D8.1

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SOLUTIONS

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MAT 3380 - Assignment #8

5.21 Given: $y' = x + \sin y$, $y(0) = 0$, $h = 0.1$

$\therefore f(x, y) = x + \sin y$, $x_0 = 0$, $y_0 = 0$

Apply the Adams - Bashforth - Moulton three-step predictor corrector method:

$$y^p_{n+1} = y^c_n + \frac{h}{12}(23 f^c_n - 16 f^c_{n-1} + 5 f^c_{n-2}), \quad f^c_k = f(x_k, y^c_k)$$
$$y^c_{n+1} = y^c_n + \frac{h}{12}(5 f^p_{n+1} + 8 f^c_n - f^c_{n-1}), \quad f^p_k = f(x_k, y^p_k)$$

In this case, $f^c_k = f(x_k, y^c_k) = x_k + \sin y^c_k$
$f^p_k = f(x_k, y^p_k) = x_k + \sin y^p_k$

$$\Rightarrow y^p_{n+1} = y^c_n + \frac{h}{12}(23(x_n + \sin y^c_n) - 16(x_{n-1} + \sin y^c_{n-1}) + 5(x_{n-2} + \sin y^c_{n-2}))$$
$$y^c_{n+1} = y^c_n + \frac{h}{12}(5(x_{n+1} + \sin y^p_{n+1}) + 8(x_n + \sin y^c_n) - (x_{n-1} + \sin y^c_{n-1}))$$

We use the starting values generated by the 4th-order Runge-Kutta method in exercise 5.12. Namely, we have that

$x_0 = 0$, $y^c_0 = 0$
$x_1 = 0.1$, $y^c_1 = 0.0051708328 4024$
$x_2 = 0.2$, $y^c_2 = 0.0214025222 8767$

Step 1: $x_3 = 0.3$

$$y^p_3 = 0.02140252228767 + \frac{0.1}{12}[23(0.2 + \sin(0.02140252228767)) - 16(0.1 + \sin(0.00517083284024)) + 5(0 + \sin(0))]$$
$$= 0.04981491791636$$

$$y^c_3 = 0.02140252228767 + \frac{0.1}{12}[5(0.3 + \sin(0.04981491791636)) + 8(0.2 + \sin(0.02140252228767)) - (0.1 + \sin(0.00517083284024))]$$
$$= 0.04986092133133$$
$$\doteq \underline{0.049861}$$

By programming the representative calculations as in step 1 into MATLAB, we obtain the following results for steps 2 - 5.

Step 2 : $x_4 = 0.4$

$$y_4^p = 0.091775637212 14$$
$$y_4^c = 0.091623885391158$$
$$\doteq \underline{0.091824}$$

Step 3 : $x_5 = 0.5$

$$y_5^p = 0.14864507506834$$
$$y_5^c = 0.14869230365041$$
$$\doteq \underline{0.148692}$$

Note: the local error estimate at $x_5 = 0.5$ is

$$\text{Error} \approx -\frac{1}{10}\left[y_5^c - y_5^p\right]$$
$$= -\frac{1}{10}\left[0.14869230365041 - 0.14864507506834\right]$$
$$= -4.72285821 \times 10^{-6} = \underline{-5 \times 10^{-6}}$$

5.24 Given: $y' = x + \sin y$, $y(0) = 0$, $h = 0.1$

$\therefore f(x,y) = x + \sin y$, $x_0 = 0$, $y_0 = 0$

Apply the Adams-Bashforth-Moulton four-step predictor-corrector method:

$$y_{n+1}^p = y_n^c + \frac{h}{24}(55 f_n^c - 59 f_{n-1}^c + 37 f_{n-2}^c - 9 f_{n-3}^c), \quad f_k^c = f(x_k, y_k^c)$$
$$y_{n+1}^c = y_n^c + \frac{h}{24}(9 f_{n+1}^p + 19 f_n^c - 5 f_{n-1}^c + f_{n-2}^c), \quad f_k^p = f(x_k, y_k^p)$$

In this case, $f_k^c = f(x_k, y_k^c) = x_k + \sin y_k^c$
$f_k^p = f(x_k, y_k^p) = x_k + \sin y_k^p$

$$\Rightarrow y_{n+1}^p = y_n^c + \frac{h}{24}(55(x_n + \sin y_n^c) - 59(x_{n-1} + \sin y_{n-1}^c) + 37(x_{n-2} + \sin y_{n-2}^c) - 9(x_{n-3} + \sin y_{n-3}^c))$$
$$y_{n+1}^c = y_n^c + \frac{h}{24}(9(x_{n+1} + \sin y_{n+1}^p) + 19(x_n + \sin y_n^c) - 5(x_{n-1} + \sin y_{n-1}^c) + (x_{n-2} + \sin y_{n-2}^c))$$

We use the starting values generated by the 4th-order Runge-Kutta method in exercise 5.12. Namely, we have that

$x_0 = 0$, $y_0^c = 0$
$x_1 = 0.1$, $y_1^c = 0.00517083284024$
$x_2 = 0.2$, $y_2^c = 0.0214025222876 7$
$x_3 = 0.3$, $y_3^c = 0.04985760532776$

Step 1: $x_4 = 0.4$

$$y_4^p = 0.04985760532776 + \frac{0.1}{24}[55(0.3 + \sin(0.04985760532776)) - 59(0.2 + \sin(0.02140252228767)) + 37(0.1 + \sin(0.00517083284024)) - 9(0 + \sin(0))]$$
$$= 0.09181468829498$$
$$y_4^c = 0.04985760532776 + \frac{0.1}{24}[9(0.4 + \sin(0.09181468829498)) + 19(0.3 + \sin(0.04985760532776)) - 5(0.2 + \sin(0.02140252228767)) + (0.2 + \sin(0.00517083284024))]$$
$$= 0.0918169392977 2$$
$$= \underline{0.091817}$$

By programming the representative calculations as in step 1 into MATLAB, we obtain the following results for steps 2 - 5.

Step 2: $x_5 = 0.5$

$$y_5^p = 0.148682583351830$$
$$y_5^c = 0.148681548476189$$
$$\doteq \underline{\underline{0.148682}}$$

Note: the local error estimate at $x_5 = 0.5$ is

$$\text{Error} \approx -\frac{19}{270}(y_5^c - y_5^p)$$
$$= -\frac{19}{270}(0.148681548476189 - 0.148682583351830)$$
$$= 7.281619181 \times 10^{-8}$$
$$\doteq \underline{\underline{7 \times 10^{-8}}}$$

Step 3: $x_6 = 0.6$

$$y_6^p = 0.221969705820449$$
$$y_6^c = 0.221962018190 12$$
$$\doteq \underline{\underline{0.221962}}$$

P10.2.1

$$\begin{aligned} r_{k+1} &= b - Ax_{k+1} \\ &= b - A(x_k + \alpha_{k+1} r_k) \\ &= b - Ax_k - A\alpha_{k+1} r_k \\ &= b - Ax_k - A\frac{r_k^T r_k}{r_k^T A r_k} r_k \end{aligned}$$

But note that r_k is a $n \times 1$ column vector.
So $r_k^T r_k$ is a 1×1 matrix, i.e. a scalar.
Also, $A \in \mathbb{R}^{n \times n} \Rightarrow r_k^T A r_k$ a 1×1 matrix $\Rightarrow r_k^T A r_k$ scalar

$$\begin{aligned} \therefore\ r_{k+1} &= b - Ax_k - \frac{r_k^T r_k}{r_k^T A r_k} A r_k \\ &= r_k - \frac{r_k^T r_k}{r_k^T A r_k} A r_k \quad (\text{by } r_k = b - Ax_k) \end{aligned}$$

$$\begin{aligned} \therefore\ r_k^T r_{k+1} &= r_k^T \left(r_k - \frac{r_k^T r_k}{r_k^T A r_k} A r_k \right) \\ &= r_k^T r_k - \frac{r_k^T r_k}{r_k^T A r_k} r_k^T A r_k \\ &= r_k^T r_k - r_k^T r_k \\ &= 0 \end{aligned}$$

$\therefore$ $r_i^T r_j = 0$ whenever $j = i+1$, as wanted

P10.2.3 We saw in class in general, $\phi(\vec{x}_c + \vec{y})$ has Taylor expansion

$$\phi(x_c + y) = \phi(x_c) + \nabla(\phi(x_c))^T p_k + \frac{1}{2} y^T \nabla^2 \phi(x_c) y$$

Substitute x_c by x_{k-1} and y by $\alpha_k p_k$, we have that

$$\phi(x_{k-1} + \alpha_k p_k) = \phi(x_{k-1}) + \nabla(\phi(x_{k-1}))^T \alpha_k p_k + \frac{1}{2} (\alpha_k p_k)^T \nabla^2(\phi(x_{k-1})) \alpha_k p_k$$

Note that $\nabla \phi(x_{k-1}) = Ax_{k-1} - b$ (this was shown in class)

$$= \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_{k-1,1} \\ \vdots \\ x_{k-1,n} \end{bmatrix} - \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} x_{k-1,1} + a_{12} x_{k-1,2} + \dots + a_{1n} x_{k-1,n} - b_1 \\ \vdots \\ a_{n1} x_{k-1,1} + a_{n2} x_{k-1,2} + \dots + a_{nn} x_{k-1,n} - b_n \end{bmatrix}$$

$$\frac{\partial \nabla \phi(x_{k-1})}{\partial x_l} = \begin{bmatrix} a_{1l} \\ \vdots \\ a_{nl} \end{bmatrix}$$

$$\therefore \nabla^2 \phi(x_{k-1}) = \begin{bmatrix} \frac{\partial \nabla \phi(x_{k-1})}{\partial x_1} & \frac{\partial \nabla \phi(x_{k-1})}{\partial x_2} & \dots & \frac{\partial \nabla \phi(x_{k-1})}{\partial x_n} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$$

$$= A$$

Also, $\alpha_k = \frac{p_k^T r_k}{p_k^T A p_k}$

p_k^T is a $1 \times n$ row vector, and r_k is a $n \times 1$ column vector. So $p_k^T r_k$ is a 1×1 matrix, i.e. scalar. $p_k^T A p_k$ is also a 1×1 matrix (scalar). So α_k is a scalar.

$$\therefore \quad \phi(x_{k-1} + \alpha_k p_k) = \phi(x_{k-1}) + \alpha_k \nabla(\phi(x_{k-1}))^T p_k + \tfrac{1}{2} p_k^T \alpha_k^T A \alpha_k p_k$$
$$= \phi(x_{k-1}) + \alpha_k \nabla(\phi(x_{k-1}))^T p_k + \tfrac{1}{2} \alpha_k^2 p_k^T A p_k$$

(note: $\alpha_k^T = \alpha_k$ since α_k is scalar)

But $-\nabla\phi(x_{k-1}) = b - Ax_{k-1} = r_{k-1}$

$$\therefore \quad \phi(x_{k-1} + \alpha_k p_k) = \phi(x_{k-1}) - \alpha_k r_{k-1}^T p_k + \tfrac{1}{2}\alpha_k^2 p_k^T A p_k$$
$$= \phi(x_{k-1}) - \frac{p_k^T r_{k-1}}{p_k^T A p_k} r_{k-1}^T p_k + \frac{1}{2}\left(\frac{p_k^T r_{k-1}}{p_k^T A p_k}\right)^2 p_k^T A p_k$$
$$= \phi(x_{k-1}) - \frac{p_k^T r_{k-1}}{p_k^T A p_k} (r_{k-1}^T p_k)^T + \frac{1}{2}\frac{(p_k^T r_{k-1})^2}{(p_k^T A p_k)^2} p_k^T A p_k$$

Note: $r_{k-1}^T p_k$ is a scalar $\Rightarrow r_{k-1}^T p_k = (r_{k-1}^T p_k)^T$

$$\therefore \quad \phi(x_{k-1} + \alpha_k p_k) = \phi(x_{k-1}) - \frac{p_k^T r_{k-1}}{p_k^T A p_k}(p_k^T r_{k-1}^{T^T}) + \frac{1}{2}\frac{(p_k^T r_{k-1})^2}{p_k^T A p_k}$$
$$= \phi(x_{k-1}) - \frac{(p_k^T r_{k-1})^2}{p_k^T A p_k} + \frac{1}{2}\frac{(p_k^T r_{k-1})^2}{p_k^T A p_k}$$
$$= \underline{\underline{\phi(x_{k-1}) - \frac{1}{2}\frac{(p_k^T r_{k-1})^2}{p_k^T A p_k}}}, \text{ as wanted}$$