Numerical Analysis Assignment 3

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Course: AMATH 740

Problem 1

Consider the CG method for $A\mathbf{x} = \mathbf{b}$ with A SPD. Show that, in the update formula

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \alpha_k \mathbf{p}_{k-1},$$

CG chooses the step length that minimizes $\phi(\mathbf{x})$ along direction $\mathbf{p}_{k-1}$, as in steepest descent,

$$\frac{\mathrm{d}}{\mathrm{d}\alpha_k}\phi(\mathbf{x}_k(\alpha_k)) = 0.$$

(a) Show that this requires step length

$$\alpha_k = \frac{\mathbf{r}_{k-1}^\intercal \mathbf{p}_{k-1}}{\mathbf{p}_{k-1}^\intercal A \mathbf{p}_{k-1}}$$

(b) Using properties we showed in class for the CG method, show that his α_k equals the α_k used in the CG algorithm:

$$\alpha_k = \frac{\mathbf{r}_{k-1}^\intercal \mathbf{r}_{k-1}}{\mathbf{p}_{k-1}^\intercal A \mathbf{p}_{k-1}}$$

Solution. (a) Let's first recall the following derivative:

$$\frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\phi(\mathbf{x}) = \frac{\mathrm{d}}{\mathrm{d}\mathbf{x}}\left[\frac{1}{2}\mathbf{x}^\intercal A\mathbf{x} - \mathbf{b}^\intercal\mathbf{x} + c\right] = \mathbf{x}^\intercal A - \mathbf{b}^\intercal.$$

With that let's calculate the derivative of ϕ with respect to α_k.

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}\alpha_k}\phi(\mathbf{x}_k(\alpha_k)) &= \phi'(\mathbf{x}_k(\alpha_k))\mathbf{p}_{k-1} \\
&= \phi'(\mathbf{x}_{k-1} + \alpha_k\mathbf{p}_{k-1})\mathbf{p}_{k-1} \\
&= \left[\mathbf{x}_{k-1}^\intercal A + \alpha_k\mathbf{p}_{k-1}^\intercal A - \mathbf{b}^\intercal\right]\mathbf{p}_{k-1} \\
&= \left[-(\mathbf{b} - A\mathbf{x}_{k-1})^\intercal + \alpha_k\mathbf{p}_{k-1}^\intercal A\right]\mathbf{p}_{k-1} \\
&= \left[-\mathbf{r}_{k-1}^\intercal + \alpha_k\mathbf{p}_{k-1}^\intercal A\right]\mathbf{p}_{k-1} \\
&= -\mathbf{r}_{k-1}^\intercal\mathbf{p}_{k-1} + \alpha_k\mathbf{p}_{k-1}^\intercal A\mathbf{p}_{k-1}
\end{aligned}$$

Setting this equal to 0 we can move one term over and divide by the other to obtain

$$\alpha_k = \frac{\mathbf{r}_{k-1}^\intercal \mathbf{p}_{k-1}}{\mathbf{p}_{k-1}^\intercal A \mathbf{p}_{k-1}}$$

(b) First, remember we have $\mathbf{p}_k = \mathbf{r}_k + \beta_k \mathbf{p}_{k-1}$. Also, recall R_k and P_k as defined on page 69 of the courses notes are equal. This means we can write $\mathbf{p}_k$ as a linear combination of of the $\mathbf{r}_i$'s with $i \in \{0, \dots, k\}$.

$$\begin{aligned}
\mathbf{r}_{k-1}^\intercal \mathbf{p}_{k-1} &= \mathbf{r}_{k-1}^\intercal (\mathbf{r}_{k-1} + \beta_{k-1} \mathbf{p}_{k-2}) \\
&= \mathbf{r}_{k-1}^\intercal \mathbf{r}_{k-1} + \beta_{k-1} \mathbf{r}_{k-1}^\intercal \mathbf{p}_{k-2} \\
&= \mathbf{r}_{k-1}^\intercal \mathbf{r}_{k-1} + \beta_{k-1} \mathbf{r}_{k-1}^\intercal \sum_{i=0}^{k-2} a_i \mathbf{r}_i \\
&= \mathbf{r}_{k-1}^\intercal \mathbf{r}_{k-1}
\end{aligned}$$

Where we've used the fact that $\mathbf{r}_i^\intercal \mathbf{r}_j = 0$ when $i \neq j$. Thus we can conclude the above forms of α_k are equivalent.

Problem 2

Write the following third-order ODE as a first-order ODE system:

$$y'''(x) + 3y''(x) - 4y'(x) + 7y(x) = x^2 + 7,$$

and give the system in matrix form.

Solution. Let's first define the following functions:

$$y_1(x) = y(x) \qquad y_2(x) = y'(x) \qquad y_3(x) = y''(x).$$

We then have the following relations between them.

$$y_1'(x) - y_2(x) = 0 \qquad y_2'(x) - y_3(x) = 0.$$

This allows us to construct the following matrix system

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}' = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -7 & 4 & -3 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} - \begin{bmatrix} 0 \\ 0 \\ x^2 + 7 \end{bmatrix}$$

This is equivalent to the above third order ODE.

Problem 3

Consider the Ralston method for ODE $y' = f(x,y)$:

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\left(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\right), \\ y_{n+1} &= y_n + h\left(\frac{1}{4}k_1 + \frac{3}{4}k_2\right). \end{aligned}$$

Show that the local truncation error at x_{n+1} given by $l_{n+1} = \hat{y}(x_{n+1}) - y_{n+1}$, is $\mathcal{O}(h^3)$. (Note: We assume as usual that f and it's derivatives are sufficiently smooth and bounded. The Ralston method is a 2-stage RK method.)

Solution. To begin, let's expand k_2 to order h (we don't need beyond this because it's multiplied by h in the equation for y_{n+1}). Here we use the notation $a \overset{h^n}{=} b$ to mean $a = b + \mathcal{O}(h^n)$.

$$\begin{aligned} k_2 &:= f\left(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\right) \\ &\overset{h^2}{=} f(x_n, y_n) + \frac{2h}{3}f_x(x_n, y_n) + \frac{2hk_1}{3}f_y(x_n, y_n) \\ &\overset{h^2}{=} k_1 + \frac{2h}{3}f_x(x_n, y_n) + \frac{2hk_1}{3}f_y(x_n, y_n) \end{aligned}$$

Now let's expand $\hat{y}(x_{n+1})$ to order h^2.

$$\begin{aligned} \hat{y}(x_{n+1}) &\overset{h^3}{=} \hat{y}(x_n) + h\hat{y}'(x_n) + \frac{h^2}{2}\hat{y}''(x_n) \\ &\overset{h^3}{=} y_n + hf(x_n, y_n) + \frac{h^2}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(x_n, \hat{y}(x_n)) \\ &\overset{h^3}{=} y_n + hf(x_n, y_n) + \frac{h^2}{2}\left[f_x(x_n, \hat{y}(x_n)) + f_y(x_n, \hat{y}(x_n))\hat{y}'(x_n)\right] \\ &\overset{h^3}{=} y_n + hf(x_n, y_n) + \frac{h^2}{2}\left[f_x(x_n, y_n) + f_y(x_n, y_n)f(x_n, y_n)\right] \\ &\overset{h^3}{=} y_n + hk_1 + \frac{h^2}{2}\left[f_x(x_n, y_n) + k_1 f_y(x_n, y_n)\right] \end{aligned}$$

Now let's try and calculate the local truncation error.

$$\begin{aligned} \ell_{n+1} &:= \hat{y}(x_{n+1}) - y_{n+1} \\ &\overset{h^3}{=} y_n + hk_1 + \frac{h^2}{2}\left[f_x(x_n, y_n) + k_1 f_y(x_n, y_n)\right] - y_n - h\left(\frac{1}{4}k_1 + \frac{3}{4}k_2\right) \\ &\overset{h^3}{=} \frac{3}{4}hk_1 + \frac{h^2}{2}\left[f_x(x_n, y_n) + k_1 f_y(x_n, y_n)\right] - \frac{3}{4}hk_2 \\ &\overset{h^3}{=} \frac{3}{4}hk_1 + \frac{h^2}{2}\left[f_x(x_n, y_n) + k_1 f_y(x_n, y_n)\right] - \frac{3}{4}hk_1 - \frac{h^2}{2}f_x(x_n, y_n) - \frac{h^2 k_1}{2}f_y(x_n, y_n) \\ &\overset{h^3}{=} 0 \end{aligned}$$

Thus we can conclude ℓ_{n+1} is $\mathcal{O}\left(h^3\right)$.

Problem 4

Consider numerical method

$$y_{n+1} = y_n + hf(x_n + (1-\eta)h, \eta y_n + (1-\eta)y_{n+1}) \qquad \eta \in [0,1]$$

for $y' = f(x,y)$. Show that the local truncation error $l_{n+1} = \mathcal{O}(h^2)$ for any $\eta \in [0,1]$. Is there a value of η for which $l_{n+1} = \mathcal{O}(h^3)$?
(Note: We assume as usual that f and it's derivatives are sufficiently smooth and bounded.)

Solution. The first thing we will do (which is the thing that took me the longest to figure out), is rewrite the second argument of f.

$$\eta y_n + (1-\eta)y_{n+1} = y_n + (1-\eta)(y_{n+1} - y_n)$$

This allows us to get that pesky η out of our way so we can Taylor expand properly. We'll start by expanding y_{n+1} up to order h^2.

$$\begin{aligned} y_{n+1} &= y_n + hf(x_n + (1-\eta)h, y_n + (1-\eta)(y_{n+1} - y_n)) \\ &\overset{h^3}{=} y_n + h\big[f(x_n, y_n) + f_x(x_n, y_n)(1-\eta)h + f_y(x_n, y_n)(1-\eta)(y_{n+1} - y_n)\big] \end{aligned}$$

Here we use our formula for y_{n+1} and subtract over y_n to obtain an equation for the difference. We know to first order $f(x_n + (1-\eta)h, \eta y_n + (1-\eta)y_{n+1}) = f(x_n, y_n)$ from our above expansion, so we can simply use that since we don't want higher order terms of h.

$$y_{n+1} \overset{h^3}{=} y_n + h\big[f(x_n, y_n) + f_x(x_n, y_n)(1-\eta)h + f_y(x_n, y_n)(1-\eta)hf(x_n, y_n)\big]$$

Now we expand the perfect answer.

$$\begin{aligned} \hat{y}(x_{n+1}) &\overset{h^3}{=} \hat{y}(x_n) + \hat{y}'(x_n)h + \hat{y}''(x_n)\frac{h^2}{2} \\ &\overset{h^3}{=} y_n + f(x_n, y_n)h + \frac{h^2}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(x, y(x))\Big|_{x=x_n} \\ &\overset{h^3}{=} y_n + f(x_n, y_n)h + \frac{h^2}{2}\big(f_x(x_n, y_n) + f_y(x_n, y_n)y'(x_n)\big) \end{aligned}$$

Now we can take their difference.

$$\begin{aligned} \ell_{n+1} &:= \hat{y}(x_{n+1}) - y_{n+1} \\ &\overset{h^3}{=} \frac{h^2}{2}(f_x + f_y f) - f_x(1-\eta)h^2 - f_y f(1-\eta)h^2 \\ &\overset{h^3}{=} \left(\eta - \frac{h^2}{2}\right)(f_x + f_y f) \end{aligned}$$

From here we can see ℓ_{n+1} is always $\mathcal{O}(h^2)$ (because the h^1 terms cancelled out) and when $\eta = \frac{h^2}{2}$, then ℓ_{n+1} is $\mathcal{O}(h^3)$.

Problem 5

You are given the ODE

$$y'(x) = f(x,y)$$

with explicit knowledge of $f(x,y)$ as a function of x and y. Assume that, given the initial condition $y_0 = y(x_0)$, you need a starting value for y_1 at $x_1 = x_0 + h$ that is accurate with order h^4. Find an explicit method for calculating such an accurate starting value y_1, using only evaluations of $f(x,y)$ and it's partial derivatives at x_0. (Hint: as always, Taylor is your best friend.)

Solution. Not much to say here, so let's just get into the calculation.

$$\begin{aligned}
y_1 &= y(x_1) = y(x_0 + h) \\
&\overset{h^4}{=} y(x_0) + hy'(x_0) + \frac{h^2}{2}y''(x_0) + \frac{h^3}{3!}y'''(x_0) \\
&\overset{h^4}{=} y_0 + hf(x_0,y_0) + \frac{h^2}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(x,y(x))\bigg|_{x=x_0} + \frac{h^3}{3!}\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x,y(x))\bigg|_{x=x_0}
\end{aligned}$$

Now let's calculate each of the last two terms separately so we avoid a giant mess.

$$\begin{aligned}
\frac{h^2}{2}\frac{\mathrm{d}}{\mathrm{d}x}f(x,y(x))\bigg|_{x=x_0} &= \frac{h^2}{2}\left[f_x(x_0,y_0) + f_y(x_0,y_0)y'(x_0)\right] \\
&= \frac{h^2}{2}\left[f_x(x_0,y_0) + f_y(x_0,y_0)f(x_0,y_0)\right] \\
\frac{h^3}{3!}\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x,y(x))\bigg|_{x=x_0} &= \frac{h^3}{3!}\big[f_{xx}(x_0,y_0) + f_{yx}(x_0,y_0)f(x_0,y_0) + f_y(x_0,y_0)f_x(x_0,y_0) \\
&\quad + f_{xy}(x_0,y_0)y'(x_0) + f_{yy}(x_0,y_0)f(x_0,y_0)y'(x_0) \\
&\quad + f_y(x_0,y_0)f_y(x_0,y_0)y'(x_0)\big] \\
&= \frac{h^3}{3!}\left[f_{xx} + f_{yx}f + f_yf_x + f_{xy}f + f_{yy}f^2 + f_y^2f\right] \\
&= \frac{h^3}{3!}\left[f_{xx} + 2f_{yx}f + f_yf_x + f_{yy}f^2 + f_y^2f\right]
\end{aligned}$$

Where I've taken away all the function parameters because they're all (x_0, y_0). So, putting this all together we have

$$y_1 \overset{h^4}{=} y_0 + hf + \frac{h^2}{2}\left[f_x + f_yf\right] + \frac{h^3}{3!}\left[f_{xx} + 2f_{yx}f + f_yf_x + f_{yy}f^2 + f_y^2f\right].$$

Problem 6

Find the region D of absolute stability for the backward Euler method

$$y_{n+1} = y_n + hf(x_{n+1}, y_{n+1})$$

in the complex $h\lambda$ plane.
(Note: this is an implicit one-step method, and can be derived similar to the forward Euler method.)

Solution. As per the "test equation" we have

$$\begin{aligned} y_{n+1} &= y_n + hf(x_{n+1}, y_{n+1}) \\ &= y_n + h\lambda y_{n+1} \\ &= \frac{y_n}{1 - h\lambda} \\ &= \frac{y_0}{(1 - h\lambda)^n} \end{aligned}$$

Thus for stability we have

$$1 < |1 - h\lambda|.$$

Thus our region of stability is $D = \{z \in \mathbb{C} \mid \text{Re}(z) < 0\} =: \mathbb{C}_-$.

Problem 7

Consider the Ralston method

$$\begin{aligned} k_1 &= f(x_n, y_n), \\ k_2 &= f\left(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hk_1\right), \\ y_{n+1} &= y_n + h\left(\frac{1}{4}k_1 + \frac{3}{4}k_2\right). \end{aligned}$$

(a) Show that the region D of absolute stability for this method in the complex $h\lambda$ plane is described by the condition

$$\left|1 + h\lambda + h^2\lambda^2/2\right| < 1.$$

(b) Consider this inequality for the case of real $\lambda < 0$, and derive an upper stability bound for the step length h.

Solution. (a) In order to find the region of stability we take the model equation $y'(x) = \lambda y(x)$. This translates into $k_1 = f(x_n, y_n) = \lambda y_n$. In order to start this problem we start by simplifying the k_2 term.

$$\begin{aligned} k_2 &= f\left(x_n + \frac{2}{3}h, y_n + \frac{2}{3}hf(x_n, y_n)\right) \\ &= f\left(x_n + \frac{2}{3}h, y_n + \frac{2}{3}h\lambda y_n\right) \\ &= \lambda\left(y_n + \frac{2}{3}h\lambda y_n\right) \end{aligned}$$

Now we can take a look at the expression for y_{n+1}.

$$\begin{aligned} y_{n+1} &= y_n + h\left(\frac{\lambda y_n}{4} + \frac{3\lambda}{4}\left[y_n + \frac{2}{3}h\lambda y_n\right]\right) \\ &= y_n + h\lambda y_n + \frac{1}{2}h^2\lambda^2 y_n \\ &= \left(1 + h\lambda + \frac{1}{2}h^2\lambda^2\right)y_n \end{aligned}$$

Thus for stability we require

$$\left|1 + h\lambda + \frac{1}{2}h^2\lambda^2\right| < 1.$$

(b) Let $\lambda = -\gamma$ where $\gamma \in \mathbb{R}_{>0}$.

$$\begin{aligned} 1 - h\gamma + \frac{1}{2}h^2\gamma^2 &< 1 \\ -h\gamma + \frac{1}{2}h^2\gamma^2 &< 0 \\ h &< \frac{2}{\lambda} \end{aligned}$$