k+1}) = s_k & \qquad (1.2b) \end{cases}$$

  where $s_k \in \mathbb{R}^n$ and $A_k, B_k \in \mathbb{R}^{n \times n}$. Let $y_k(x;s)$ denote the solution of (1.2) on $[x_k,x_{k+1}]$.
- Define the function f(s), containing the continuity condition of the solution of (1.1) and the boundary conditions by

$$f(s) := \begin{bmatrix} y_1(x_2;s) - y_2(x_2;s) \\ \cdot \\ \cdot \\ y_{N-1}(x_N;s) - y_N(x_N;s) \\ g(y_1(x_1;s), y_N(x_{N+1};s)) \end{bmatrix} \qquad (1.3)$$

  with $s := (s_1^T, s_2^T, \ldots, s_N^T)^T$.
- Find the zero of f(s) by applying Newton's method to f.

Usually in the multiple shooting method one defines initial value problems on subintervals of [a,b], i.e. $A_k = I$ and $B_k = 0$ for all k. However, if the linearization of the BVP at $y^*(x)$ contains any growing modes, these IVP's cannot be well–conditioned (cf. [AsMaRu] Th. 3.106). In section 2 we will show that consequently the convergence domain for f(s) as stated in the Newton–Kantorovich theorem can become very small. Furthermore it will be shown that this area is considerably larger if well–conditioned BVP's are defined on the subintervals.

This generalized form of multiple shooting that uses well–conditioned BVP's on the subintervals will be called unbiased multiple shooting. This method is somewhat more complicated, because the local solutions $y_k(x;s)$ can no longer be computed by an initial value integrator. In this paper we use a one–step finite difference method to obtain an estimate for $y_k(x;s)$.

Using the unbiased multiple shooting method in combination with finite differences on the subintervals is in some respect preferable to using a finite difference method on the entire interval [a,b].

1 One Newton iteration requires less flops, for one has to solve
- 1 system of order nN + N systems of order $n\cdot|\Pi_k|$ for unbiased multiple shooting
- 1 sytem of order $N\cdot n\cdot|\Pi_k|$ for a finite difference method

2 The finite difference method requires approximately N–times more memory space, than unbiased multiple shooting.

The algorithm considered in this paper contains two iterative processes.

1 the "outer" iteration of the Newton method on $f(s) = 0$ generating a sequence $\{ s^j \}$.

2 the "inner" iteration on the finite difference scheme to approximate $y_k(x;s^j)$.

Let Π_k be the finite difference mesh of $[x_k,x_{k+1}]$ and y_π^k the vector containing the concatenation of the vectors approximating the solution $y_k(x;s)$ at the meshpoints.

In section 3 it will be proven that, if for all $1 \le k \le N$

1 the matrices A_k and B_k are such that the BVP (1.2) is well–conditioned

2 the initial estimates for $(y_\pi^k)^0$ and s^0 are sufficiently good

3 the mesh Π_k is sufficiently fine

the following algorithm converges super–linear (order approx. 1.4)

for j:=1 to ∞

do begin

$s_j := s_{j-1} - \left[\frac{df}{ds}((y_\pi)^{j-1}) \right]^{-1} \cdot f((y_\pi)^{j-1})$ i.e. the evaluation of $\frac{df}{ds}$ and f respectively at the discrete approximation $(y_\pi^k)^{j-1}$ to $y_k(x;s^{j-1})$, $k = 1,\ldots,N$;

for k := 1 to N do $(y_\pi^k)^j$ is formed by applying one Newton iteration to the finite difference discretization of (1.2) at $(y_\pi^k)^{j-1}$.

end;

Finally we have to address to the choice of A_k and B_k. In most cases $A_k = B_k = I$ will yield a well–conditioned BVP (1.2). Some more work on this part has still to be done.

§2 Comparison of the Newton–Kantorovich convergence domain

Both for ordinary and unbiased multiple shooting a zero of the non–linear function f(s) (see (1.3)) describing the continuity of the solution and the global boundary conditions has to be found. In this section it will be shown that the convergence domain mentioned in the Newton-Kantorovich theorem is considerably larger for the unbiased multiple shooting method. This is due to the equilibration of the Jacobian resulting from using well–conditioned BVP's on the subintervals instead of initial value problems.

2.1 Newton–Kantorovich theorem (see [RhOr] p.421)

Let $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$ be Frechet–differentiable on a convex set D_1. Assume that

1 $\forall_{x,y \in D_1}$: $\| F'(x) - F'(y) \| \le \gamma \| x-y \|$

and that there is a $x_0 \in D_1$ such that

2 $\| F'(x_0)^{-1} \| \le \beta$

3 $\| F'(x_0)^{-1} \cdot F(x_0) \| \le \eta$

and $\alpha := \beta\gamma\eta < \frac{1}{2}$. Define

$$t^* = (\beta\gamma)^{-1}[1-\sqrt{1-2\alpha}], \qquad t^{**} = (\beta\gamma)^{-1}[1+\sqrt{1-2\alpha}]$$

and assume finally that $B(x_0,t^*) \subset D_1$. Then the iterates x_k generated by

$$x_{k+1} = x_k - F'(x_k)^{-1}F(x_k) \qquad k = 0,1,2,..$$

are well–defined, remain in $B(x_0,t^*)$ and converge to a solution x^* of $F(x) = 0$, which is unique in $B(x_0,t^{**}) \cap D_1$.

∎

Consider the BVP (1.1) and let $y^*(x)$ be a solution at which it is well–conditioned. Let the interval [a,b] be divided into subintervals $[x_k,x_{k+1}]$ with $a = x_1 < x_2 < \ldots < x_{N+1} = b$.

2.2 Notational convention

Define the operators

a $\mathcal{N} : C^1([a,b]\to\mathbb{R}^n) \to C([a,b]\to\mathbb{R}^n)$ by $\qquad \mathcal{N}y := \dot{y} - h(x,y(x))$ (2.1)

the non–linear differential equation.

b $\forall_{1\le k\le N}$: $\mathcal{N}_k : C^1([x_k,x_{k+1}]\to\mathbb{R}^n) \to C([x_k,x_{k+1}]\to\mathbb{R}^n)$ by $\qquad \mathcal{N}_k y := \dot{y} - h(x,y(x))$ (2.2)

the restriction of $\mathcal{N}$ to $[x_k,x_{k+1}]$

c $\forall_{1\le k\le N}$: $\mathcal{B}_k : C([x_k,x_{k+1}]\to\mathbb{R}^n) \to \mathbb{R}^n$ by $\qquad \mathcal{B}_k y := A_k y(x_k) + B_k y(x_{k+1})$ (2.3)

the boundary conditions on $[x_k,x_{k+1}]$.

d With $s \in \mathbb{R}^{nN}$ subdivided into N subvectors of length n, ($s = (s_1^T, s_2^T, \ldots, s_N^T)^T$),

$y_k(x;s)$ denotes the solution of the BVP

$$\begin{cases} \mathcal{N}_k y_k = 0 \\ \mathcal{B}_k y_k = s_k \end{cases} \tag{2.4}$$

e Define the function $L_k : [x_k, x_{k+1}] \times \mathbb{R}^{nN} \rightarrow C([x_k, x_{k+1}] \rightarrow \mathbb{R}^n \times \mathbb{R}^n)$ by

$$L_k(x;s) = \left.\frac{\partial h(x,y)}{\partial y}\right|_{y=y_k(x;s)} \tag{2.5}$$

the linearization of $h(x,y(x))$ at $y_k(x;s)$.

f Define the operator $\mathcal{L}_k(s) : C^1([x_k, x_{k+1}] \rightarrow \mathbb{R}^n) \rightarrow C([x_k, x_{k+1}] \rightarrow \mathbb{R}^n)$ for all $s \in \mathbb{R}^{nN}$ by

$$\mathcal{L}_k(s)y := \dot{y} - L_k(x;s)y \tag{2.6}$$

the linearization of $\mathcal{N}_k$ at $y(x;s)$.

g Let $Y_k(x;s) \in C(\mathbb{R} \times \mathbb{R}^{nN} \rightarrow \mathbb{R}^{n \times n})$ denote the fundamental solution of

$$\begin{cases} \mathcal{L}_k(s)Y = 0 \\ \mathcal{B}_k Y = I \end{cases} \tag{2.7}$$

h Furthermore define

$$B_a(s) = \left.\frac{\partial g(u, y_N(x_{N+1};s))}{\partial u}\right|_{u=y_1(x_1;s)} \quad \text{and} \quad B_b(s) = \left.\frac{\partial g(y_1(x_1;s), v)}{\partial v}\right|_{v=y_N(x_{N+1};s)} \tag{2.8}$$

the linearization of the boundary conditions.

i Let s^* be the solution of $f(s) = 0$ with $\forall_k \; \forall_{x \in [x_k, x_{k+1}]} : y^*(x) = y_k(x;s^*)$

j Let $\mathcal{L}$ denote a linear diffential equation on [a,b] and $\mathcal{B}$ a set of linear boundary conditions on [a,b]. Then the conditioning constant, κ, of $(\mathcal{L}, \mathcal{B})$ is defined by :

$$\kappa := \max\left(\max_{a \leq t \leq b} \| Y(t) \| , \max_{a \leq x, t \leq b} \| G(x,t) \| \right) \tag{2.9}$$

with $Y(t)$ the fundamental solution of $\mathcal{L}$ with $\mathcal{B}Y = I$ and $G(x,t)$ the Green's function of the linear BVP $(\mathcal{L}, \mathcal{B})$.

▬

To guarantee the well–conditioning of the BVP (1.1) at $y^*(x)$, some smoothness of the functions g and h has to be assumed.

<u>2.3 Assumption</u>

The function $g : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ is two times continuously differentiable with respect to both variables and the function $h : \mathbb{R} \times \mathbb{R}^n \rightarrow \mathbb{R}^n$ is two times continuously differentiable with respect to its second variable. There is an open set $D_y \subset C([a,b] \rightarrow \mathbb{R}^n)$ with $y^*(x) \in D_y$ such that there is a moderate upperbound C_{gh} on all first and second derivatives of $h(x,y)$ and $g(u,v)$ at any function $y \in D_y$.

▬

We will now investigate the constants appearing in the Newton–Kantorovich theorem.

1 The Lipschitz constant of J(s)

The Jacobian J(s) of f(s) has the form

$$J(s) = \begin{bmatrix} Y_1(x_2) & -Y_2(x_2) & & & \\ & Y_2(x_3) & -Y_3(x_3) & & \\ & & \ddots & \ddots & \\ & & & Y_{N-1}(x_N) & -Y_N(x_N) \\ B_a Y_1(x_1) & & & & B_b Y_N(x_{N+1}) \end{bmatrix} \qquad (2.10)$$

because $Y_k(x;s) = \frac{\partial y_k(x;s)}{\partial s}$

For notational convenience we have dropped the s in $Y_k(x;s)$, $B_a(s)$ and $B_b(s)$.

2.4 Property

Let D_s be the neighbourhood of s* such that $\{ y(x;s) \mid s \in D_s \} \subset D_y$ and

$\forall_{s \in D_s}$: $Y_k(x;s)$ exists (i.e. (2.6) has a f.s. Y with $\mathcal{B}_k Y$ non–singular)

Then

$\forall_{s,\sigma \in D_s}$: $\| J(s) - J(\sigma) \| \leq C \cdot (b-a) \cdot \kappa^3 \cdot \| s-\sigma \|$

for some constant C of moderate size and

$\kappa = \sup \{$ conditioning constant of $(\mathcal{L}_k(\tau), \mathcal{B}_k) \mid 1 \leq k \leq N$ and $\tau = ts + (1-t)\sigma$, $t \in [0,1] \}$

∎

Proof

From (2.10) we see that it is sufficient to estimate

1 $\| Y_k(x;s) - Y_k(x;\sigma) \|$

2 $\| B_a(s) Y_1(x_1;s) - B_a(\sigma) Y_1(x_1;\sigma) \|$

3 $\| B_b(s) Y_N(x_{N+1};s) - B_b(\sigma) Y_N(x_{N+1};\sigma) \|$

in terms of $\| s-\sigma \|$.

1 Because $Y_k(x;s)$ and $Y_k(x;\sigma)$ are fundamental solutions to different ODE's, Theorem A.6 can be applied to them. So, $\mathcal{B}_k Y_k(x;s) = \mathcal{B}_k Y_k(x;\sigma) = I$, implies that

$$Y_k(x;\sigma) = Y_k(x;s) + \int_a^b G(x,t) \cdot (L_k(t;\sigma) - L_k(t;s)) \cdot Y_k(t;\sigma) \, dt$$

and $\| Y_k(x;s) - Y_k(x;\sigma) \| \leq \kappa^2 \cdot (b-a) \cdot \max_t \| L_k(t;s) - L_k(t;\sigma) \|$

The differences in $L_k(x;s)$ can be estimated by

$$\| L_k(x;s) - L_k(x;\sigma) \| = \| \left. \frac{\partial h(x;y)}{\partial y} \right|_{y=y_k(x;s)} - \left. \frac{\partial h(x;y)}{\partial y} \right|_{y=y_k(x;\sigma)} \|$$

$$\le \sup \{ \| \frac{\partial^2 h(x,y)}{\partial y^2}\Big|_{y=ty_k(x;s)+(1-t)y_k(x;\sigma)} \| \mid t\in[0,1] \} \cdot \| y_k(x;s) - y_k(x;\sigma) \|$$
$$\le C_{gh} \cdot \sup \{ \| \frac{\partial y_k(x;\tau)}{\partial \tau}\Big|_{\tau=ts+(1-t)\sigma} \| \mid t\in[0,1] \} \cdot \| s-\sigma \|$$
$$\le C_{gh} \cdot \kappa \cdot \| s-\sigma \|$$

2 $\| B_a(s)Y_1(x_1;s) - B_a(\sigma)Y_1(x_1;\sigma) \|$

$$\le \| B_a(s) - B_a(\sigma) \| \cdot \| Y_1(x_1;s) \| + \| B_a(\sigma) \| \cdot \| Y_1(x_1;s) - Y_1(x_1;\sigma) \|$$
$$\le \kappa \cdot \| \frac{\partial g(u;y_N(x_{N+1};s))}{\partial u}\Big|_{u=y_1(x_1;s)} - \frac{\partial g(u;y_N(x_{N+1};\sigma))}{\partial u}\Big|_{u=y_1(x_1;s)} \|$$
$$+ \kappa \cdot \| \frac{\partial g(u;y_N(x_{N+1};\sigma))}{\partial u}\Big|_{u=y_1(x_1;s)} - \frac{\partial g(u;y_N(x_{N+1};\sigma))}{\partial u}\Big|_{u=y_1(x_1;\sigma)} \|$$
$$+ \| B_a(\sigma) \| \cdot \| Y_1(x_1;s) - Y_1(x_1;\sigma) \|$$
$$\le \kappa \cdot C_{gh} \cdot \| y_N(x_{N+1};s) - y_N(x_{N+1};\sigma) \| + \kappa \cdot C_{gh} \cdot \| y_1(x_1;s) - y_1(x_1;\sigma) \|$$
$$+ C_{gh} \| Y_1(x_1;s) - Y_1(x_1;\sigma) \|$$
$$\le 2 \cdot \kappa^2 \cdot C_{gh} \cdot \| s-\sigma \| + C_{gh} \cdot \kappa^2 \cdot (b-a) \cdot C_{gh} \cdot \kappa \cdot \| s-\sigma \|$$
$$\le C_{gh} \cdot \kappa^2 \cdot (2+(b-a) \cdot C_{gh} \cdot \kappa) \cdot \| s-\sigma \|$$

3 For $\| B_b(s)Y_N(x_{N+1};s) - B_b(\sigma)Y_N(x_{N+1};\sigma) \|$ the same upperbound can be derived.

This yields

$$\| J(s) - J(\sigma) \| \le \max (\max_k \| Y_k(x_{k+1};s) - Y_k(x_{k+1};\sigma) \| + \| Y_{k+1}(x_{k+1};s) - Y_{k+1}(x_{k+1};\sigma) \| ,$$
$$\| B_a(s)Y_1(x_1;s) - B_a(\sigma)Y_1(x_1;\sigma) \| + \| B_b(s)Y_N(x_{N+1};s) - B_b(\sigma)Y_N(x_{N+1};\sigma) \|)$$
$$\le C \cdot \kappa^3 \cdot \| s-\sigma \| \qquad \text{for some constant C of moderate size.}$$

∎

In order to determine the Lipschitz constant of the Jacobian of f(s) we need an estimate of the conditioning constant of the linearized BVP's $(\mathcal{L}_k(s),\mathcal{B}_k)$ for s in the vicinity of s*.
If the differential equation $(\mathcal{N}_k,\mathcal{B}_k)$ is well-conditioned at its solution $y_k(x;s^*)$, then small changes in s induce only small changes in $y_k(x;s)$. Consequently the linearization $L_k[y_k(x;s)]$ is only slightly perturbed and the conditioning constant of $(\mathcal{L}_k(s),\mathcal{B}_k)$ will not increase considerably. So the Lipschitz constant of the Jacobian for the unbiased multiple shooting method will be of moderate size on a reasonably sized neighbourhood of s*.
If on the other hand, IVP's are defined on the subintervals and its f.s. $Y_k(x;s^*)$ is dichotomic with constants (K,λ,μ) (see A.1), then $\kappa \ge \| Y_k(x_{k+1};s^*) \| \ge K^{-1}e^{\mu(x_{k+1}-x_k)}$, i.e. the IVP becomes more ill-conditioned, if $\mu(x_{k+1}-x_k)$ increases. So small changes in some directions of s induce major changes in $y_k(x;s)$ and thus in $L_k(s)$. Consequently the conditioning constants of the neighboring problems are difficult to estimate. But the Lipschitz constant

will be at least $C \cdot (b-a) \cdot K^{-3} \cdot e^{3\mu(x_{k+1}-x_k)}$ and it is difficult to estimate the size of this Lipschitz area.

2 The inverse of J(s)

The inverse of the Jacobian J(s) can be written in terms of Green's functions.
Let $s \in \mathbb{R}^{nN}$ be such that $Y_k(x;s)$ is non–singular for all k, $1 \le k \le N$.
Subdivide $J^{-1}(s)$ into N^2 blocks $J_{kj} \in \mathbb{R}^{n \times n}$ and drop the argument s. Then J_{kj} satisfies

$$\forall_{1 \le j \le N,\ 1 \le k \le N-1} : \ Y_k(x_{k+1})J_{kj} - Y_{k+1}(x_{k+1})J_{k+1,j} = \delta_{kj}\, I$$

$$\text{and } \forall_{1 \le j \le N} : \ B_aY_1(x_1)J_{1j} + B_bY_N(x_{N+1})J_{Nj} = \delta_{Nj}\, I$$

This shows that J_{kj}, $1 \le k \le N$ and $1 \le j \le N-1$, is the Green's function of the difference equation

$$\begin{cases} Y_{k+1}(x_{k+1})\, z_{k+1} = Y_k(x_{k+1})\, z_k & 1 \le k \le N-1 \\ B_aY_1(x_1)z_1 + B_bY_N(x_{N+1})z_N = 0 & \end{cases} \tag{2.11}$$

and that J_{kN} equals the fundamental solution of (2.11) with boundary condition equal to the unit–matrix. Unfortunately the conditioning constant of (2.11) is not known. But G_{kj} can also be expressed in terms of the Green's function of the differential equation

$$\begin{cases} \dot{y} = L_k(x;s) \cdot y & \text{if } x \in [x_k, x_{k+1}] \\ B_a(s)y(a) + B_b(s)y(b) = \beta & \end{cases} \tag{2.12}$$

whose conditioning constant is supposed to be of moderate size on a neighbourhood of s*.

2.5 Lemma

Let F(x), $x \in [a,b]$ be the fundamental solution of (2.12) satisfying $B_aF(a) + B_bF(b) = I$. Let G(x,t) denote the Green's function of (2.12). Then

$$J_{kj} = \begin{cases} A_kG(x_k,x_{j+1}) + B_kG(x_{k+1},x_{j+1}) - \delta_{kj}B_k & \text{if } j \ne N \\ A_kF(x_k) + B_kF(x_{k+1}) & \text{if } j = N \end{cases} \tag{2.13}$$

∎

Proof

Let $1 \le k \le N$. On the interval $[x_k,x_{k+1}]$ both F(x) and $Y_k(x)$ are fundamental solutions of

$$\dot{z} = L_k(x)z$$

So there is a non–singular matrix X_k with $F(x) = Y_k(x) \cdot X_k$ all $x \in [x_k,x_{k+1}]$. And

$$X_k = \mathcal{B}_kY_k \cdot X_k = \mathcal{B}_kF = A_kF(x_k) + B_kF(x_{k+1})$$

The difference equation for J_{kj} can be rewritten into

$$Y_{k+1}(x_{k+1})\, J_{k+1,j} = Y_k(x_{k+1})\, J_{kj} - \delta_{kj}\, I \qquad 1 \le k \le N-1$$

$$\Leftrightarrow\ F(x_{k+1}) \cdot X_{k+1}^{-1}\, J_{k+1,j} = F(x_{k+1}) \cdot X_k^{-1}\, J_{kj} - \delta_{kj}\, I$$

$$\Leftrightarrow\ X_{k+1}^{-1}\, J_{k+1,j} = X_k^{-1}\, J_{kj} - \delta_{kj}\, F^{-1}(x_{k+1})$$

Let $\{ G_{kj} \}$ denote the Green's function of the difference equation

$$\begin{cases} X_{k+1}^{-1} z_{k+1} = X_k^{-1} z_k + q_k & 1 \le k \le N-1 \\ B_a Y_1(x_1) z_1 + B_b Y_N(x_{N+1}) = \beta \end{cases}$$

$$\text{Then } J_{kj} = \begin{cases} -G_{kj}\, F^{-1}(x_{j+1}) & j \ne N \\ X_k & j = N \end{cases}$$

$$\text{and } G_{kj} = \begin{cases} X_k B_a Y_1(x_1) \quad X_1 X_{j+1}^{-1} (X_{j+1}^{-1})^{-1} & k > j \\ -X_k B_b Y_N(x_{N+1}) X_N X_{j+1}^{-1} (X_{j+1}^{-1})^{-1} & k \le j \end{cases}$$

$$= \begin{cases} (A_k F(x_k) + B_k F(x_{k+1})) B_a F(x_1) & k > j \\ -(A_k F(x_k) + B_k F(x_{k+1})) B_b F(x_{N+1}) & k \le j \end{cases}$$

This finally yields

$$J_{kj} = \begin{cases} A_k G(x_k, x_{j+1}) + B_k G(x_{k+1}, x_{j+1}) - \delta_{kj} B_k & j \ne N \\ A_k F(x_k) \qquad\qquad + B_k F(x_{k+1}) & j = N \end{cases}$$

∎

2.6 Theorem

If $\| \ \|$ denotes a Hölder–norm, then

$$\forall_s \ : \ \| J^{-1}(s) \| \le N \cdot \kappa \cdot \max_k (\|A_k\| + 2 \cdot \|B_k\|), \quad \text{with } \kappa \text{ the conditioning constant of (2.12)}$$

∎

Proof

Let $y \in \mathbb{R}^{nN}$ and $1 \le k \le N$. Then

$$\| (J^{-1}y)_k \| = \| \sum_j G_{kj} y_j \|$$

$$= \| \sum_j A_k G(x_k, x_{j+1}) y_j + A_k F(x_k) y_N + \sum_j B_k G(x_{k+1}, x_{j+1}) y_j + B_k F(x_{k+1}) y_N - B_k y_k \|$$

And with

$$\sum_j A_k G(x_k, x_{j+1}) y_j = A_k \cdot \int_a^b G(x_k, \tau) \sum_{j=1}^{N-1} \delta(\tau - x_{j+1}) y_j \, d\tau$$

$$\| (J^{-1}y)_k \| \le \|A_k\| \cdot [\|F(x_k)\| \cdot \|y_N\| + \max_\tau \| G(x_k, \tau) \| \sum_{j=1}^{N-1} \|y_j\|]$$

$$+ \|B_k\| \cdot [\|F(x_{k+1})\| \cdot \|y_N\| + \max \| G(x_{k+1}, \tau) \| \sum_{j=1}^{N-1} \|y_j\| + \|y_k\|]$$

$$\le (\|A_k\| + 2\|B_k\|) \cdot \kappa \cdot \sum_{j=1}^{N} \|y_j\|$$

Let $\| \;\|$ denote the p–Hölder norm, then

$$\| J^{-1}y \| = (\sum_{k=1}^{N} \| (J^{-1}y)_k \|^p)^{\frac{1}{p}} \le (\sum_{k=1}^{N}((\|A_k\|+2\|B_k\|)\cdot\kappa)^p \sum_{j=1}^{N} \| y_j \|^p)^{\frac{1}{p}}$$

$$\le N\cdot\kappa\cdot\max_k(\|A_k\|+2\|B_k\|)\cdot\|y\|$$

∎

The above theorem shows that $\| J^{-1}(s) \| \le C\cdot N\cdot\kappa$, with κ the conditioning constant of the BVP (2.12). For s close to s^* this is almost equal to the conditioning constant for s^*, i.e. the conditioning constant of the original BVP (1.1). The bound on J^{-1} is not influenced by the choice of the boundary conditions on the subintervals, but only by the amount of subintervals.

3 The norm of $J^{-1}(s)f(s)$

The norm of $J^{-1}(s)$ has already been estimated in the previous part.
If the BVP's on the subintervals are well–conditioned, then small changes in s^* wil induce only small changes in $y(x;s^*)$ and in f(s). So the set $\{ s \mid \| f(s) \| < \varepsilon \}$ will be reasonably sized, $\varepsilon > 0$. If, however, ill–conditioned IVP's are defined on the subintervals , small changes in s^* can cause major changes in y(x;s) and thus in f(s). So the sets $\{s \mid \|f(s)\| < \varepsilon \}$ are considerably smaller in this case and may vary strongly in different directions.

Conclusion

The use of initial value problems on the subintervals may influence the size of the Newton-Kantorovich convergence domain negatively in two ways

- the Lipschitz constant of J(s) is larger; presumably on a smaller domain.
- the value of f(s) increases more rapidly when s moves away from s^*.

§3 Convergence of the unbiased multiple shooting method

In the previous section it was shown that the unbiased multiple shooting method with its well-conditioned BVP's on the subintervals may have a much larger Newton–Kantorovich convergence domain than ordinary multiple shooting. However, this was shown under the assumption that the exact solutions to the local BVP's were available on request. Here we will investigate the situation in case the local solutions are estimated by a one–step finite difference scheme. We will show that the algorithm described in section 1 converges superlinear if the grids for the finite differences are sufficiently small.

Recall that we were trying to solve the non–linear two point BVP

$$\begin{cases} \dot{y} = h(x,y(x)) & a \le x \le b \\ g(y(a),y(b)) = 0 \end{cases} \tag{1.1}$$

Consider a subinterval $[x_k,x_{k+1}]$ and let $\Pi_k : x_k = \xi_1^k < \xi_2^k < \ldots < \xi_{M+1}^k = x_{k+1}$ be a mesh on it. For simplicity we assume that M is independent of k.

In this section the superscript k denotes the number of the subinterval and the subscript m denotes the position within the subinterval.

3.1 Notational convention

- $y_m^k \in \mathbb{R}^n$ denotes an approximation of a solution of a differential equation at ξ_m^k
- $y^k = \begin{bmatrix} y_1^k \\ \hline \cdot \\ \cdot \\ \hline y_{M+1}^k \end{bmatrix} \in \mathbb{R}^{n(M+1)}$ is an approximation to that same solution at the mesh points ξ_m^k, $1 \le m \le M+1$
- $y = \begin{bmatrix} y^1 \\ \hline \cdot \\ \cdot \\ \hline y^N \end{bmatrix} \in \mathbb{R}^{n(M+1)N}$ is an approximation to that solution at all mesh points and with two values at x_k, $2 \le k \le N$, viz. y_{M+1}^{k-1} and y_1^k.
- Define the discretisation of the differential equation at $[x_k,x_{k+1}]$ by

  $\mathcal{N}_\pi^k : \mathbb{R}^{n(M+1)} \to \mathbb{R}^{nM}$

  and $$(\mathcal{N}_\pi^k y^k)_m = (h_m^k)^{-1}(y_{m+1}^k - y_m^k) - \Phi(y_m^k,y_{m+1}^k;\xi_m^k,h_m^k) \tag{3.1}$$

  , here Φ denotes a one–step discretisation scheme, e.g. a higher order Runge–Kutta scheme
- Let $y^k(s)$ denote the discrete solution of $$\begin{cases} \mathcal{N}_\pi^k y = 0 \\ \mathcal{B}_k y = s \end{cases} \tag{3.2}$$

- Furthermore $\mathcal{L}_\pi^k$ is the linearisation of $\mathcal{N}_\pi^k$ at a vector y^k :

$$\mathcal{L}_\pi^k : \mathbb{R}^{n(M+1)} \to C(\mathbb{R}^{n(M+1)} \to \mathbb{R}^{nM}) \text{ and}$$

$$\mathcal{L}_\pi^k[y^k]\, w = \begin{bmatrix} S_1^k\, R_1^k & & & \\ & S_2^k\, R_2^k & . & \\ & & \ddots & \\ & & & S_M^k\, R_M^k \end{bmatrix} \cdot w,\ w \in \mathbb{R}^{n(M+1)} \tag{3.3}$$

with

$$S_m^k := -(h_m^k)^{-1} I - \frac{\partial \Phi}{\partial u}(u, y_{m+1}, \xi_m^k, h_m^k)\Big|_{u=y_m} \tag{3.4a}$$

and $$R_m^k := (h_m^k)^{-1} I - \frac{\partial \Phi}{\partial v}(y_m, v, \xi_m, h_m^k)\Big|_{v=y_{m+1}} \tag{3.4b}$$

- Let $\{ Y_m^k \}_m$ denote the fundamental solution of the linearized difference equation :

$$\begin{cases} \mathcal{L}_\pi^k[y^k]\{Y^k\} = 0 \\ \mathcal{B}_k\{Y^k\} = I \end{cases} \tag{3.5}$$

- $\mathcal{L}_\pi[y]$ is the linearisation of the global difference equation :

$$\mathcal{L}_\pi : \mathbb{R}^{n(M+1)N} \to C(\mathbb{R}^{n(MN+1)} \to \mathbb{R}^{nMN}) \text{ and for any } w \in \mathbb{R}^{n(MN+1)}$$

$$\mathcal{L}_\pi[y] \cdot w = \begin{bmatrix} S_1^1\, R_1^1 & & & & & \\ & \ddots\ S_M^1\, R_M^1 & & & & \\ & & S_1^2\, R_1^2 & . & & \\ & & & \ddots\ S_M^2\, R_M^2 & & \\ & & & & \ddots & \\ & & & & & S_M^N\, R_M^N \end{bmatrix} \cdot w \tag{3.6}$$

- h is the maximum stepsize, i.e. $h = \max_{k\ m} h_m^k$

-

Normally the finite difference method with Newton iteration for the BVP

$$\mathcal{N}_\pi^k y = 0 \quad \text{with} \quad \mathcal{B}_k y = s_k$$

given an initial guess $(y^k)^0$, reads

for j := 0 to ∞ do

solve $\begin{bmatrix} \mathcal{L}_\pi^k[(y^k)^j] \\ A_k\ 0..0\ B_k \end{bmatrix} w = -\begin{bmatrix} \mathcal{N}_\pi^k(y^k)^j \\ \mathcal{B}_k(y^k)^j - s_k \end{bmatrix}$ and $(y^k)^{j+1} := (y^k)^j + w$ for $1 \le k \le N$

Here the situation is somewhat different. The boundary value s is not known at the start of the iteration. So we have the following situation

Given an initial 'solution' $(y^k)^0$ and a sequence $\{ s^j \}$ of vectors

for j:=0 to ∞ do

$$\text{solve} \begin{bmatrix} \mathcal{L}_\pi^k[(y^k)^j] \\ A_k\ 0..0\ B_k \end{bmatrix} w = - \begin{bmatrix} \mathcal{N}_\pi^k(y^k)^j \\ \mathcal{B}_k(y^k)^j - s_k^{j+1} \end{bmatrix} \quad \text{and} \quad (y^k)^{j+1} := (y^k)^j + w \quad \text{for } 1 \le k \le N$$

i.e. at every step of the algorithm we want to approximate the solution of

$\mathcal{N}_\pi^k y = 0$ and $\mathcal{B}_k y = s_k^{j+1}$

by applying a Newton iteration to it with y^j as an initial guess.

Notice that $\mathcal{B}_k(y^k)^{j+1} = \mathcal{B}_k(y^k)^j + \mathcal{B}_k w = \mathcal{B}_k(y^k)^j - \mathcal{B}_k(y^k)^j + s_k^{j+1} = s_k^{j+1}$, i.e. if $j \ge 1$ then $(y^k)^j$ satisfies the local boundary conditions. If the sequence $\{ s^j \}$ converges, taking y^j as an initial guess for y^{j+1} might do rather well.

In the previous section we considered the sequence $\{ s^j \}$ to result from Newton iteration on a function depending on the continuous differential equations at the subintervals. In this setting with only discrete approximations to the solution known, it is more natural to consider the continuity requirements and boundary conditions on the discretized problem. Define $f_\pi(s)$ by

$$f_\pi(s) := \begin{bmatrix} y_{M+1}^1(s) - y_1^2(s) \\ \vdots \\ y_{M+1}^{N-1}(s) - y_1^N(s) \\ g(y_1^1(s), y_{M+1}^N(s)) \end{bmatrix} \tag{3.7}$$

Let s_π denote a zero of $f_\pi(s)$. The the Jacobian of $f_\pi(s)$ has the form

$$J_\pi(s) = \begin{bmatrix} Y_{M+1}^1 & -Y_1^2 & & & \\ & Y_{M+1}^2 & -Y_1^3 & & \\ & & \ddots & \ddots & \\ & & & Y_{M+1}^{N-1} & -Y_1^N \\ B_a Y_1^1 & & & & B_b Y_{M+1}^N \end{bmatrix} \tag{3.8}$$

where $\{ Y_m^k \}_m$ is the f.s. of $\mathcal{L}_\pi^k[y^k(s)]$ with $A_k Y_1^k + B_k Y_{M+1}^k = I$.

Although f_π and J_π are functions of s, their formulas can be evaluated for any vector $y \in \mathbb{R}^{n(M+1)N}$ for which $(\mathcal{L}_\pi^k[y^k], \mathcal{B}_k)$ is well–defined. These evalutions at an appropriate vector y will be denoted by $f_\pi(y)$ and $J_\pi(y)$.

The algorithm for unbiased multiple shooting now reads

– given an initial guess s^0 and $(y)^0$ (Alg.3.1)

for $j := 0$ to ∞ do

$s^{j+1} := s^j - J_\pi((y)^j)^{-1} \cdot f_\pi((y)^j)$;

for $k := 1$ to N do $\quad (y^k)^{j+1} := (y^k)^j - \begin{bmatrix} \mathcal{L}_\pi^k[(y^k)^j] \\ A_k\ 0.\ .0\ B_k \end{bmatrix}^{-1} \cdot \begin{bmatrix} \mathcal{N}_\pi^k(y^k)^j \\ \mathcal{B}_k(y^k)^j - s_k^{j+1} \end{bmatrix}$

In this section the local convergence of this algorithm will be shown, i.e.

If $\| s^0 - s_\pi \|$ and $\| (y)^0 - y(s_\pi) \|$ are sufficiently small, then both $\| s^j - s_\pi \|$ and $\| (y)^j - y(s^j) \|$ tend to zero.

Of course this can only be established if the BVP and the finite difference method satisfy some neatness conditions.

3.2 Assumption

There are constants h_0, r_s ans r_y such that if the meshsize of all Π_k is smaller than h_0 and $S_s := B(s_\pi, r_s)$, $S_y := \{ y \in \mathbb{R}^{n\times(NM+1)} \mid \exists_{s\in S_s} : y \in B(y(s); r_y) \}$ and $S_y^k := \{ y \in \mathbb{R}^{n\times(N+1)} \mid \exists_{s\in S_s} : y^k \in B(y^k(s); r_y) \}$, then there is a constant κ of moderate size such that

1 $\forall_k$: The discretisation $\mathcal{N}_\pi^k$ of $\mathcal{N}$ at $[x_k, x_{k+1}]$ is consistent of order p and stable. And S_y^k is contained in its stability region and the stability constant is bounded by κ.

2 $\forall_{y\in S_y}$: The linearisation of the discrete BVP at y, $(\mathcal{L}_\pi[y], \mathcal{B})$, is consistent of order p and stable with stability constant less or equal to κ.

3 $\forall_k \ \forall_{y^k \in S_y^k}$: The local difference equation $(\mathcal{L}_\pi^k[y^k], \mathcal{B}_k)$ is consistent and stable, with stability constant less or equal to κ.

4 $\exists_{C_\phi} \ \forall_{k,m} \ \forall_{y\in S_y}$: $\| \frac{\partial \Phi}{\partial u}(u, y_{m+1}^k, \xi_m^k, h_m^k)\Big|_{u=y_m^k} \| \le C_\phi$

and $\| \frac{\partial \Phi}{\partial v}(y_m^k, v, \xi_m^k, h_m^k)\Big|_{u=y_{m+1}^k} \| \le C_\phi$

5 $\exists_{L_1} \ \forall_k \ \forall_{y^k, z^k \in S_y^k}$: $\| \mathcal{L}_\pi^k[y^k] - \mathcal{L}_\pi^k[z^k] \| \le L_1 \max_m \| y_m^k - z_m^k \|$

∎

The conditions 2–5 also occur in Assumption 5.51 in [AsMaRu].

3.3 Property

1 The stability of $\mathcal{N}_\pi^k$ implies that $\forall_{s,\sigma\in S_s}$: $\| y_m^k(s) - y_m^k(\sigma) \| \le \kappa \| s - \sigma \|$

2 In [AsMaRu] Th.5.52 it is shown that under the conditions mentioned in Assumption 3.1

$$\exists_{C_i} \ \forall_k \ \forall_{y\in S_y^k} : \left\| \begin{bmatrix} \mathcal{L}_\pi^k[y^k] \\ A_k \, 0. \ .0 \, B_k \end{bmatrix}^{-1} \right\| \le C_i$$

3 $\forall_{k,m}$: If $h_m^k < C_\phi^{-1}$, then R_m^k is invertible and $\| (R_m^k)^{-1} \| \le h_m^k (1 - h_m^k C_\phi)^{-1}$,

for $R_m^k = (h_m^k)^{-1} I - \frac{\partial \Phi}{\partial v}(y_m, v, \xi_m, h_m^k)\Big|_{v=y_{m+1}}$ and the second term is bounded by C_ϕ.

∎

Let y be a vector obtained from application of algorithm 3.1 . The error in y as an approximation for the solution $y(x;s^*)$ of BVP (1.1) can be bounded in terms of the discretisation error of $\mathcal{N}_\pi$ and the error in the Newton approximations of s_π and $y^k_m(s_\pi)$.

3.4 Theorem

Let $s \in S_s$ and $y \in S_y$ (see Ass.3.2) , where y^k is an approximation to $y^k(s)$, the exact solution to the difference equation $\mathcal{N}^k_\pi$ with $\mathcal{B}_k y^k = s_k$. Then

$$\forall_{k,m} : \| y^k_m - y(\xi^k_m;s^*) \| \le \| y^k_m - y^k_m(s) \| + \kappa\|s-s_\pi\| + \tilde{C}h^p , \tag{3.9}$$

with $\tilde{C}$ a constant of moderate size.

∎

Proof

Let $1 \le k \le N$ and $1 \le m \le M+1$. Recall that $y_k(x;s)$ denotes the ontinuous solution of the BVP $\mathcal{N}_k y = 0$ with $\mathcal{B}_k y = s_k$. Then

$$\| y^k_m - y(\xi^k_m;s^*) \| \le \| y^k_m - y^k_m(s) \| + \| y^k_m(s) - y^k_m(s_\pi) \|$$

$$+ \| y^k_m(s_\pi) - y_k(\xi^k_m;s_\pi) \| + \| y_k(\xi^k_m;s_\pi) - y_k(\xi^k_m;s^*) \|$$

$$\le \| y^k_m - y^k_m(s) \| + \kappa \|s-s_\pi\| + Ch^p + \kappa\|s_\pi-s^*\|$$

An estimate of $\| s_\pi-s^*\|$ is needed. To this end we estimate $f(s_\pi)$ (the continuous version).

$$\| y_k(x_{k+1};s_\pi) - y_{k+1}(x_{k+1};s_\pi) \|$$

$$\le \| y_k(x_{k+1};s_\pi) - y^k_{M+1}(s_\pi) \| + \| y^k_{M+1}(s_\pi) - y^{k+1}_1(s_\pi) \| + \| y^{k+1}_1(s_\pi) - y_{k+1}(x_{k+1};s_\pi) \|$$

$$\le Ch^p + 0 + Ch^p$$

and

$$\| g(y_1(x_1;s_\pi),y_N(x_{N+1};s_\pi)) \| = \| g(y_1(x_1;s_\pi),y_N(x_{N+1};s_\pi)) - g(y^1_1(s_\pi),y^N_{M+1}(s_\pi)) \|$$

$$\le C_{gh} (\| y_1(x_1;s_\pi) - y^1_1(s_\pi) \| + \| y_N(x_{N+1};s_\pi) - y^N_{M+1}(s_\pi) \|)$$

$$\le C_{gh} \cdot 2Ch^p$$

So $\| f(s_\pi) \| \le 2Ch^p \cdot \max(1,C_{gh})$

Because $f(s^*)=0$ and $J(s^*)$ is non–singular the inverse funtion theorem states that on some neighbourhood D of zero

$$\exists_{C_{finv}} \forall_{f(s) \in D} : \| s - s^* \| \le C_{finv} \| f(s) - f(s^*) \| \le C_{finv} \| f(s) \|$$

For sufficiently small h this yields

$$\| s^* - s_\pi \| \le C_{finv} \cdot 2CC_{gh} \cdot h^2$$

∎

The above theorem shows that the error in y^k_m as an approximation for $y_k(\xi^k_m;s^*)$ depends on the truncation error if Algorithm 1.3. converges, in the sense that both $\| s^j - s_\pi \|$ and $\| (y)^j - y(s^j) \|$ tend to zero. To proof the convergence of the algorithm, some estimates of the Jacobian $J_\pi(s)$ are required.

3.5 Lemma

1 $\exists_{C_j} \quad \forall_{y \in S_y} \quad : \| J_\pi(y) \| \le C_j$

2 $\exists_{L_j} \quad \forall_{y,z \in S_y} \quad : \| J_\pi(y) - J_\pi(z) \| \le L_j \| y-z \|$

If $\| \ \|$ is a Hölder norm, then

3 $\exists_{C_{jinv}} \quad \forall_{y \in S_y} \quad : \| J_\pi(y)^{-1} \| \le C_{jinv}$

4 $\exists_{L_{jinv}} \quad \forall_{y,z \in S_y} \quad : \| J_\pi(y)^{-1} - J_\pi(z)^{-1} \| \le L_{jinv} \| y-z \|$

∎

Proof

Let $y,z \in S_y$.

1 Because κ is a bound on the norm of the fundamental solution $\{ Y^k_m \}$ of the difference equation $(\mathcal{L}^k_\pi[y^k],\mathcal{B}_k)$, the Jacobian of $f_\pi(s)$ given by (3.8) can be bounded by

$$\| J_\pi(y) \| \le \max \left(2\kappa, \max_k (\| A_k \| + \| B_k \|)\right)$$

2 Let $\{ Y^k_m \}$ and $\{ Z^k_m \}$ be the fundamental solutions of $(\mathcal{L}^k_\pi[y^k],\mathcal{B}_k)$ and $(\mathcal{L}^k_\pi[z^k],\mathcal{B}_k)$ resp..

$$\text{Then} \begin{bmatrix} \mathcal{L}^k_\pi[y^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix} Y^k - \begin{bmatrix} \mathcal{L}^k_\pi[z^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix} Z^k = 0$$

$$\Rightarrow \begin{bmatrix} \mathcal{L}^k_\pi[y^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix} (Y^k - Z^k) + \left(\begin{bmatrix} \mathcal{L}^k_\pi[y^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix} - \begin{bmatrix} \mathcal{L}^k_\pi[z^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix} \right) Z^k = 0$$

$$\Rightarrow \| Y^k - Z^k \| \le \left\| \begin{bmatrix} \mathcal{L}^k_\pi[y^k] \\ A_k\, 0. \ \ .0\, B_k \end{bmatrix}^{-1} \right\| \cdot \| \mathcal{L}^k_\pi[y^k] - \mathcal{L}^k_\pi[z^k] \| \cdot \| Z^k \|$$

$$\le C_j \cdot L_1 \cdot \kappa \cdot \| y^k - z^k \|$$

3 Let $\{ F_k \}$ be the fundamental solution of $\mathcal{L}[y]$ with $B_a(y)\, F_1 + B_b(y)\, F_{NM+1} = I$ and let $\{ G_{kj} \}$ denote its Green's function. Subdivide $J_\pi(y)^{-1}$ into N^2 blocks of size n×n. Analoguous to Th.2.6 it can be proven that

$$[J_\pi(y)]^{-1}_{kj} = \begin{cases} A_k G_{(k-1)M+1,jM} R^j_M + B_k G_{kM+1,jM} R^j_M - \delta_{kj} B_k & \text{if } j \ne N \\ A_k F_{(k-1)M+1} \qquad + B_k F_{kM+1} & \text{if } j = N \end{cases}$$

and that consequently $\| J_\pi(y)^{-1} \| \le 2\, N\, \kappa \max_k (\| A_k \| + \| B_k \|)$ in any Hölder–norm.

4 Analoguous to the continuous case proven in Th.A.7 it can be shown that

$$\forall_{ij} : G_{ij}(y) - G_{ij}(z) = Y_k[(B_a(z) - B_a(y))G_{1j}(z) + (B_b(z) - B_b(y))G_{NM+1,j}(z)]$$
$$+ G_{ij}(y)\cdot(I-R_m^k(y)R_m^k(z)^{-1})$$
$$+ \sum_{c=1}^{N}\sum_{d=1}^{M} G_{i,(c-1)M+d}(y)\,(S_d^c(y) - R_d^c(y)R_d^c(z)^{-1}S_d^c(z))\,G_{(c-1)M+d,j}(z)$$

where k and m are obtained from $j = (k-1)M + m$ and $1 \le m \le M$.

So

$$\| G_{ij}(y) - G_{ij}(z) \| \le \kappa^2 (\| (B_a(z) - B_a(y)) \| + \| (B_b(z) - B_b(y)) \|)$$
$$+ \kappa\cdot \max_{k,m} \| I-R_m^k(y)R_m^k(z)^{-1} \| + NM\cdot\kappa^2\cdot \max_{k,m} \| S_m^k(y) - R_m^k(y)R_m^k(z)^{-1}S_m^k(z) \|$$

Because $\mathcal{L}_\pi^k[y^k]$ is Lipschitz continuous with respect to y^k on S_y^k, so are $R_m^k(y)$ and $S_m^k(y)$.

Say with constant L_h. Then

$$\| I-R_m^k(y)R_m^k(z)^{-1} \| = \| (R_m^k(y) - R_m^k(z)\,)\, R_m^k(z)^{-1} \| \le (h_m^k)^{-1}(1-h_m^kC)^{-1}\, L_h \, \| y-z \|$$

and $\| S_m^k(y) - R_m^k(y)R_m^k(z)^{-1}S_m^k(z) \|$

$$\le \| [I-R_m^k(y)R_m^k(z)^{-1}]\, S_m^k(y) \| + \| R_m^k(y)R_m^k(z)^{-1}\, [\, S_m^k(y) - S_m^k(z)\,] \|$$
$$\le \tilde{C} \, \| y-z \|$$

So

$$\| [J_\pi(y)]_{kj}^{-1} - [J_\pi(z)]_{kj}^{-1} \| \le \kappa^2 (2C_{gh} \| y-z \| + NMh\, \tilde{C} \, \| y-z \|),$$

And $NMh \approx N(x_{k+1} - x_k) \approx (b-a)$, this is the interval length.

∎

To show convergence of Algorithm 3.1 it is necessary to estimate the errors $\| s^j - s_\pi \|$ and $\| y_m^k(s^j) - (y_m^k)^j \|$. The next theorem shows that the alternate character of the algorithm disturbes the quadratic convergence of s and y. As it turns out the approximate solutions $\{ (y)^j \}$ converges quadratically in $\| \partial y \| + \| \partial s \|$. And moreover the quadratic convergence of s is contaminated with a linear term in $\| \partial y \|$. Considering the combined convergence of s^j and $(y)^j$ shows that the process is super-linear convergent.

Notational convention : $\| y - z \| = \max_{k\ m} \| y_m^k - z_m^k \|$, $y,z\in\mathbb{R}^{n(M+1)N}$.

<u>3.6 Theorem</u>

If $s^j\in S_s$ and $(y)^j\in B(y(s^j);r_y)$, $1 \le k \le N$, and s^{j+1} and $(y)^{j+1}$ are obtained from application of algorithm (Alg.3.1) then

$$\| s^{j+1} - s_\pi \| \le C_{jinv} \cdot L_j \cdot \| s^j - s_\pi \|^2 \tag{3.10}$$
$$+ \| y(s^j) - (y)^j \| \cdot (L_{jinv} \cdot C_j \cdot \| s^j - s_\pi \| + C_{jinv} \cdot \max(2, C_{gh}))$$

and

$$\| y(s^{j+1}) - (y)^{j+1} \| \tag{3.11}$$
$$\le 2\kappa L_1 [(1+\kappa \cdot C_{jinv} \cdot \max(2,C_{gh})) \cdot \| y(s^j) - y^j \| + \max(2,C_{gh}) \cdot C_{jinv} \cdot \kappa^2 \cdot \| s^j - s_\pi \|]^2$$

∎

<u>Proof</u>

$$\| s^{j+1} - s_\pi \| =$$
$$= \| s^j - s_\pi - J_\pi(y(s^j))^{-1} f_\pi(y(s^j)) + J_\pi(y(s^j))^{-1} f_\pi(y(s^j)) - J_\pi((y)^j)^{-1} f_\pi(y^j) \|$$
$$\le \| J_\pi^{-1}(s^j)[f_\pi(s_\pi) - f_\pi(s^j) + J_\pi(s^j)(s^j - s_\pi)] \|$$
$$+ \| J_\pi(y(s^j))^{-1} - J_\pi((y)^j)^{-1} \| \cdot \| f_\pi(y(s^j)) \| + \| J_\pi((y)^j)^{-1} \| \cdot \| f_\pi(y(s^j)) - f_\pi((y)^j) \|$$
$$\le C_{jinv} \cdot L_j \cdot \| s^j - s_\pi \|^2 + L_{jinv} \cdot \| y(s^j) - (y)^j \| \cdot \| f_\pi(s^j) - f_\pi(s_\pi) \|$$
$$+ C_{jinv} \cdot \max(2,C_{gh}) \cdot \| y(s^j) - (y)^j \|$$
$$\le C_{jinv} \cdot L_j \cdot \|s^j - s_\pi\|^2 + \| y(s^j) - (y)^j \| \, (L_{jinv} \cdot C_j \cdot \|s^j - s_\pi\| + C_{jinv} \cdot \max(2,C_{gh}))$$

and

$$\| (y^k)^{j+1} - y^k(s^{j+1}) \| \le \| (y^k)^j - y^k(s^{j+1}) - \begin{bmatrix} \mathcal{L}_\pi^k[y^k] \\ A_k\, 0. \;\; .0\, B_k \end{bmatrix}^{-1} \cdot \begin{bmatrix} \mathcal{N}_\pi^k(y^k)^j \\ \mathcal{B}_k(y^k)^j - s_k^{j+1} \end{bmatrix} \|$$
$$\le \| \begin{bmatrix} \mathcal{L}_\pi^k[y^k] \\ A_k\, 0. \;\; .0\, B_k \end{bmatrix} ((y^k)^j - y^k(s^{j+1})) - \begin{bmatrix} \mathcal{N}_\pi^k(y^k)^j \\ \mathcal{B}_k(y^k)^j - s_k^{j+1} \end{bmatrix} + \begin{bmatrix} \mathcal{N}_\pi^k(y^k)^{j+1} \\ \mathcal{B}_k(y^k)^{j+1} - s_k^{j+1} \end{bmatrix} \| \cdot$$
$$\cdot \| \begin{bmatrix} \mathcal{L}_\pi^k[y^k] \\ A_k\, 0. \;\; .0\, B_k \end{bmatrix}^{-1} \|$$
$$\le 2\kappa L_1 \| (y^k)^j - y^k(s^{j+1}) \|^2$$
$$\le 2\kappa L_1 (\| (y^k)^j - y^k(s^j) \| + \| y^k(s^j) - y^k(s^{j+1}) \|)^2$$
$$\le \{ \text{ stability of } \mathcal{N}_\pi^k \}$$
$$2\kappa L_1 (\| (y^k)^j - y^k(s^j) \| + \kappa \cdot \| s^j - s^{j+1} \|)^2$$
$$\le \{ \text{ algorithm for } s^{j+1} \}$$
$$2\kappa L_1 (\| (y^k)^j - y^k(s^j) \| + \kappa \cdot \| J_\pi^{-1}((y)^j) f_\pi((y)^j) \|)^2$$
$$\le 2\kappa L_1 (\| (y^k)^j - y^k(s^j) \| + \kappa \cdot C_{jinv} \cdot (\|f_\pi((y)^j) - f_\pi(y(s^j))\| + \| f_\pi(y(s^j)) - f_\pi(y(s_\pi)) \|))^2$$
$$\le 2\kappa L_1 ((1+ \kappa \cdot C_{jinv} \cdot \max(2,C_{gh})) \cdot \| (y)^j - y(s^j) \| + \kappa^2 \cdot C_{jinv} \cdot \max(2,C_{gh}) \cdot \| s^j - s_\pi \|)^2$$

∎

From the upperbounds derived above one can see that y^j converges quadratically to $y(s^j)$ if during the whole process s^j remains in $B(s_\pi,r_s)$ and converges to s_π . It is not straightforward however that this condition is satisfied for sufficiently small s^0, because the quadratic convergence of s^j is disturbed by a linear term. This problem can be overcome by substituting the acquired upperbound for $\| y^j - y(s^j) \|$ into the bound on $\| s^j - s_\pi \|$:

$$\| s^{j+1} - s_\pi \| \leq C_1 \| s^j - s_\pi \|^2$$
$$+ C_2((1+\kappa \cdot C_4) \cdot \| y^{j-1} - y(s^{j-1}) \| + \kappa^2 \cdot C_4 \cdot \| s^j - s_\pi \|)^2 \cdot (C_3 \| s^j - s_\pi \| + C_4)$$

with $C_1 := C_{jinv} \cdot L_j$, $C_2 := 2\kappa L_1$, $C_3 := L_{jinv} \cdot C_j$ and $C_4 := C_{jinv} \cdot \max(2,C_{gh})$

Now define the function F: $\mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{R}^2$ by

$$F\left(\begin{bmatrix} \varphi_{j-1} \\ \sigma_j \end{bmatrix},\begin{bmatrix} \varphi_{j-2} \\ \sigma_{j-1} \end{bmatrix}\right) := \begin{bmatrix} C_2((1+C_4\kappa)\varphi_{j-1} + C_4\kappa^2\sigma_{j-1})^2 \\ C_1\sigma_j^2 + C_2((1+C_4\kappa)\varphi_{j-1} + C_4\kappa^2\sigma_{j-1})^2 \cdot (C_3\sigma_j + C_4) \end{bmatrix} \tag{3.12}$$

Then with $\varphi_{-1} = 0$, $\varphi_0 = \| (y)^0 - y(s^0) \|$, $\sigma_j = \| s^j - s_\pi \|$, j=0,1 and

$$\begin{bmatrix} \varphi_j \\ \sigma_{j+1} \end{bmatrix} = F\left(\begin{bmatrix} \varphi_{j-1} \\ \sigma_j \end{bmatrix},\begin{bmatrix} \varphi_{j-2} \\ \sigma_{j-1} \end{bmatrix}\right) \qquad j \geq 1,$$

φ_j and σ_j will be upperbounds for $\| (y)^j - y(s^j) \|$ and $\| s^j - s_\pi \|$ respectively, if s^j and y^j stay in the area where the estimates (3.10) and (3.11) hold. Now the upperbound for the errors in s and y are considered to be formed by a two-step successive substitution process. In the appendix some theory about such a process is derived.

<u>3.7 Theorem</u>

<u>1</u> $\exists_{r>0}\ \exists_{C<1}\ \forall_{x,y\in\mathbb{R}^2}$: $x,y \in B(\underline{0},r) \Rightarrow \| F(x,y) \| \leq C \| x-y \|$

<u>2</u> Let $s^0,s^1 \in B(s_\pi,\min(r_s,r))$ and let $y^0 \in B(y(s^0);\min(r_y,r))$. Then

$$\forall_j : s^j \in B(s_\pi,\min(r_s,r)) \text{ and } y^j \in B(y(s^j),\min(r_y,r))$$

and the vector sequence $\begin{bmatrix} \varphi_{j-1} \\ \sigma_j \end{bmatrix}$ converges locally, super–linear to zero. The order of convergence is almost 1,4 .

■

<u>Proof</u>

<u>1</u> Because $F(\underline{0},\underline{0}) = \underline{0}$ and both partial derivatives of F at $\underline{0}$ are zero, F will have a contraction area around $\underline{x} = \underline{0}$.

<u>2</u> This follows immediately from Th A.8 (see appendix).

■

From the theory presented in this paper it follows that the generalized form of multiple shooting, that involves well–conditioned linear boundary conditions on the subintervals may

have a larger convergence area than ordinary multiple shooting, if the local BVP's can be solved exactly.
In practice a one–step finite difference method is used for solving the local BVP's. An algorithm that alternately makes a Newton update for the shooting vector s and the finite difference approximation y_m^k converges super–linear provided

- the initial guesses for s and y are sufficiently good
- the finite difference grid is sufficiently fine.

Although the method has not yet been implemented, we expect that it will not require much less execution time or memory space, then ordinary multiple shooting. But that its merit will be an enlarged convergence area. This is especially important if the convergence area is extremely small for ordinary multiple shooting or a proper initial guess cannot be obtained.

This paper presents a first draft of the generalized multiple shooting method. Issues that are to be investigated are

- the choice of the local boundary conditions
- mesh choice for both the finite differences and the 'shooting' intervals
- a posteriori error bounds and stop criteria
- experimental comparison of the convergence rate and –area for
    - normal multiple shooting
    - unbiased multiple shooting
    - finite differences on the entire interval
- the influence of more finite difference updates per Newton iteration on the 'shooting' vectors.

Appendix

A.1 Definition

Consider the linear differential equation

$$\dot{y} = A(x)\cdot y \qquad x\in[a,b] \tag{A.1}$$

Its fundamental solution (f.s.) Y(x) is dichotomic, if there is an orthogonal projection P and constants $K,\lambda,\mu \geq 0$, with K of moderate size, such that

$$\forall_{a\leq t\leq x\leq b} \quad : \quad \| Y(x)PY^{-1}(t) \| \leq Ke^{-\lambda(x-t)} \tag{A.2a}$$

$$\forall_{a\leq x\leq t\leq b} \quad : \quad \| Y(x)(I-P)Y^{-1}(t) \| \leq Ke^{-\mu(t-x)} \tag{A.2b}$$

The f.s. is called dichotomic with projection P and constants (K,λ,μ).

If λ and μ are both positive the fundamental solution is called exponentially dichotomic.

∎

A.2 Corollary

If the f.s. Y(x) of (A.1) is dichotomic with projection P and constants (K,λ,μ), then

$$\forall_{\xi\in\mathbb{R}^n} \; \forall_{a\leq x\leq t\leq b} : \quad \| Y(t)P\xi \| \leq Ke^{-\lambda(t-x)} \| Y(x)P\xi \| \tag{A.3a}$$

$$\text{and} \quad \| Y(x)(I-P)\xi \| \leq Ke^{-\mu(t-x)} \| Y(t)(I-P)\xi \| \tag{A.3b}$$

∎

A.3 Definition

a The linear BVP

$$\dot{y} = A(x)\, y + q(x) \qquad a\leq x\leq b$$

$$B_a y(a) + B_b y(b) = \beta$$

is well–conditioned , if for every smooth function q(x) and every vector β there is a unique solution $y_{q\beta}(x)$ and there is a constant κ of moderate size such that

$$\forall_{q(x)} \; \forall_{\beta} \; : \; \max_x \| y_{q\beta}(x) \| \leq \kappa \, (\| \beta \| + \| q \|)$$

b The non–linear BVP

$$\dot{y} = h(x,y(x)) \qquad a\leq x\leq b$$

$$g(y(a),y(b)) = 0$$

is well–conditoned at the solution $y^*(x)$, if there is a $r > 0$ such that for all $y\in B(y^*(x),r)$ the problem linearized at y(x) is well-conditioned.

∎

The fundamental solutions of two linear differential equations can be related to each other in several ways. Here two possibilities will be shown.
Consider two linear BVP's

$$\begin{cases} \dot{y} = A(x)y & a \le x \le b \\ \mathcal{B}y = \beta \end{cases} \tag{A.4}$$

$$\begin{cases} \dot{z} = \tilde{A}(x)z & a \le x \le b \\ \tilde{\mathcal{B}}z = \beta \end{cases} \tag{A.5}$$

with $\mathcal{B}$ and $\tilde{\mathcal{B}}$ linear boundary conditions on [a.b] and both A(x) and $\tilde{A}(x)$ Riemann-integrable.

<u>A.4 Definition</u>

Suppose Y(x) is a dichtomic fundamental solution of (A.4) with projection P . Define the operator $\mathcal{P} : C([a,b] \to \mathbb{R}^{n\times n}) \to C([a,b] \to \mathbb{R}^{n\times n})$ by

$$\forall_{\Phi} : (\mathcal{P}\,\Phi)(x) := \int_a^x Y(x)PY^{-1}(t)\cdot(\tilde{A}(t) - A(t))\cdot\Phi(t)\,dt - \int_x^b Y(x)(I-P)Y^{-1}(t)\cdot(\tilde{A}(t) - A(t))\cdot\Phi(t)\,dt \tag{A.6}$$

▬

<u>A.5 Theorem</u>

The operator $\mathcal{P}$ is linear and bounded with $\| \mathcal{P} \| \le C\cdot \| \tilde{A}-A \|$ for some moderate constant C. And for every fundamental solution Z(x) of (A.5) there is a matrix X_1 such that

$$\forall_{x\in[a,b]} : (\mathcal{I}-\mathcal{P})Z(x) = Y(x)X_1 \tag{A.7}$$

The matrix X_1 is determined by

$$\mathcal{B}Y\cdot X_1 = \mathcal{B}Z - \mathcal{B}(\mathcal{P}Z) \tag{A.8}$$

if $\mathcal{B}Y$ is non–singular.

▬

<u>Proof</u> see [KrMa] Th. 4.7

The fundamental solutions of different ODE's can also be related to one another by the Green's function

<u>A.6 Lemma</u>

Let Y(x) be a f.s. of (A.4) and let G(x,t) be the Green's function of (A.4). Then for every f.s. Z(x) of (A.5) there is a matrix X_1 such that

$$Z(x) = Y(x)X_1 + \int_a^b G(x,t)(\tilde{A}(t)-A(t))Z(t)dt$$

Where X_1 has to satisfy $\mathcal{B}Z = \mathcal{B}Y\cdot X_1$.

▬

Another feature used, is the relationship between the Green's functions of the differential equations (A.4) and (A.5).

A.7 Theorem

Let Y(x) be the fundamental solution of (A.4) with $\mathcal{B}Y = I$. Furthermore let $G(x,t)$ and $\tilde{G}(x,t)$ denote the Green's function of the BVP's (A.4) and (A.5) resp.. Then

$$\forall_{a\leq x,t\leq b}:\ \tilde{G}(x,t) = G(x,t) + Y(x)\mathcal{B}\tilde{G}(\cdot,t) - \int_a^b G(x,s)\cdot(\tilde{A}(s)-A(s))\cdot\tilde{G}(s,t)\,ds \qquad (A.11)$$

and $\| \tilde{G}(x,t) - G(x,t) \| \leq \kappa\tilde{\kappa}\cdot\left(\| \tilde{\mathcal{B}} - \mathcal{B} \| + \int_a^b \| \tilde{A}(\tau) - A(\tau) \| \,d\tau \right)$

■

Proof

Let $f\in C([a,b])$. Define $y(x) := \int_a^b G(x,t)\, f(t)\, dt$ and $\tilde{y} := \int_a^b \tilde{G}(x,t)\, f(t)\, dt$.

Then $\dot{y}(x) = A(x)\cdot y(x) + f(x)$ and $\mathcal{B}y = 0$. So

$$\frac{d}{dx}[\, \tilde{y}(x) - y(x)\,] = A(x)\cdot(\tilde{y}(x)-y(x)) + (\tilde{A}(x)-A(x))\tilde{y}(x)$$

and $\tilde{y}(x) - y(x) = Y(x)c + \int_a^b G(x,u)\cdot(\tilde{A}(u)-A(u))\cdot\tilde{y}(u)\, du$. (*)

The vector c is determined by the boundary value : $c = (\mathcal{B}Y)c = \mathcal{B}(\tilde{y}-y) = \mathcal{B}\tilde{y}$.
Combining this result with (*) and the definitions of y(x) and $\tilde{y}(x)$ yields

$$\int_a^b \tilde{G}(x,t)\, f(t)\, dt = \int_a^b G(x,t)\, f(t)\, dt + Y(x)\int_a^b \mathcal{B}\tilde{G}(\cdot,t)\, f(t)\, dt$$
$$+ \int_a^b\int_a^b G(x,s)\cdot(\tilde{A}(s)-A(s))\cdot\tilde{G}(s,t)\, f(t)\, dt\, ds$$

holds for all functions $f\in C([a,b])$. This results in

$$\tilde{G}(x,t) = G(x,t) + Y(x)\cdot\mathcal{B}\tilde{G}(\cdot,t) + \int_a^b G(x,s)\cdot(\tilde{A}(s)-A(s))\cdot\tilde{G}(s,t)\, ds$$

Because $\mathcal{B}\tilde{G}(\cdot,t) = (\mathcal{B}-\tilde{\mathcal{B}})\tilde{G}(\cdot,t) + \tilde{\mathcal{B}}\tilde{G}(\cdot,t) = (\mathcal{B}-\tilde{\mathcal{B}})\tilde{G}(\cdot,t)$ this gives

$$\| G(x,t) - \tilde{G}(x,t) \| \leq \kappa\tilde{\kappa}\cdot\| \mathcal{B}-\tilde{\mathcal{B}} \| + \kappa\tilde{\kappa}\int_a^b \| A(\tau) - \tilde{A}(\tau) \|\, d\tau$$

■

In the process presented in this paper a two–step successive substitution process occurs. For this the following convergence properties can be derived.

A.8 Theorem

Consider the two step process of successive substitution

$$x_{k+1} = F(x_k,x_{k-1}) \qquad k \geq 1$$

with initial values x_0 and x_1.

a Suppose there is a vector ξ with $F(\xi,\xi) = \xi$ and

$$\exists_{r>0}\ \exists_{K_1,K_2}\ \forall_{x_1,x_2,y_1,y_2 \in B(\xi,r)} :$$

$$\| F(x_1,y_1) - F(x_2,y_2) \| \le K_1 \| x_1 - x_2 \| + K_2 \| y_1 - y_2 \| \quad \text{and} \quad K := K_1 + K_2 < 1$$

Then for all $x_0, x_1 \in B(\xi,r)$ the sequence $\{ x_k \}$ remains in $B(\xi,r)$ and converges to ξ with

$$\| x_k - \xi \| \le K^{k \operatorname{div} 2}\, r$$

b If additionally $\frac{\partial F}{\partial u}(\xi,\xi) = \frac{\partial F}{\partial v}(\xi,\xi) = 0$ and F is twice differentiable on $B(\xi,r)$, then

$$\exists_{C>0}\ \forall_k : \| x_{k+1} - \xi \| \le C \cdot (\| x_k - \xi \| + \| x_{k-1} - \xi \|)^2$$

and the order of convergence is almost 1.4 .

∎

Proof

a Proof by induction to (k div 2). Initial step.

$$\| x_2 - \xi \| = \| F(x_1,x_0) - F(\xi,\xi) \|$$
$$\le K_1 \| x_1 - \xi \| + K_2 \| x_0 - \xi \| \le (K_1 + K_2)\cdot r = Kr$$

and $\| x_3 - \xi \| = \| F(x_2,x_1) - F(\xi,\xi) \|$

$$\le K_1 \| x_2 - \xi \| + K_2 \| x_1 - \xi \| \le (K_1 + K_2)\cdot \max(Kr,r) \le Kr$$

Induction step.

$$\| x_{k+1} - \xi \| \le K_1 \| x_k - \xi \| + K_2 \| x_{k-1} - \xi \|$$
$$\le K_1 K^{k \operatorname{div} 2}\, r + K_2 K^{(k-1) \operatorname{div} 2}\, r$$
$$\le K\, K^{(k \operatorname{div} 2) - 1}\, r$$

b Now suppose that $\frac{\partial F}{\partial u}(\xi,\xi) = \frac{\partial F}{\partial v}(\xi,\xi) = 0$ and that F is twice differentiable on $B(\xi,r)$. Then

$$\| x_{k+1} - \xi \| = \| F(x_k,x_{k-1}) - F(\xi,\xi) \|$$
$$= \| F(x_k,x_{k-1}) - F(\xi,x_{k-1}) + F(\xi,x_{k-1}) - F(\xi,\xi) \|$$
$$= \| F(x_k,x_{k-1}) - F(\xi,x_{k-1}) - \frac{\partial F}{\partial u}(\xi,x_{k-1})\cdot(x_k - \xi)$$
$$+ \frac{\partial F}{\partial u}(\xi,x_{k-1})\cdot(x_k-\xi) - \frac{\partial F}{\partial u}(\xi,\xi)\cdot(x_k-\xi) + F(\xi,x_{k-1}) - F(\xi,\xi) - \frac{\partial F}{\partial v}(\xi,\xi)\cdot(x_{k-1}-\xi) \|$$
$$\le \sup_{0<t<1} \| \frac{\partial^2 F}{\partial u^2}(tx_k + (1-t)\xi, x_{k+1}) \| \cdot \| x_k - \xi \|^2$$
$$+ \sup_{0<t<1} \| \frac{\partial^2 F}{\partial u \partial v}(\xi, tx_{k-1} + (1-t)\xi) \| \cdot \| x_k - \xi \| \cdot \| x_{k+1} - \xi \|$$
$$+ \sup_{0<t<1} \| \frac{\partial^2 F}{\partial v^2}(\xi, tx_{k-1} + (1-t)\xi) \| \cdot \| x_{k-1} - \xi \|^2$$
$$\le C (\| x_k - \xi \| + \| x_{k+1} - \xi \|)^2$$

where C is a upperbound for the second–order partial derivatives of F on $B(\xi,r)$.

Let d_k satisfy

$$d_{k+1} = (d_k + d_{k-1})^2 ,\ k \ge 1,$$
$$d_k = C\cdot \| x_k - \xi \| \text{ for } k = 0,1 ,$$

then d_k is an upperbound for $C\cdot \| x_k - \xi \|$, $k \in \mathbb{N}$.

Let θ be such that $d_{k+1}{}^{\theta} = d_k$, then

$$d_{k+1} = (d_{k+1}{}^{\theta} + d_k{}^{\theta})^2 = (d_{k+1}{}^{\theta} + (d_{k+1}{}^{\theta})^{\theta})^2 = d_{k+1}{}^{\theta^2} + 2d_{k+1}{}^{\theta^3} + d_{k+1}{}^{\theta^4}$$

$$\Rightarrow \ln(d_{k+1})\cdot[\theta^4 + \frac{\ln(2d_{k+1})}{\ln(d_{k+1})}\theta^3 + \theta^2 - 1] = 0$$

and with $\lim_{d\to 0} \frac{\ln(2d)}{\ln(d)} = \frac{1}{2}$, θ satisfies approximately

$$\theta^4 + \frac{1}{2}\theta^3 + \theta^2 - 1 = 0 \quad \text{so } \theta \approx 0.73 , \theta^{-1} \approx 1.4$$

This shows that $d_{k+1} \approx (d_k)^{1.4}$

∎

<u>A.9 Theorem</u> (perturbed two–step SUCSUB)

Consider the perturbed two step succesive substitution process

$$x_{k+1} = F(x_k,x_{k-1}) + \delta_{k+1} \qquad k \geq 1$$

If the conditions of theorem A.8 hold and $\forall_k : \| \delta_k \| < (1-K)r$ and $\| \delta_{k+1} \| \leq \| \delta_k \|$ then

$$\forall_k : \| x_k - \xi \| \leq K^{k \text{ div } 2} r + \sum_{j=1}^{k \text{ div } 2} K^{k \text{ div } 2 - j} \varepsilon_j$$

where $\varepsilon_k := \max (\| \delta_{2k} \| , \| \delta_{2k+1} \|)$

If additionally $\exists_{L<1} \ \forall_k : \varepsilon_{k+1} \leq L\,\varepsilon_k$, then $\lim_{k\to\infty} \| x_k - \xi \| = 0.$

∎

<u>Proof</u>

Initial step

$$\| x_2 - \xi \| \leq K \max(\| x_0 - \xi \|,\| x_1 - \xi \|) + \|\delta_2\| \leq K \max(r,r) + \varepsilon_1$$

$$\| x_3 - \xi \| \leq K \max(\| x_2 - \xi \|,\| x_1 - \xi \|) + \|\delta_3\| \leq K \max(Kr+\varepsilon_1,r) + \varepsilon_1 \leq Kr + \varepsilon_1$$

Induction step

If k = 2l , l > 1 then

$$\| x_k - \xi \| \leq K \max (\| x_{k-1} - \xi \| , \| x_{k-2} - \xi \|) + \| \delta_k \|$$

$$\leq K \max (K^{l-1} r + \sum_{j=1}^{l-1} K^{l-j-1} \varepsilon_j , K^{l-1} r + \sum_{j=1}^{k-1} K^{l-j-1} \varepsilon_j) + \varepsilon_1$$

$$\leq K^l r + \sum_{j=1}^{l} K^{l-j} \varepsilon_j$$

If k = 2l + 1 , l > 1 then

$$\| x_k - \xi \| \leq K \max (\| x_{k-1} - \xi \| , \| x_{k-2} - \xi \|) + \| \delta_k \|$$

$$\leq K \max (K^l r + \sum_{j=1}^{l} K^{l-j} \varepsilon_j , K^{l-1} r + \sum_{j=1}^{l-1} K^{l-j-1} \varepsilon_j) + \varepsilon_1$$

$$\leq \{ \eta := K^{l-1} r + \sum_{j=1}^{l-1} K^{l-j-1} \varepsilon_j \}$$

$$K \max (K\eta + \varepsilon_1 , \eta) + \varepsilon_k \leq K\eta + \varepsilon_k \leq K^l r + \sum_{j=1}^{l} K^{l-j}\varepsilon_j$$

because

$$\eta - K\eta - \varepsilon_1 = (K^{l-1} - K^l)r + \sum_{j=1}^{l-1} (K^{l-j-1} - K^{l-j})\varepsilon_j - \varepsilon_1$$

$$\geq K^{l-1}(1-K)r + \varepsilon_1(1-K)\sum_{j=0}^{l-2} K^j - \varepsilon_1$$

$$> K^{l-1}\varepsilon_1 + \varepsilon_1(1-K^{l-1}-1) \ = 0$$

Next suppose that $\exists_{L>1} \ \forall_k \ : \| \varepsilon_{k+1} \| \leq L \| \varepsilon_k \|$.

Now $\| x_{2k+1} - \xi \| = \| x_{2k} - \xi \| = K^k r + \sum_{j=1}^{k} K^{k-j} L^{j-1}\varepsilon_1$

$$= \begin{cases} K^k r + \varepsilon_1 \sum_{j=1}^{k} \left[\frac{K}{L}\right]^{k-j} L^{k-1} & \text{if } K < L \\ K^k r + \varepsilon_1 k \cdot K^{k-1} & \text{if } K = L \\ K^k r + \varepsilon_1 \sum_{j=1}^{k} \left[\frac{L}{K}\right]^{j-1} K^{k-1} & \text{if } K > L \end{cases}$$

$\to 0$ if $k \to \infty$.

∎

References

[AsMaRu] U.Ascher, R.Mattheij, R.Russell, *Numerical solution of boundary value problems for ordinary differential equations*. Englewood Cliffs,N.J. : Prentice–Hall, 1988.

[KrMa] M.Kramer, R.Mattheij, *Combining multiple shooting and time–stepping for solving non–linear BVP's*. RANA report 89–04, Technische Universiteit, Eindhoven, 1989.

[OrRh] J.Ortega, W.Rheinboldt, *Iterative solution of nonlinear equations in several variables*. Sandiego : Academic Press inc. ,1970.