Predictor Corrector Methods[-1-]

Predictor Corrector Methods form the basis of the most successful codes (Variable Step Variable Order Methods) for the solution of initial value problems of ordinary differential equations. Briefly, these methods have been successful because they occur in naturally arising families covering a range of orders, they have reasonable stability properties, and they allow for easy error control via suitable step size/order changing policies and techniques. A thorough discussion is in chapter 4 of J.D. Lambert, *Numerical Methods for Ordinary Differential Systems*, Wiley, 1991. This handout extracts some main points from Lambert's discussion and mostly employs the same notation.

Consider the implicit linear multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}. \tag{1}$$

A possible way of solving the nonlinear system (1) is via the fixed point iteration

$$y_{n+k}^{[v+1]} = h\beta_k f\left(x_{n+k}, y_{n+k}^{[v]}\right) - \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h \sum_{j=0}^{k-1} \beta_j f_{n+j}, \quad v = 0, 1, \cdots. \tag{2}$$

where $y_{n+k}^{[0]}$ is given. This iteration will converge to the unique solution of (1) provided

$$|h\beta_k L| < 1 \tag{3}$$

where L is the Lipschitz constant of f. Thus it converges for sufficiently small h.

The basic idea of predictor corrector methods is to compute the initial approximation $y_{n+k}^{[0]}$ by an explicit linear multistep method (the *predictor*) and then run the iteration (2) for a *predetermined number* of steps. The implicit method (1) is called the *corrector*.

Predictor Corrector Modes

We denote the corrector by (1) and the predictor by

$$\sum_{j=0}^{k} \alpha_j^* y_{n+j} = h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}, \tag{4}$$

and assume that the predictor and corrector have the same step number k (if not we pad one of them with zero coefficients).

$$
\begin{aligned}
&\mathbf{P}: \quad y_{n+k}^{[0]} = -\sum_{j=0}^{k-1} \alpha_j^* y_{n+j} + h \sum_{j=0}^{k-1} \beta_j^* f_{n+j} \\
&\mathbf{E}: \qquad\qquad\qquad\qquad\qquad f_{n+k}^{[v]} = f\left(x_{n+k}, y_{n+k}^{[v]}\right) \left.\right\} \\
&\mathbf{C}: \quad y_{n+k}^{[v+1]} = h\beta_k f\left(x_{n+k}, y_{n+k}^{[v]}\right) - \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h \sum_{j=0}^{k-1} \beta_j f_{n+j} \left.\right\} \quad v = 0, 1, \cdots, \mu-1 \\
&\mathbf{E}: \quad f_{n+k} = f\left(x_{n+k}, y_{n+k}^{[\mu]}\right)
\end{aligned}
\tag{5}
$$

There are various *modes* of predictor corrector methods. Denoting by **P** the prediction, **C** one iteration of (2), and **E** an evaluation of f, these are denoted by $P(EC)^\mu E$ and defined by the boxed equations (5).

Note: There's also a mode where the final evaluation is omitted, denoted by **P(EC)$^\mu$**, which, however, is rarely used in practice.

Example: Suppose the predictor is Euler's Method, and the corrector is the Backward Euler Method. Then the corresponding Predictor Corrector Method in **PECE** mode is given by

$$
\boxed{
\begin{aligned}
&\mathbf{P} : y_{n+1}^{[0]} = y_n + h f_n \\
&\mathbf{E} : f_{n+1}^{[0]} = f\left(x_{n+1}, y_{n+1}^{[0]}\right) \\
&\mathbf{C} : y_{n+1} = y_{n+1}^{[1]} = y_n + h f_{n+1}^{[0]} \\
&\mathbf{E} : f_{n+1} = f\left(x_{n+1}, y_{n+1}^{[1]}\right)
\end{aligned}
}
\tag{6}
$$

Note: Thus predictor corrector methods constitute explicit methods in their own right. They do not constitute a particular way of implementing implicit methods (i.e., the corrector). Indeed, since they are explicit methods their stability properties may be quite distinct from those of the corrector.

The Local Truncation Error of Predictor Corrector Methods

The following is a simplified discussion of the local truncation error under the assumption that f is scalar valued, **the orders of the predictor and corrector are the same** (and both denoted by p), and the mode of the predictor corrector method is **PECE**. The discussion is followed by a statement of more general results. A full discussion of the subject can be found in the above mentioned book by Lambert.

For our purposes, by the *local truncation error* **LTE** of the **PECE** method we mean the difference

$$
\boxed{\mathbf{LTE}_{PECE} = y\left(x_{n+k}\right) - y_{n+k}}
\tag{7}
$$

under the *localizing assumption*

$$
\boxed{y_{n+j} = y\left(x_{n+j}\right) \quad j = 0, 1, \cdots, k-1.}
\tag{8}
$$

We also recall the definition of the local truncation error of the predictor and corrector, i.e., using **H.O.T.** to denote *higher order terms* as usual:

$$
\mathbf{LTE}_P = \sum_{j=0}^{k} \alpha_j^* y\left(x_{n+j}\right) - h \sum_{j=0}^{k-1} \beta_j^* y'\left(x_{n+j}\right) = C_{p+1}^* h^{p+1} y^{(p+1)}\left(x_n\right) + \mathbf{H.O.T.}
\tag{9}
$$

and

$$
\mathbf{LTE}_C = \sum_{j=0}^{k} \alpha_j y\left(x_{n+j}\right) - h \sum_{j=0}^{k} \beta_j y'\left(x_{n+j}\right) = C_{p+1} h^{p+1} y^{(p+1)}\left(x_n\right) + \mathbf{H.O.T.}
\tag{10}
$$

Note: The local truncation error as defined here is identical to the error under the localizing assumption for explicit linear multistep methods, and differs only in

higher order terms for implicit liner multistep methods. To see this consider a general (not necessarily implicit) linear multistep method (1) and subtract (10) from (1). If (1) is explicit the statement follows immediately, if it is implicit the statement follows upon applying the mean value theorem and absorbing the term $h\beta_k...$ in the **H.O.T.**, exercise!

Upon subtracting

$$y^{[0]}_{n+k} + \sum_{j=0}^{k-1} \alpha^*_j y_{n+j} - h \sum_{j=0}^{k-1} \beta^*_j f_{n+j} = 0 \qquad (11)$$

from (9) and using (8) we obtain

$$y(x_{n+k}) - y^{[0]}_{n+k} = \mathbf{LTE}_P. \qquad (12)$$

Similarly, subtracting

$$y_{n+k} + \sum_{j=0}^{k-1} \alpha_j y_{n+j} - h \sum_{j=0}^{k-1} \beta_j f_{n+j} - h\beta_k f\left(x_{n+k}, y^{[0]}_{n+k}\right) = 0 \qquad (13)$$

from (10) we obtain

$$\mathbf{LTE}_C = y(x_{n+k}) - y_{n+k} - h\beta_k \left(y'(x_{n+k}) - f\left(x_{n+k}, y^{[0]}_{n+k}\right)\right) =$$

$$= y(x_{n+k}) - y_{n+k} - h\beta_k \left(f(x_{n+k}, y(x_{n+k})) - f\left(x_{n+k}, y^{[0]}_{n+k}\right)\right)$$

$$= y(x_{n+k}) - y_{n+k} - h\beta_k \frac{\partial f}{\partial y}(x_{n+k}, \xi)\left(y(x_{n+k}) - y^{[0]}_{n+k}\right)$$

$$= y(x_{n+k}) - y_{n+k} - h\beta_k \frac{\partial f}{\partial y}(x_{n+k}, \xi)\left(C^*_{p+1} h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.}\right)$$

using (10) again

$$= C_{p+1} h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.}$$

$$(14)$$

Absorbing $h\beta_k \frac{\partial f}{\partial y}(x_{n+k}, \xi) C^*_{p+1} h^{p+1} y^{(p+1)}(x_n)$ in the higher order terms in the final expression of (14) we obtain

$$y(x_{n+k}) - y_{n+k} = C_{p+1} h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.} = \mathbf{LTE}_C + \mathbf{H.O.T.} \qquad (15)$$

The leading term of the local truncation error of the **PECE** *method is therefore the same as that of the corrector alone.*

In general, if P is a predictor of order p^* and C is a corrector of order p, the leading term local truncation error of the $\mathbf{P(EC)^\mu E}$ method is

> **i**   the same as that of the corrector if $\mu > p - p^*$,
>
> **ii** of the same order, but with a different constant,
>   as that of the corrector if $\mu = p - p^*$,
>
> **iii** of order $p^* + \mu < p$ if $\mu < p - p^*$.

$$(16)$$

If you think this was heavy going, the next section will be easier!

Absolute Stability of Predictor Corrector Methods

We proceed as we did for linear multistep methods. Consider the test equation

$$y' = \lambda y \tag{17}$$

where λ is complex. We say that the predictor corrector method is *absolutely stable* for a given $h\lambda$ if all solutions y_n of the test equation (17) with step size h tend to zero as n tends to infinity.

Consider again a PECE method. For the test equation we have

$$f_n = \lambda y_n \tag{18}$$

thus we obtain

$$y_{n+k}^{[0]} = -\sum_{j=0}^{k-1} \left(\alpha_j^* - h\lambda\beta_j^* \right) y_{n+j}. \tag{19}$$

Similarly

$$y_{n+k} = -\sum_{j=0}^{k-1} \left(\alpha_j - h\lambda\beta_j \right) y_{n+j} + h\lambda\beta_k y_{n+k}^{[0]}. \tag{20}$$

Substituting (19) in (20), rearranging, and noting that $\alpha_k^* = 1$, yields

$$\sum_{j=0}^{k} \left(\alpha_j - h\lambda\beta_j + h\lambda\beta_k\left(\alpha_j^* - h\lambda\beta_j^* \right) \right) y_{n+j} = 0. \tag{21}$$

Despite its complicated appearance this is just a homogeneous constant coefficient linear difference equations whose solutions are linear combinations of powers of the roots of its characteristic polynomial. Clearly, this is given by

$$\boxed{\pi_{\mathbf{PECE}}(\xi, h\lambda) = \pi_C(\xi, h\lambda) + h\lambda\beta_k\pi_P(\xi, h\lambda)} \tag{22}$$

where

$$\pi_P(\xi, h\lambda) = \rho_P(\xi) - h\lambda\sigma_P(\xi), \tag{23}$$

$$\pi_C(\xi, h\lambda) = \rho_C(\xi) - h\lambda\sigma_C(\xi), \tag{24}$$

and

$$\begin{aligned}
\rho_P(\xi) &= \sum_{j=0}^{k} \alpha_j^* \xi^j, \\
\sigma_P(\xi) &= \sum_{j=0}^{k-1} \beta_j^* \xi^j, \\
\rho_C(\xi) &= \sum_{j=0}^{k} \alpha_j \xi^j, \\
\sigma_C(\xi) &= \sum_{j=0}^{k} \beta_j \xi^j.
\end{aligned} \tag{25}$$

In general (exercise) we obtain

$$\pi_{\mathbf{P(EC)^\mu E}}(\xi, h\lambda) = \frac{1 - (h\lambda\beta_k)^\mu}{1 - h\lambda\beta_k}\pi_c + (h\lambda\beta_k)^\mu\pi_P \tag{26}$$

Note: As for explicit linear multistep methods, the leading coefficient of the stability polynomial $\pi_{\mathbf{P(EC)^\mu E}}(\xi, h\lambda)$ (which is 1) becomes small relative to some others as $h\lambda$ tends to infinity. As a consequence (at least) one of the roots must tend to infinity and thus become larger than 1. Hence there can be no predictor corrector method whose region of absolute stability includes the entire left half plane. Indeed, no explicit convergent method of any type with an unbounded region of absolute stability has been found.

Milne's Device

Crucial to any adaptive technique is an error estimate. As we have seen several times, these are usually based on the comparison of two different approximations of the same thing. Since predictor corrector methods compute several approximations of $y(x_{n+k})$ they come with their built in error estimate. The exploitation of this fact is called *Milne's Device*. Once again, we consider the case of a **PECE** method and assume that predictor and corrector have the same order p. Modifications of the idea apply to other cases. Recall from our discussion of the local truncation error that

$$y(x_{n+k}) - y_{n+k}^{[0]} = C_{p+1}^* h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.} \tag{27}$$

and

$$y(x_{n+k}) - y_{n+k} = C_{p+1} h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.} \tag{28}$$

Subtracting these equations yields

$$y_{n+k} - y_{n+k}^{[0]} = \left(C_{p+1}^* - C_{p+1}\right) h^{p+1} y^{(p+1)}(x_n) + \mathbf{H.O.T.} \tag{29}$$

Solving for $h^{p+1} y^{(p+1)}(x_n)$ and plugging this into (28) yields

$$y(x_{n+k}) - y_{n+k} = \frac{C_{p+1}}{C_{p+1}^* - C_{p+1}}\left(y_{n+k} - y_{n+k}^{[0]}\right) + \mathbf{H.O.T.}. \tag{30}$$

Ignoring the higher order terms this yields a *computable* estimate of the local error $y(x_{n+k}) - y_{n+k}$ which can be used to decide whether or not a step is accepted, and also can be employed in the selection of the next step size (and order).

Choice of Predictor and Corrector

The linear multistep methods used most widely as predictors and correctors are the Adams-Bashforth and Adams-Moulton methods, respectively.