Scientific Computing Comprehensive Exam - January 2013

Answer all of the following questions. Present a full motivation of your answers. Present a full explanation of the process by which your answers are derived, including any assumptions you make which are not stated in the problem.

1. Write a floating point pseudo code that takes in as input an analytical function f, a point x, and error bound ϵ, and returns the value of the derivative $f'(x)$ with error less than ϵ.

2. Assume you know f and f' at $x_0, x_1 = x_0 + h$. Compute the best approximation method for the value and first derivative at $h/2$. Compute the order of the methods and find the leading order for the error for each method.

3. Assume X is a positive definite symmetric matrix given by

$$X = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}.$$

Let S be the Schur complement of A in X given by

$$S = C - B^T A^{-1} B.$$

Show that both A and S are positive definite.

4. (a) For the following numerical ODE method, show that it is convergent and find the order.

$$y_{n+1} = y_n + \frac{h}{2}(3f_n - f_{n-1}).$$

(b) Consider the following Runge-Kutta method

$$\begin{aligned} y_{n+1} &= y_n + hK_2; \\ K_1 &= f(x_n, y_n); \\ K_2 &= f\left(x_n + \frac{h}{2}, y_n + \frac{h}{2}K_1\right), \end{aligned}$$

apply it to the model problem $y' = \lambda y$, what restriction is necessary on $h\lambda$ in order to have reasonable results? (Write out the equation for $h\lambda$, you don't have to solve it)

5. The general form of an s-stage Runge-Kutta method to solve the ODE system $y' = F(t, y)$ is

$$\begin{aligned} y_{k+1} &= y_k + \sum_{i=1}^{s} w_i K_i, \\ K_i &= hf\left(t_k + \alpha_i h, y_k + \sum_{j=1}^{i-1} \beta_{ij} K_j\right), \end{aligned}$$

where $h = t_{k+1} - t_k$

(a) What are the storage requirements to carry out one step of the general s-stage method?

(b) Discuss the storage benefits of reorganizing the computation as

$$\begin{aligned} & K_1 = y_k \\ & \text{for } i = 1, 2, \ldots, s \\ & \qquad K_2 = A_i K_2 + hf(t_k + \alpha_i h, K_1) \\ & \qquad K_1 = K_1 + B_i K_2 \\ & y_{k+1} = K_1 \end{aligned}$$

, where $A_1 = 0$.

(c) Express coefficients A_i, B_i in terms of w_i, β_{ij}.

6. Find a 2 point Gaussian quadrature for the integral

$$F(s) = \int_0^{\infty} e^{-st} f(t)dt, s > 0.$$

Derive the error expression, its leading order, and how it scales with s as $s \to \infty$.

Problem 6

- Define inner product: $\langle p(t), q(t) \rangle = \int_0^\infty e^{-st} p(t) q(t)\, dt$

- Find orthogonal polynomials. Need quadratic to get two nodes

$B = \{1, t, t^2\}$

$v_1 = 1$

$v_2 = t - \frac{\langle t, 1\rangle}{\langle 1, 1\rangle} \cdot 1 = t - \frac{1}{s}$

$v_3 = t^2 - \frac{\langle t^2, v_2\rangle}{\langle v_2, v_2\rangle} \cdot v_2 - \frac{\langle t^2, 1\rangle}{\langle 1, 1\rangle} \cdot 1 = t^2 - \frac{6-2s}{s} t - \frac{2}{s^2}$

$\langle 1, 1\rangle = \int_0^\infty e^{-st}\, dt = -\frac{1}{s} e^{-st}\Big|_0^\infty = \frac{1}{s}$

$\langle t, 1\rangle = \int_0^\infty t e^{-st}\, dt = -\frac{1}{s} t e^{-st}\Big|_0^\infty + \frac{1}{s}\int_0^\infty e^{-st}\, dt = -\frac{1}{s^2}\left[st e^{-st} + e^{-st}\right]_0^\infty$

$= -\frac{1}{s^2} \lim_{t \to \infty} \left(\frac{t+1}{e^{st}}\right) + \frac{1}{s^2} = 1/s^2$

$\langle t^2, 1\rangle = \int_0^\infty t^2 e^{-st}\, dt = \cancel{-\frac{1}{s} t^2 e^{-st}\Big|_0^\infty}^{\to 0} + \frac{2}{s}\int_0^\infty t e^{-st}\, dt = \frac{2}{s}\left(1/s^2\right) = \frac{2}{s^3}$

$\langle t^2, t - \frac{1}{s}\rangle = \int_0^\infty \left(t^3 - \frac{t^2}{s}\right) e^{-st}\, dt = \int_0^\infty t^3 e^{-st}\, dt - \frac{1}{s}\left(2/s^2\right)$

$= \cancel{-\frac{1}{s} t^3 e^{-st}\Big|_0^\infty}^{\to 0} + \frac{3}{s}\int_0^\infty t^2 e^{-st}\, dt - 2/s^3 = \frac{3}{s}\left(2/s^3\right) - 2/s^3 = \frac{6-2s}{s^4}$

$\langle t - 1/s, t - 1/s\rangle = \int_0^\infty \left(t^2 - \frac{2t}{s} - \frac{1}{s^2}\right) e^{-st}\, dt = \frac{2}{s^3} - \frac{2}{s}\left(1/s^2\right) - \frac{1}{s^2}\left(\frac{1}{s}\right) = -\frac{1}{s^3}$

- Find nodes:

$36 - 24s + 4s^2 + 8 = 4s^2 - 24s + 44$

$$t_{1,2} = \frac{2 - \frac{6}{s} \pm \sqrt{\frac{(6-2s)^2}{s^2} - 4\left(-2/s^2\right)}}{2} = 1 - \frac{3}{s} \pm \frac{1}{s}\sqrt{s^2 - 6s + 11}$$

- Find weights:

$f(t) = 1$: $\int_0^\infty e^{-st}\, dt = \frac{1}{s} = \omega_1 + \omega_2$

$f(t) = t$: $\int_0^\infty t e^{-st}\, dt = 1/s^2 = \omega_1 t_1 + \omega_2 t_2$

} solve for ω_1 and ω_2

Error:

$$E(f) = \int_0^\infty e^{-st} f(t)\,dt - \sum_{i=1}^{2} w_i f(t_i)$$

interpolates: $\{(t_1, f(t_1)), (t_2, f(t_2))\}$

$$= \int_0^\infty e^{-st} f(t)\,dt - \int_0^\infty e^{-st} p(t)\,dt$$

$$= \int_0^\infty e^{-st} \left(f(t) - p(t)\right) dt$$

$$= \int_0^\infty e^{-st} \left(\frac{f'''(\xi)}{3!} \prod_{i=1}^{2} (t - t_i)^2 \right) dt$$

$$= \frac{f'''(\xi)}{6} \underbrace{\int_0^\infty e^{-st} (t-t_1)^2 (t-t_2)^2\,dt}_{I(s)}$$

$I(s)$ is findable via Watson's Lemma

Problem 6

Jan 2013

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt \qquad s > 0$$

1) Find inner prod

$$\langle p, q \rangle = \int_0^\infty p(t) q(t) e^{-st}\, dt$$

2) Construct basis

$$B = \{1, t, t^2\}$$

By G.S. $u_0 = 1$

$$u_1 = t - \frac{\langle 1, t \rangle}{\langle 1, 1 \rangle} \cdot 1 = t - \frac{1}{3}$$

$$u_2 = t - \frac{\langle t^2, u_1 \rangle}{\langle u_1, u_1 \rangle} u_1 - \frac{\langle t^2, 1 \rangle}{\langle 1, 1 \rangle} \cdot 1 = t^2 - \frac{4t}{5} + \frac{2}{5}$$

3) Find roots of u_2

$$t_{1,2} = \frac{2 \pm \sqrt{2}}{5}$$

4) Make weights

$$f(t) = 1: \quad \int_0^\infty e^{-st}\, dt = \frac{1}{s} = w_1 + w_2$$

$$f(t) = t: \quad \int_0^\infty t e^{-st}\, dt = \frac{1}{s^3} = w_1 \left(\frac{2+\sqrt{2}}{5}\right) + w_2 \left(\frac{2-\sqrt{2}}{5}\right)$$

$$w_1 = \frac{2-\sqrt{2}}{4s} \qquad w_2 = \frac{2+\sqrt{2}}{4s}$$

Error:

Interpolates $\{(t_i, f(t_i)), (t_i, f'(t_i)$

$$E(f) = \int_0^\infty e^{-st} f(t)\, dt - \sum_{i=1}^{2} w_i f(t_i) = \int_0^\infty e^{-st} f(t) dt - \int_0^\infty e^{-st} p(t)\, dt$$

$$= \int_0^\infty e^{-st} \left(f(t) - p(t)\right) dt = \int_0^\infty e^{-st} \frac{f'''(\xi)}{6} \underbrace{(t - t_1)^2 (t - t_2)^2}_{\text{Doesn't change signs}} dt$$

$$= \frac{f'''(\eta)}{6} \underbrace{\int_0^\infty e^{-st} (t - t_1)^2 (t - t_2)^2\, dt}_{I(s)}$$

Use Watson's Lemma

$$\underline{I}(s) = \int_0^\infty e^{-st} (t-t_1)^2 (t-t_2)^2 \, dt$$

$\alpha = 0 \qquad \beta = 1 \qquad a_0 = t_1^2 t_2^2$

dependant on s...

$$\Rightarrow E(f,s) \sim \frac{f'''(\eta)\, t_1^2 t_2^2}{6s}$$