Numerical Solutions to Differential Equations

Lecture Notes #9 — Predictor-Corrector Methods

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Outline

Implicit Linear Multistep Methods

Suppose we want to solve $y'(t) = f(t, y)$, $y(t_0) = y_0$ by an implicit linear multistep method.

At each step we have to solve the implicit system

$$\mathbf{y_{n+k}} - h\beta_k f(t_{n+k}, \mathbf{y_{n+k}}) = -\sum_{j=0}^{k-1} \alpha_j y_{n+j} + h\sum_{j=0}^{k-1} \beta_j f_{n+j}$$

Usually this is done by the fixed point iteration

$$\mathbf{y}_{\mathbf{n+k}}^{[\nu+1]} = h\beta_k f(t_{n+k}, \mathbf{y}_{\mathbf{n+k}}^{[\nu]}) - \sum_{j=0}^{k-1} \alpha_j y_{n+j} + h\sum_{j=0}^{k-1} \beta_j f_{n+j}$$

where $y_{n+k}^{[0]}$ is arbitrary (but typically y_{n+k-1}).

Fixed Point Iteration for Implicit LMMs

The fixed point iteration*Math 541* converges to the unique solution provided that

$$h < \frac{1}{|\beta_k| L},$$

where L is the Lipschitz constant of f with respect to y, *i.e.*

$$\|f(t,y) - f(t,y+\epsilon)\| \leq L\epsilon, \quad \epsilon > 0.$$

This is usually not very restrictive. In most cases accuracy places tighter constraints on h.

Convergence of Fixed Point Iteration

- Although the fixed point iteration **will converge** for arbitrary starting values $y_{n+k}^{[0]}$, **convergence may be slow** (linear unless we are extremely lucky.)
- Obviously, it would help to have a good initial guess!
- We will obtain the good initial guess from an **explicit** Linear Multistep Method.
- The explicit method is called the **predictor**, and the implicit method the **corrector**. Together they are a **predictor-corrector pair.**

Predictor-Corrector Methods

It is an advantage to have the predictor and corrector to be accurate to the same order.

This usually means the step-number for the explicit predictor is greater than that of the implicit corrector, *e.g.*

$$\begin{array}{ll} (p) & y_{n+2} - y_{n+1} = \frac{h}{2}(3f_{n+1} - f_n) \\ (c) & y_{n+2} - y_{n+1} = \frac{h}{2}(f_{n+2} + f_{n+1}) \end{array}$$

is regarded a PC-method with step-number 2, even though the corrector is a 1-step method (and, as written, it also violates $|\alpha_0| + |\beta_0| \neq 0$, *i.e.* it does not have any term on the n-level).

A General Predictor-Corrector Pair

We write a general k-step PC-method:

$$(p) \qquad \sum_{j=0}^{k} \alpha_j^* y_{n+j} = h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}$$

$$(c) \qquad \sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}$$

We will look at different types of predictor-corrector pairs, initially we will be concerned with predictors of Adams-Bashforth type, and correctors of Adams-Moulton type.

Predictor-Corrector Modes I/IV

Remember:

We are using the predictor to get an initial guess for the fixed point iteration for the corrector method. How many fixed point steps should we take???

[Mode] Correcting to convergence:

In this mode we iterate until

$$\|y_{n+k}^{[\nu+1]} - y_{n+k}^{[\nu]}\| < \epsilon, \quad \text{or} \quad \frac{\|y_{n+k}^{[\nu+1]} - y_{n+k}^{[\nu]}\|}{\|y_{n+k}^{[\nu+1]}\|} < \epsilon,$$

where ϵ usually is of the order of machine-precision (round-off error).

Predictor-Corrector Modes

[Mode] Correcting to convergence:

In this mode the predictor plays a very small role. The local truncation error and the linear stability characteristics of the PC-pair are those of the corrector alone.

This mode is not very attractive since we cannot *a priori* predict how many fixed-point iterations will be needed. In a real-time system (*e.g.* the auto-pilot in an aircraft), this may be dangerous.

Predictor-Corrector Modes III/IV

[Mode] Fixed number of Fixed-Point Corrections:

In this mode we perform a fixed number of FP-iteration at each step — usually 1 or 2.

The local truncation error and the linear stability properties of the PC-method depend both on the predictor and corrector (more complicated analysis — more work for us!)

We will use the following short-hand

P	—	Apply the predictor once
E	—	Evaluate f given t and y
C	—	Apply the corrector once

The methods described above are PEC and P(EC)^2.

Predictor-Corrector Modes IV/IV

At the end of $\mathrm{P(EC)}^2$ we have the values $y_{n+k}^{[2]}$ for y_{n+k} and $f_{n+k}^{[1]}$ for $f(t_{n+k}, y_{n+k})$, sometimes we want to update the value of f by performing a further evaluation $f_{n+k}^{[2]} = f(t_{n+k}, y_{n+k}^{[2]})$; this mode would be described as $\mathrm{P(EC)}^2\mathrm{E}$.

The two classes of modes can be written as

$$\mathrm{P(EC)}^{\mu}\mathrm{E}^{t},\ \mu \geq 1,\ t \in \{0, 1\}.$$

$\mathrm{P(EC)}^{\mu}\mathrm{E}^{t}$

$$P: \quad y_{n+k}^{[0]} = -\sum_{j=0}^{k-1} \alpha_j^* y_{n+j}^{[\mu]} + h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}^{[\mu-1+t]}$$

$$(EC)^{\mu}: \quad \left\{ \begin{array}{rcl} f_{n+k}^{[\nu]} & = & f(t_{n+k}, y_{n+k}^{[\nu]}) \\ y_{n+k}^{[\nu+1]} & = & -\sum_{j=0}^{k-1} \alpha_j y_{n+j}^{[\mu]} + h\beta_k f_{n+k}^{[\nu]} + h \sum_{j=0}^{k-1} \beta_j f_{n+j}^{[\mu-1+t]} \\ & & \nu = 0, 1, \ldots, \mu - 1 \end{array} \right\}$$

$$E^t: \quad f_{n+k}^{[\mu]} = f(t_{n+k}, y_{n+k}^{[\mu]}), \quad \text{if } t = 1.$$

Error Analysis of $\mathrm{P(EC)}^\mu\mathrm{E}^t$ [Lambert 105 – 107]

If the predictor is a p^*-order method and the corrector a p-order method, then (using notationally non-consistent LTEs)

$$
\begin{array}{llcl}
(p) & \mathrm{LTE}^*(h) & = & \mathcal{C}^* h^{p^*+1} y^{(p^*+1)}(\xi^*) + \mathcal{O}(h^{p^*+2}) \\
(c) & \mathrm{LTE}(h) & = & \mathcal{C} h^{p+1} y^{(p+1)}(\xi) + \mathcal{O}(h^{p+2})
\end{array}
$$

The local truncation error for $\mathrm{P(EC)}^\mu\mathrm{E}^t$ is $\mathcal{C}^{**} h^{p^{**}+1}$, where:

(i) if $p^* \geq p$ or ($p^* < p$ and $\mu > p - p^*$), $p^{**} = p$ and $\mathcal{C}^{**} = \mathcal{C} y^{(p+1)}(\xi)$

(ii) if $p^* < p$ and $\mu = p - p^*$, $p^{**} = p$, but $\mathcal{C}^{**} \neq \mathcal{C} y^{(p+1)}(\xi)$

(iii) if $p^* < p$ and $\mu < p - p^*$, $p^{**} = p^* + \mu < p$.

Milne's Error Estimate

If $p^* = p$ it is possible to get an estimate of the leading part of the local truncation error with two subtractions and a multiplication.
— Something for (almost) nothing!

$$\begin{array}{lllll} (p) & \text{LTE}^*(h) & = & \mathcal{C}^* h^{p+1} y^{(p+1)}(t_n) & = & y(t_{n+k}) - y_{n+k}^{[0]} + \mathcal{O}(h^{p+2}) \\ (c) & \text{LTE}(h) & = & \mathcal{C} h^{p+1} y^{(p+1)}(t_n) & = & y(t_{n+k}) - y_{n+k}^{[\mu]} + \mathcal{O}(h^{p+2}) \end{array}$$

Subtraction gives

$$(\mathcal{C}^* - \mathcal{C}) h^{p+1} y^{(p+1)}(t_n) = y_{n+k}^{[\mu]} - y_{n+k}^{[0]} + \mathcal{O}(h^{p+2})$$

Hence (multiply by $\frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}$)

$$\text{LTE}(h) \approx \mathcal{C} h^{p+1} y^{(p+1)}(t_n) = \frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}} \left[y_{n+k}^{[\mu]} - y_{n+k}^{[0]} \right]$$

Local Extrapolation

c.f. Richardson Extrapolation. Math 541

Now that we have an estimate for the error... Why not use that estimate as another correction of the solution?!?

It is really a case of being greedy and trying to eat the cake and still have it. However, local extrapolation (symbol: L) is an accepted feature in many modern codes.

It can be applied in more than one way: $\text{P(ECL)}^{\mu}\text{E}^{t}$, or $\text{P(EC)}^{\mu}\text{LE}^{t}$.

$\text{P(EC)}^{\mu}\text{LE}^{t}$

$$P: \qquad y_{n+k}^{[0]} = -\sum_{j=0}^{k-1} \alpha_j^* y_{n+j}^{[\mu]} + h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}^{[\mu-1+t]}$$

$$(EC)^{\mu}: \quad \left\{ \begin{array}{rcl} f_{n+k}^{[\nu]} & = & f(t_{n+k}, y_{n+k}^{[\nu]}) \\ \\ y_{n+k}^{[\nu+1]} & = & -\displaystyle\sum_{j=0}^{k-1} \alpha_j y_{n+j}^{[\mu]} + h\beta_k f_{n+k}^{[\nu]} + h \sum_{j=0}^{k-1} \beta_j f_{n+j}^{[\mu-1+t]} \\ & & \nu = 0, 1, \dots, \mu - 1 \end{array} \right\}$$

$$L: \qquad y_{n+k}^{[\mu]} \overset{\text{update}}{\longleftarrow} \left[1 + \frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}\right] y_{n+k}^{[\mu]} - \left[\frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}\right] y_{n+k}^{[0]}$$

$$E^t: \qquad f_{n+k}^{[\mu]} = f(t_{n+k}, y_{n+k}^{[\mu]}), \quad \text{if } t = 1.$$

$\mathrm{P(ECL)}^{\mu}\mathrm{E}^{t}$

$$P: \quad y_{n+k}^{[0]} = -\sum_{j=0}^{k-1} \alpha_j^* y_{n+j}^{[\mu]} + h \sum_{j=0}^{k-1} \beta_j^* f_{n+j}^{[\mu-1+t]}$$

$$(ECL)^{\mu}: \quad \left\{ \begin{array}{rcl} f_{n+k}^{[\nu]} & = & f(t_{n+k}, y_{n+k}^{[\nu]}) \\ y_{n+k}^{[\nu+1]} & = & -\sum_{j=0}^{k-1} \alpha_j y_{n+j}^{[\mu]} + h\beta_k f_{n+k}^{[\nu]} + h \sum_{j=0}^{k-1} \beta_j f_{n+j}^{[\mu-1+t]} \\ & & \nu = 0, 1, \dots, \mu - 1 \\ y_{n+k}^{[\nu+1]} & \overset{\text{update}}{\leftarrow} & \left[1 + \frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}\right] y_{n+k}^{[\nu+1]} - \left[\frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}\right] y_{n+k}^{[0]} \end{array} \right\}$$

$$E^t: \quad f_{n+k}^{[\mu]} = f(t_{n+k}, y_{n+k}^{[\mu]}), \quad \text{if } t = 1.$$

Linear Stability Analysis for Predictor-Corrector Methods

By applying our methods to the linear model problem

$$y'(t) = \lambda y(t), \quad y(t_0) = y_0$$

we can again find the region in $\widehat{h} = h\lambda$ space where the method produces non-exponentially growing solutions.

The idea and framework is the same as in our previous cases (LMMs, Runge-Kutta methods), but the algebra involved becomes "somewhat" tedious.

Here, we will summarize some of the key results.

Linear Stability Analysis: Notation

$$\widehat{h} = h\lambda$$

$$H = \widehat{h}\beta_k$$

$$M_\mu(H) = \frac{H^\mu(1-H)}{1-H^\mu}$$

$$W = \frac{\mathcal{C}}{\mathcal{C}^* - \mathcal{C}}$$

Notice:

$$\lim_{\mu\to\infty} M_\mu(H) = 0, \quad \text{when } |H| < 1$$

Some Stability Polynomials

P(EC)$^\mu$: (order $2k$ polynomial)

$$\pi(r,\widehat{h}) = \beta_k r^k \left[\rho(r) - \widehat{h}\sigma(r)\right] + M_\mu(H)\left[\rho^*(r)\sigma(r) - \rho(r)\sigma^*(r)\right]$$

Adding an extra evaluation changes the stability polynomial quite a bit:

P(EC)$^\mu$E: (order k polynomial)

$$\pi(r,\widehat{h}) = \rho(r) - \widehat{h}\sigma(r) + M_\mu(H)\left[\rho^*(r) - \widehat{h}\sigma^*(r)\right]$$

We notice that (in general) the stability polynomials are non-linear in $\widehat{h}$, which means plotting the region of absolute stability $\mathcal{R}_A$ or its boundary, becomes a challenge. [One exception...]

Stability Polynomial in PEC mode

In PEC mode the stability polynomial is linear in $\widehat{h}$:

$$\pi(r,\widehat{h}) = \beta_k r^k \left[\rho(r) - \widehat{h}\sigma(r)\right] + \beta_k \widehat{h}\left[\rho^*(r)\sigma(r) - \rho(r)\sigma^*(r)\right]$$

These are easy to plot, but the regions of stability are not great. — In fact PEC of order k has a smaller stability region than explicit Adams-Bashforth of the same order!

In general we have to solve a non-linear equation to find the roots of $\pi(r,h)$ — using *e.g.* Newton's method[Math 541].

Adding local extrapolation to the picture makes the stability polynomial more "interesting..."

Stability Polynomials with Local Extrapolation

P(ECL)$^\mu$E:

$$\pi(r,\widehat{h}) = (1+W)\left[\rho(r) - \widehat{h}\sigma(r)\right] + [M_\mu(H+WH) - W]\left[\rho^*(r) - \widehat{h}\sigma^*(r)\right]$$

P(ECL)$^\mu$:

$$\begin{aligned}\pi(r,\widehat{h}) &= \beta_k r^k \left\{(1+W)\left[\rho(r) - \widehat{h}\sigma(r)\right] - W\left[\rho^*(r) - \widehat{h}\sigma^*(r)\right]\right\} \\ &\quad + M_\mu(H+WH)\left[\rho^*(r)\sigma(r) - \rho(r)\sigma^*(r)\right]\end{aligned}$$

P(EC)$^\mu$LE:

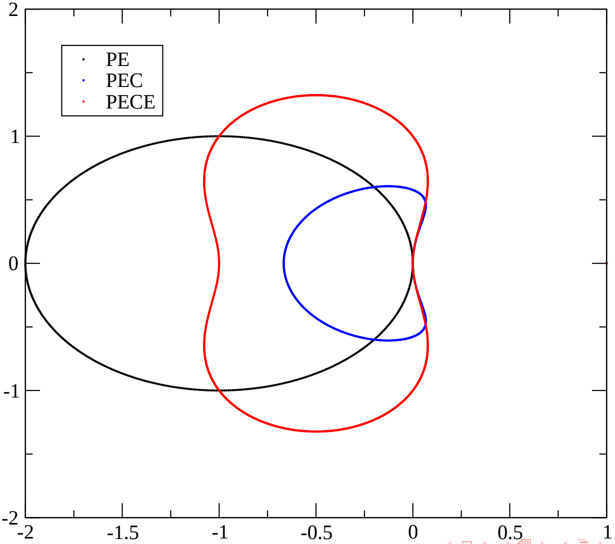
$$\pi(r,\widehat{h}) = (1+W)\left[\rho(r) - \widehat{h}\sigma(r)\right] + [M_\mu(H) + (H-1)W]\left[\rho^*(r) - \widehat{h}\sigma^*(r)\right]$$

P(EC)$^\mu$L:

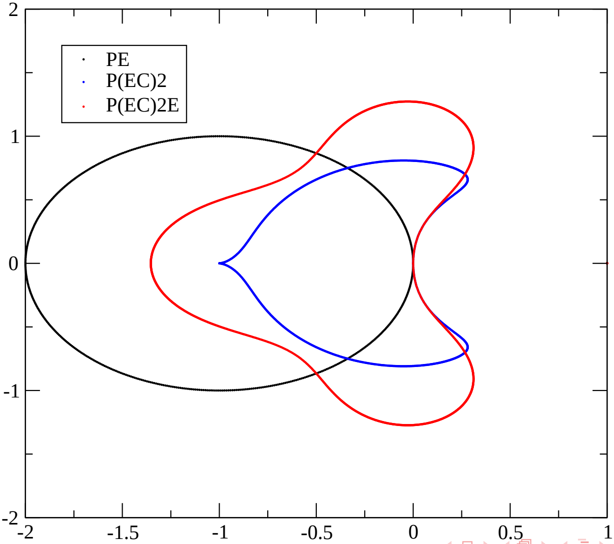
$$\begin{aligned}\pi(r,\widehat{h}) &= \beta_k r^k \left\{(1+W)\left[\rho(r) - \widehat{h}\sigma(r)\right] - W\left[\rho^*(r) - \widehat{h}\sigma^*(r)\right]\right\} \\ &\quad + [M_\mu(H) + HW]\left[\rho^*(r)\sigma(r) - \rho(r)\sigma^*(r)\right]\end{aligned}$$

Stability Regions, PE, PEC, PECE

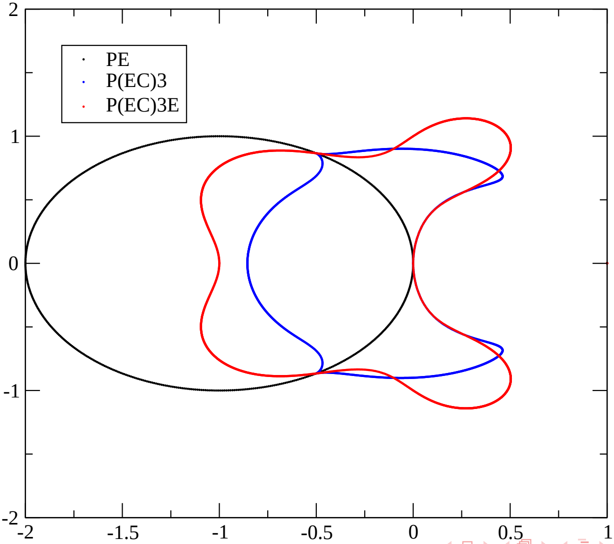
Order $k = 1$



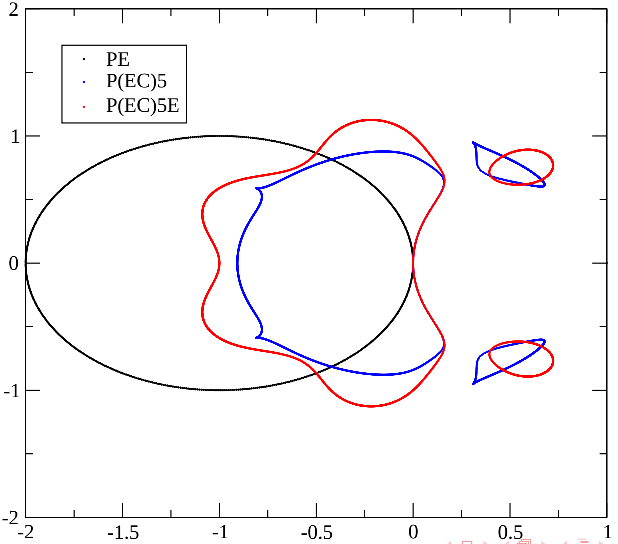
Stability Regions, PE, P(EC)^2, P(EC)^{2}E $k = 1$



Stability Regions, PE, P(EC)^3, P(EC)^{3}E $\quad k = 1$



Stability Regions, PE, P(EC)^5, P(EC)^{5}E $\quad k = 1$



Stability Analysis when $k = 1$

Predictor, $\rho^*(r) = r - 1$, $\sigma^*(r) = 1$, $\mathcal{C}^* = 1/2$

$$y_{n+1} - y_n = hf_n$$

Corrector, $\rho(r) = r - 1$, $\sigma(r) = r$, $\mathcal{C} = -1/2$

$$y_{n+1} - y_n = hf_{n+1}$$

$$H = h, \quad M_\mu = \frac{h^\mu(1-h)}{1-h^\mu}, \quad W = -\frac{1}{2}$$

Stability Analysis when $k = 1$

P(EC)$^\mu$

$$\pi(r,h) = r((r-1) - hr) + \frac{h^\mu(1-h)}{1-h^\mu}((r-1)r - (r-1)1)$$

Multiply through by $1 - h^\mu$ and solve

$$(1-h^\mu)r((r-1) - hr) + h^\mu(1-h)((r-1)r - (r-1)1) = 0$$

$$h^{\mu+2}\left[r^2 - (r-1)^2\right] + h^{\mu+1}\left[(r-1)^2 - r(r-1)\right] - hr^2 + r(r-1) = 0$$

Now we can use matlab's friendly `roots` command to solve for h!

Stability Analysis when $k = 1$

P(EC)$^\mu$E

$$\pi(r,h) = (r-1) - hr + \frac{h^\mu(1-h)}{1-h^\mu}\left[(r-1)-h\right]$$

Multiply through by $1 - h^\mu$ and solve

$$(1-h^\mu)((r-1)-hr) + h^\mu(1-h)\left[(r-1)-h\right] = 0$$
$$h^{\mu+2} - rh + (r-1) = 0$$

Now we can use matlab's friendly `roots` command to solve for h!

Homework #4, Due 3/20/2015

Pick your favorite Adams-Bashforth (P)redictor (order p^*), and Adams-Moulton (C)orrector (order p) methods, and plot the stability regions for

P(ECL)E

P(ECL)^{2}E

P(EC)LE

P(EC)^{2}LE

Note: The problem is least challenging for $p^* = p = 1$...

Project Idea? — Write a piece of code which can plot the stability regions for any PC-method, as described by P(ECL^k)$^\ell$L^{m}E^n, $(k + m \leq 1,\ k,m,n \in \{0,1\})$.