Multivalue Methods (Nordsieck 1962)

A multivalue method is a multistep predictor/corrector in disguise.

General idea: $\vec{y}_n = \begin{pmatrix} y_n \\ hf_n \\ * \\ \vdots \\ * \end{pmatrix}$ } other values of $y, y', y'' \dots$

P: $\vec{y}_n^{(0)} = B \cdot \vec{y}_{n-1}$ $\qquad$ B = constant matrix

produces $y_n^{(0)}$ = predictor for y_n

$f_n^{(0)}$ = predictor for f_n

(not in original multistep method)

repeat as desired:

EC: $\vec{y}_n^{(1)} = \vec{y}_n^{(0)} + \underbrace{h\left[f_n^{(1)} - f_n^{(0)}\right]}_{G(\vec{y}_n^{(0)})} \cdot \vec{c}$

(the evaluation step $f_n^{(1)} = f(x_n, y_n^{(0)})$ happens inside G)

The optional final evaluation step

$$f_n^{(m+1)} = f(x_n, y_n^{(m)})$$

can be written as

$$\vec{y}_n^{(m+1)} = \vec{y}_n^{(m)} + h\left[f_n^{(m+1)} - f_n^{(m)}\right] \cdot \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_{c_2}$$

<u>Example:</u> 3-step AB predictor, 2-step AB corrector

$$y_n^{(0)} = y_{n-1} + \frac{h}{12}\left[23 f_{n-1} - 16 f_{n-2} + 5 f_{n-3}\right]$$

$$y_n^{(1)} = y_{n-1} + \frac{h}{12}\left[5 f_n^{(1)} + 8 f_{n-1} - f_{n-2}\right]$$

choose $\vec{y}_n = \begin{pmatrix} y_n \\ h f_n \\ h f_{n-1} \\ h f_{n-2} \end{pmatrix}$

<u>recall:</u> 3-step AB is based on interpolating f at $x_{n-3}, x_{n-2}, x_{n-1}$. To get $y_n^{(0)}$, we integrate the interpolating polynomial $p(x)$. To get $f_n^{(0)}$, we should simply evaluate p at x_n.

$$p(x) = f_{n-3} + \frac{f_{n-2} - f_{n-3}}{h}(x - x_{n-3}) + \frac{f_{n-1} - 2f_{n-2} + f_{n-3}}{2h^2}(x - x_{n-3})(x - x_{n-2})$$

$$p(x_n) = f_{n-3} + 3(f_{n-2} - f_{n-3}) + 3(f_{n-1} - 2f_{n-2} + f_{n-3})$$

$$= 3 f_{n-1} - 3 f_{n-2} + f_{n-3}$$

P: $$\vec{y}_n^{(0)} = \underbrace{\begin{pmatrix} 1 & \frac{23}{12} & -\frac{16}{12} & \frac{5}{12} \\ 0 & 3 & -3 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}}_{B} \vec{y}_{n-1}$$

EC: $f_n^{(1)} = f(x_n, y_n^{(0)})$

$$y_n^{(1)} = y_{n-1} + \frac{h}{12}\left[5 f_n^{(1)} + 8 f_{n-1} - f_{n-2}\right]$$

$$= \left\{ y_n^{(0)} - \frac{h}{12}\left[23 f_{n-1} - 16 f_{n-2} + 5 f_{n-3}\right] \right\} + \frac{h}{12}\left[5 f_n^{(1)} + 8 f_{n-1} - f_{n-2}\right]$$

$$= \underbrace{y_n^{(0)}}_{} + \underbrace{\frac{5}{12}}_{\substack{\text{first}\\\text{component}\\\text{of } \vec{c}}} \underbrace{h\left[f_n^{(1)} - \underbrace{(3 f_{n-1} - 3 f_{n-2} + f_{n-3})}_{f_n^{(0)}} \right]}_{G(\vec{y}_n^{(0)})}$$

$$h f_n^{(1)} = h f_n^{(0)} + \underbrace{1}_{\substack{\text{second component}\\\text{of } \vec{c} \text{ is always } = 1}} \cdot \underbrace{h\left[f_n^{(1)} - f_n^{(0)} \right]}_{G(\vec{y}_n^{(0)})}$$

The rest are 0, since we don't update values at x_{n-1} or earlier

$$\vec{y}_n^{(1)} = \vec{y}_n^{(0)} + h\left[f_n^{(1)} - f_n^{(0)} \right] \cdot \underbrace{\begin{pmatrix} 5/12 \\ 1 \\ 0 \\ 0 \end{pmatrix}}_{\vec{c}}$$

Now comes the trick: the polynomial $p(x)$ which interpolates f at $x_{n-3}, x_{n-2}, x_{n-1}$ is uniquely described by $f_{n-3}, f_{n-2}, f_{n-1}$, but equally well by $f_{n-1}, f'_{n-1}, f''_{n-1}$.

By rewriting everything in terms of derivatives, we get rid of previous values, and can change the step size easily.

choose $\vec{y_n} = \begin{pmatrix} y_n \\ h f_n \\ h^2/2 \cdot f_n' \\ h^3/6 \cdot f_n'' \end{pmatrix}$

in this case

$$p(x) = f_{n-1} + f_{n-1}'(x - x_{n-1}) + \tfrac{1}{2} f_{n-1}''(x - x_{n-1})^2$$

$$y_n^{(0)} = y_{n-1} + h f_{n-1} + \tfrac{1}{2} h^2 f_{n-1}' + \tfrac{1}{6} h^3 f_{n-1}''$$

$$h f_n^{(0)} = h[\, f_{n-1} + h f_{n-1}' + \tfrac{1}{2} h^2 f_{n-1}'' \,]$$

$$= h f_{n-1} + 2 \cdot \tfrac{h^2}{2} f_{n-1}' + 3 \cdot \tfrac{1}{6} h^3 f_{n-1}''$$

$$\tfrac{1}{2} h^2 f_n'^{(0)} = \tfrac{1}{2} h^2 [\, f_{n-1}' + h f_{n-1}'' \,] = \tfrac{1}{2} h^2 f_{n-1}' + 3 \cdot \tfrac{1}{6} h^3 f_{n-1}''$$

$$\tfrac{1}{6} h^3 f_n''^{(0)} = \tfrac{1}{6} h^3 f_{n-1}''$$

This leads to $B = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

<u>Easier derivation:</u>

$$p(x) = f_{n-1} + f_{n-1}'(x - x_{n-1}) + \tfrac{1}{2} f_{n-1}''(x - x_{n-1})^2$$

$$f_{n-1} = p(x_{n-1}) = f_{n-1}$$

$$f_{n-2} = p(x_{n-2}) = f_{n-1} - h f_{n-1}' + \tfrac{1}{2} h^2 f_{n-1}''$$

$$f_{n-3} = p(x_{n-3}) = f_{n-1} - 2h f_{n-1}' + 2h^2 f_{n-1}''$$

$$\begin{pmatrix} h f_{n-1} \\ h f_{n-2} \\ h f_{n-3} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 1 & -2 & 3 \\ 1 & -4 & 12 \end{pmatrix} \begin{pmatrix} h f_{n-1} \\ h^2/2\, f_{n-1}' \\ h^3/6\, f_{n-1}'' \end{pmatrix}$$

together

$$\begin{pmatrix} y_{n-1} \\ hf_{n-1} \\ hf_{n-2} \\ hf_{n-3} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & -2 & 3 \\ 0 & 1 & -4 & 12 \end{pmatrix}}_{T^{-1}} \begin{pmatrix} y_{n-1} \\ hf_{n-1} \\ \frac{h^2}{2} f'_{n-1} \\ \frac{h^3}{6} f''_{n-1} \end{pmatrix}$$

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 3/4 & -1 & 1/4 \\ 0 & 1/6 & -1/3 & 1/6 \end{pmatrix}$$

previous method: $\vec{y}_n^{(0)} = B \cdot \vec{y}_{n-1}$

new $\vec{y}_n = T \cdot (\text{old } \vec{y}_n)$, so

$$\text{new } \vec{y}_n^{(0)} = \underbrace{\left(T \cdot B \cdot T^{-1}\right)}_{\text{new } B} \underbrace{\left(T \vec{y}_{n-1}\right)}_{\text{new } \vec{y}_{n-1}}$$

we can check:

$$T \cdot \begin{pmatrix} 1 & \frac{23}{12} & -\frac{16}{12} & \frac{5}{12} \\ 0 & 3 & -3 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \cdot T^{-1} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

likewise:

$$\text{new } \vec{c} = T \cdot (\text{old } \vec{c}) = \begin{pmatrix} 5/12 \\ 1 \\ 3/4 \\ 1/6 \end{pmatrix}$$

Here is another method for future reference:

Gear's 3-step backward differentiation formula (stiff method)

$$y_{n+3} = \frac{18}{11} y_{n+2} - \frac{9}{11} y_{n+1} + \frac{2}{11} y_n + \frac{6}{11} f_{n+3}$$

we use again $\vec{y}_n = \begin{pmatrix} y_n \\ h f_n \\ h^2/2 \, f_n' \\ h^3/6 \, f_n'' \end{pmatrix}$, and AB 3-step predictor

then

$$B = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \vec{c} = \begin{pmatrix} 6/11 \\ 1 \\ 6/11 \\ 1/11 \end{pmatrix}$$

Modification For Stiff Methods

As we saw before, stiff ODES require special treatment. Even if you use a method with large region of stability, you can't use predictor-corrector because fixed point iteration does not converge.

Here is one way to fix that:

Forget about the predictor; it is irrelevant here. Consider the corrector

$$\vec{y}_n^{(k+1)} = \vec{y}_n^{(k)} + G(\vec{y}_n^{(k)}) \cdot \vec{c}$$

Notice how all corrections are ~~of the form~~ in direction $\vec{c}$, so

$$\vec{y}_n^{(k)} = \vec{y}_n^{(0)} + \omega_k \cdot \vec{c} \qquad \text{for suitable } \omega_k.$$

Define

$$F(\omega) = G(\vec{y}_n^{(0)} + \omega \cdot \vec{c})$$

then the standard approach corresponds to

$$\omega_0 = 0$$
$$\omega_1 = \omega_0 + F(\omega_0)$$
$$\vdots$$
$$\omega_{k+1} = \omega_k + F(\omega_k)$$

This is fixed point iteration applied to

$$\omega + F(\omega) = \omega$$

Let us solve instead

$$F(\omega) = 0$$

by Newton's method.

$$\omega_{k+1} = \omega_k - \frac{F(\omega_k)}{F'(\omega_k)} = \omega_k + W \cdot F(\omega_k)$$

where $$W = -\frac{1}{F'(\omega_k)} = \frac{-1}{DG \cdot \vec{c}}$$

After retracing the steps, this corresponds to

$$\boxed{\vec{y}_n^{(k+1)} = \vec{y}_n^{(k)} + W \cdot G(\vec{y}_n^{(k)}) \cdot \vec{c}}$$

<u>Example:</u>

In the special case $y' = \lambda y$, for Gear's 3-step method

$$DG \cdot \vec{c} = (h\lambda, -1, 0, 0) \cdot \begin{pmatrix} 6/11 \\ 1 \\ 6/11 \\ 1/11 \end{pmatrix} = \frac{6}{11} h\lambda - 1$$

$$W = \frac{1}{1 - \frac{6}{11} h\lambda}$$