Numerical Analysis & Scientific Computing II

Module 2

Initial Value Problems

2.5 Stiffness

2.6 Linear Multistep Method

2.7 Non-Linear Methods

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Initial Value Problems: Non-Linear Methods

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To implement any implicit method, we need a way to solve, at least approximately, the non-linear algebraic equation that arise at each step.

One common strategy is to solve the equation approximately using a small number of fixed point iterations starting from an initial approximation obtained by an explicit method.

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- Predictor-Corrector Schemes

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One common strategy is to solve the equation approximately using a small number of fixed point iterations starting from an initial approximation obtained by an explicit method.

A predictor-corrector scheme takes the following form:

1. $p_{n+1} = E(y_n, y_{n-1}, \dots, f_n, f_{n-1}, \dots)$ *(PREDICT)*
2. $f_{n+1}^{p} = f(t_{n+1}, p_{n+1})$ *(EVALUATE)*
3. $y_{n+1}^{(1)} = I(y_n, y_{n-1}, \dots, f_{n+1}^{p}, f_n, f_{n-1}, \dots)$ *(CORRECT)*
4. $f_{n+1}^{(1)} = f(t_{n+1}, y_{n+1}^{(1)})$ *(EVALUATE)*
5. $y_{n+1}^{(2)} = I(y_n, y_{n-1}, \dots, f_{n+1}^{(1)}, f_n, f_{n-1}, \dots)$ *(CORRECT)*
6. $f_{n+1}^{(2)} = f(t_{n+1}, y_{n+1}^{(2)})$ *(EVALUATE)*

$$\vdots$$

where $E(y_n, y_{n-1}, \dots, f_n, f_{n-1}, \dots)$ refers to some explicit scheme and $I(y_n, y_{n-1}, \dots, f_{n+1}, f_n, f_{n-1}, \dots)$ stands for an implicit method.

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It is common to use a fixed number of iterations, but other suitable stopping criterion can also be adopted to stop.

Initial Value Problems: Non-Linear Methods

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Example

Consider the following predictor-corrector scheme where Euler's method is used as predictor and Trapezoidal method as corrector:

1. $p_{n+1} = y_n + h_k f(t_n, y_n)$ *(PREDICT)*
2. $f_{n+1}^{p} = f(t_{n+1}, p_{n+1})$ *(EVALUATE)*
3. $y_{n+1} = y_n + h_k\big(f(t_n, y_n) + f_{n+1}^{p}\big)/2$ *(CORRECT)*

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3. $y_{n+1} = y_n + h_k\big(f(t_n, y_n) + f_{n+1}^{p}\big)/2$ *(CORRECT)*

This can be expressed more concisely as

$$y_{n+1} = y_n + h_k(f(t_n, y_n) + f(t_{n+1}, y_n + h_k f(t_n, y_n)))/2$$

and is commonly known as Heun's method, a non-linear one step method.

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Example

Consider the following PECE scheme with 2-step Adam-Bashford predictor and 2-step Adam-Moulton corrector.

$$p_{n+1} = y_n + h[3f(t_n, y_n) - f(t_{n-1}, y_{n-1})]/2$$
$$y_{n+1} = y_n + h[5f(t_{n+1}, p_{n+1}) + 8f(t_n, y_n) - f(t_{n-1}, y_{n-1})]/12.$$

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Consider the following PECE scheme with 2-step Adam-Bashford predictor and 2-step Adam-Moulton corrector.

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$$y_{n+1} = y_n + h[5f(t_{n+1}, p_{n+1}) + 8f(t_n, y_n) - f(t_{n-1}, y_{n-1})]/12.$$

Thus, the resulting method

$$y_{n+1} = y_n + h[5f(t_{n+1}, y_n + h[3f(t_n, y_n) - f(t_{n-1}, y_{n-1})]/2\,) + 8f(t_n, y_n) - f(t_{n-1}, y_{n-1})]/12$$

is a nonlinear 2-step method.

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Error Analysis

There are two contributions to the local truncation error, one arising from predictor formula and one arising from corrector formula. Let the predictor be of order p *and the corrector be of order* q*.*

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$$\left|\ell_{n+1}^{PECE}(y,h)\right|$$
$$=\left|hb_{-1}^{I}f\left(t_{n+1},h\sum_{j=-1}^{k}b_j^E y'(t_n-jh)-\sum_{j=0}^{k}a_j^E y(t_n-jh)\right)+h\sum_{j=0}^{k}b_j^I y'(t_n-jh)-\sum_{j=-1}^{k}a_j^I y(t_n-jh)\right|$$

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$$\begin{aligned}
&\left|\ell_{n+1}^{PECE}(y,h)\right| \\
&= \left| hb_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh)\right) + h\sum_{j=0}^{k} b_j^I y'(t_n - jh) - \sum_{j=-1}^{k} a_j^I y(t_n - jh)\right| \\
&= \left| hb_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh)\right) - hb_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h)\right|
\end{aligned}$$

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\begin{aligned}
&\left|\ell_{n+1}^{PECE}(y,h)\right| \\
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&= \left| h b_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) \right) - h b_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h) \right| \\
&\le h\left|b_{-1}^{I}\right| L \left| \left(h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) - y(t_{n+1}) \right) \right| + \left|\ell_{n+1}^{I}(y,h)\right|
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&= \left| h b_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh)\right) - h b_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h)\right| \\
&\le h\left|b_{-1}^{I}\right| L \left|\left(h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) - y(t_{n+1})\right)\right| + \left|\ell_{n+1}^{I}(y,h)\right| \\
&= h\left|b_{-1}^{I}\right| L \left|\ell_{n+1}^{E}(y,h)\right| + \left|\ell_{n+1}^{I}(y,h)\right|
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&= \left| hb_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) \right) - hb_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h) \right| \\
&\le h\left|b_{-1}^{I}\right| L \left| \left(h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) - y(t_{n+1}) \right) \right| + \left|\ell_{n+1}^{I}(y,h)\right| \\
&= h\left|b_{-1}^{I}\right| L \left|\ell_{n+1}^{E}(y,h)\right| + \left|\ell_{n+1}^{I}(y,h)\right| \le C_1 h \left|b_{-1}^{I}\right| L h^{p+1} + C_2 h^{q+1}
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&= \left| h b_{-1}^{I} f\left(t_{n+1}, h \sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) \right) - h b_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h) \right| \\
&\leq h \left| b_{-1}^{I} \right| L \left| \left(h \sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) - y(t_{n+1}) \right) \right| + \left| \ell_{n+1}^{I}(y,h) \right| \\
&= h \left| b_{-1}^{I} \right| L \left| \ell_{n+1}^{E}(y,h) \right| + \left| \ell_{n+1}^{I}(y,h) \right| \leq C_1 h \left| b_{-1}^{I} \right| L h^{p+1} + C_2 h^{q+1} \leq C h^{\min\{p+2, q+1\}}
\end{aligned}
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where $C = \max\left\{ \left| b_{-1}^{I} \right| C_1, C_2 \right\}$.

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&= \left| hb_{-1}^{I} f\left(t_{n+1}, h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh)\right) - hb_{-1}^{I} f\big(t_{n+1}, y(t_n + h)\big) + \ell_{n+1}^{I}(y,h)\right| \\
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where $C = \max\left\{\left|b_{-1}^{I}\right| C_1, C_2\right\}$. *Thus, for* $p \ge q-1$, *the local error is* $O(h^{q+1})$.

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&\leq h\left|b_{-1}^{I}\right| L \left|\left(h\sum_{j=-1}^{k} b_j^E y'(t_n - jh) - \sum_{j=0}^{k} a_j^E y(t_n - jh) - y(t_{n+1})\right)\right| + \left|\ell_{n+1}^{I}(y,h)\right| \\
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\end{aligned}$$

where $C = \max\{\left|b_{-1}^{I}\right| C_1, C_2\}$. Thus, for $p \geq q-1$, the local error is $O(h^{q+1})$. Most common choice is $p = q-1$.

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- One step methods

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One step methods

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One step methods

Are there ways to develop one step methods that are high order? Here is an idea! Consider the Taylor series

$$y(t+h) = y(t) + hy'(t) + \frac{h^2}{2}y''(t) + \frac{h^3}{6}y'''(t) + \cdots$$

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Therefore,

$$y(t+h) = y(t) + hy'(t) + \frac{h^2}{2}y''(t)$$

yields a second-order method.

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Thus the method reads

$$y_{n+1} = y_n + h_n f(t_n, y_n) + \frac{h_n^2}{2}\Big(f_t(t_n,y_n) + f_y(t_n,y_n)f(t_n,y_n)\Big).$$

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One can use this idea to construct higher order methods. For example, we have

$$y'''(t) = f_{tt}(t,y) + 2f_{ty}(t,y)f(t,y) + f_{yy}(t,y)f^2(t,y) + f_t(t,y)f_y(t,y) + f_y^2(t,y)f(t,y),$$

therefore,

$$y_{n+1} = y_n + h_n f(t_n, y_n) + \frac{h_n^2}{2}\Big(f_t(t_n,y_n) + f_y(t_n,y_n)f(t_n,y_n)\Big) + \frac{h_n^3}{6}y'''(t_n)$$

has order 3.

Initial Value Problems: Non-Linear Methods

More generally, by defining the total derivative of f as

$$Df := f_t + f f_y$$

and by further differentiating

$$D^2 f := f_{tt} + 2f f_{ty} + f^2 f_{yy} + f_t f_y + f f_y^2,$$

$D^3 f = y^{(4)}(t)$, etc., an order p single step method takes the form

$$y_{n+1} = y_n + h_n f + \frac{h_n^2}{2} D f_n + \cdots + \frac{h_n^p}{p!} D^{p-1} f_n.$$

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$$y_{n+1} = y_n + h_n f + \frac{h_n^2}{2} D f_n + \cdots + \frac{h_n^p}{p!} D^{p-1} f_n.$$

Such methods are called Taylor series methods.

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$$Df \coloneqq f_t + f f_y$$

and by further differentiating

$$D^2 f \coloneqq f_{tt} + 2 f f_{ty} + f^2 f_{yy} + f_t f_y + f f_y^2,$$

$D^3 f = y^{(4)}(t)$, *etc., an order p single step method takes the form*

$$y_{n+1} = y_n + h_n f + \frac{h_n^2}{2} D f_n + \cdots + \frac{h_n^p}{p!} D^{p-1} f_n.$$

Such methods are called Taylor series methods.

Remark

These methods can be implemented in some cases but require evaluation of partial derivatives of f. They are, therefore, not commonly used.

More generally, by defining the total derivative of f as

$$Df := f_t + f f_y$$

and by further differentiating

$$D^2 f := f_{tt} + 2f f_{ty} + f^2 f_{yy} + f_t f_y + f f_y^2,$$

$D^3 f = y^{(4)}(t)$, etc., an order p single step method takes the form

$$y_{n+1} = y_n + h_n f + \frac{h_n^2}{2} D f_n + \cdots + \frac{h_n^p}{p!} D^{p-1} f_n.$$

Such methods are called Taylor series methods.

Remark

These methods can be implemented in some cases but require evaluation of partial derivatives of f. They are, therefore, not commonly used.

What else can we do?