SciComp Practice Exam 5/12/14

*Answer the following questions explaining all steps that lead to a solution. Results presented without motivation will **not** receive any credit.*

1. Approximate $I = \int_0^1 \log(x) \sin(x^2/100)\, \mathrm{d}x$ to a relative error $\varepsilon = 10^{-4}$.

Solution. Construct a Gauss quadrature formula for integrals of form

$$I = \int_0^1 \log(x)\, f(x)\, \mathrm{d}x = \sum_{i=1}^{n} w_i\, f(x_i) + e_n.$$

For $f(x) = \sin(x^2/100)$ and $x \in [0, 1]$, Taylor-series expansion gives $f(x) \cong (x/10)^2 + \mathcal{O}((x/10)^6)$ so Gauss quadrature with $n = 2$, exact for quadratics will have $|e_n| < 10^{-6}$. The evaluation nodes x_1, x_2 are roots of $p_2(x)$ from the orthogonal polynomial set $\{p_0(x),\ p_1(x),\ p_2(x)\}$, obtained by applying the Gram-Schmidt algorithm to $\{1, x, x^2\}$ with scalar product

$$(u, v) = -\int_0^1 \log(x)\, u(x)\, v(x)\, \mathrm{d}x,$$

and associated norm $\|u\| = (u, u)^{1/2}$. Compute:

$$-\int_0^1 \log(x)\, x^k\, \mathrm{d}x = \frac{1}{(k+1)^2},$$

arising in application of Gram-Schmidt

$$p_0(x) = 1/(1,1)^{1/2} = 1.$$

$$q_1(x) = x - (x, p_0)\, p_0(x) = x - 1/4.$$

$$p_1(x) = q_1(x)/\|q\| = 144(x - 1/4)/7$$

$$q_2(x) = x^2 - (x^2, p_0)p_0(x) - (x^2, p_1)p_1(x)$$

The polynomial $p_2(x) = q_2(x)/\|q_2\|$ has same roots x_1, x_2 as $q_2(x)$. The weights w_1, w_2 are determined by imposing exact quadrature results for integrands $1, x$

$$\int_0^1 \log(x)\, \mathrm{d}x = -1 = w_1 + w_2$$

$$\int_0^1 \log(x) x\, \mathrm{d}x = -\frac{1}{4} = w_1\, x_1 + w_2\, x_2.$$

2. Assume the real-valued sequence $\{x_n\}_{n \in \mathbb{N}}$ exhibits first-order convergence to $a \in \mathbb{R}$.

   a) What is the limit of the sequence

$$y_n = \frac{x_n\, x_{n+2} - x_{n+1}^2}{x_{n+2} - 2x_{n+1} + x_n}\ ?$$

   b) At what rate does $\{y_n\}_{n \in \mathbb{N}}$ converge?

Solution. Change origin to make $a=0$ and simplify calculations. First-order convergence $x_n \to 0$ as $n \to \infty$ implies

$$\lim_{n \to \infty} \frac{|x_{n+1}|}{|x_n|} = C \in (0,1)$$

Assume $x_n > 0$, such that $x_{n+2} \cong C x_{n+1} \cong C^2 x_n$, for large enough n

$$y_n \to \frac{(C^2 - C^2) x_n^2}{(C^2 - 2C + 1)\, x_n} = 0,$$

so y_n sequence has the same limit. Consider now second-order terms $x_{n+2} \cong C x_{n+1} + D x_{n+1}^2$

$$y_n = \frac{x_n\,[C(C x_n + D x_n^2) + D\,(C x_n + D x_n^2)^2] - (C x_n + D x_n^2)^2}{C(C x_n + D x_n^2) + D\,(C x_n + D x_n^2)^2_{n+1} - 2\,(C x_n + D x_n^2) + x_n} = \frac{CD}{C-1} x_n^2 + \mathcal{O}(x_n^3),$$

showing that y_n exhibits second-order convergence.

3. Find the best approximation of $\sqrt{x}$ by a first-degree polynomial on the interval $[0,1]$.

Solution. Introduce the error $e(x;a,b) = a x + b - \sqrt{x}$, and consider the p-norms for functions $f\colon [0,1] \to \mathbb{R}$

$$\|f\|_p = \left(\int_0^1 |f(x)|^p \, \mathrm{d}x \right)^{1/p}.$$

Interpret "best approximation" to mean minimal 2-norm

$$\min_{a,b \in \mathbb{R}} \|e\|_2.$$

(Note: choice of a specific norm when nothing is specified in the problem is fine. It is not acceptable however to choose a set of discrete points $x_0, \ldots, x_n$ since the problem specifically requests a best approximation over the *interval* $[0,1]$.)

Compute

$$g(a,b) = \|e\|_2^2 = \left(\int_0^1 (a x + b - \sqrt{x})^2 \, \mathrm{d}x \right) = \frac{a^2}{3} + a\left(b - \frac{4}{5}\right) - \frac{4b}{3} + b^2 + \frac{1}{2}$$

and seek minima by solving

$$\frac{\partial g}{\partial a} = \frac{2a}{3} + b - \frac{4}{5} = 0, \quad \frac{\partial g}{\partial b} = a + 2b - \frac{4}{3} = 0$$

with solution $a = 4/5$, $b = 4/15$.

4. Approximate $x(1/2)$ to relative error $\varepsilon = 10^{-3}$ with $x(t)$ solution of the two-point boundary value problem

$$\begin{array}{l} x'' + 2x' + 10x = 0 \\ x(0) = 1, x(1) = 2 \end{array}.$$

Solution. The characteristic equation of the ODE is $r^2 + 2r + 10 = 0$, with roots $r_{1,2} = -1 \pm 3i$, so the solution has form

$$x(t) = e^{-t}(a \cos 3t + b \sin 3t).$$

Boundary conditions give

$$1 = a, 2 = e^{-1}(\cos 3 + b \sin 3) \Rightarrow b = (2e - \cos 3)/\sin 3$$

so

$$x\left(\frac{1}{2}\right) = e^{-1/2}\left(\cos\frac{3}{2} + \frac{2e - \cos 3}{\sin 3}\sin\frac{3}{2}\right)$$

Euler's number is $e = 2.71828$. Construct a numerical approximation of $e^{-1/2}$ by applying Newton's method to

$$f(z) = 1/z^2 - e = 0,\ f'(z) = -2/z^3$$

$$z_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)} = z_n + \frac{z_n^3}{2}\left(\frac{1}{z_n^2} - e\right) = (3 - e z_n^2)\frac{z_n}{2}.$$

Start from $z_0 = 1/1.6 = 0.625$ (since $1.6^2 = 2.56$), giving $z_1 = 0.60568$, $z_2 = 0.6065 \cong e^{-1/2}$. Next,

$$\sin\frac{3}{2} = \sin\left(\frac{\pi}{2} - 0.0708\right) = \cos(0.0708) \cong 1 - \frac{0.0708^2}{2} \cong 0.9975$$

$$\cos\frac{3}{2} = \cos\left(\frac{\pi}{2} - 0.0708\right) = \sin(0.0708) \cong 0.0708$$

$$\sin 3 = 2\sin\frac{3}{2}\cos\frac{3}{2} \cong 0.141$$

$$\cos 3 = \cos^2\frac{3}{2} - \sin^2\frac{3}{2} \cong -0.99$$

Using these numerical approximations

$$x\left(\frac{1}{2}\right) = 0.6065\left[0.0708 + \frac{2 \times 2.71828 + 0.99}{0.141}0.9975\right] \cong 27.62$$

5. Consider the Cholesky factorization $A = LL^T$ of $A \in \mathbb{R}^{m \times m}$, symmetric positive definite. Given L write the pseudocode to compute A with minimal use of computational resources (memory, floating point operations). Specify the algorithm complexity.

Solution. Start from matrix multiplication formula

$$a_{i,j} = \sum_{k=1}^{m} l_{i,k} l_{j,k}$$

and use $l_{i,k} = 0$ for $k > i$, $l_{j,k} = 0$ for $k > j$ to obtain

$$a_{i,j} = \sum_{k=1}^{\min(i,j)} l_{i,k} l_{j,k}$$

It is possible to return A by overwriting L, hence no additional memory is required

Algorithm

```
for i = 1 to m
  for j = i downto 1
    n = min(i, j)
    s = 0
    for k = 1 to n
      s = s + l_{i,k} l_{j,k}
    l_{i,j} = s
return L
```

Memory: $1+2+\ldots+m = m(m+1)/2 = \mathcal{O}(m^2/2)$ locations

Floating point ops (count along principal minors): $\frac{1}{2}\sum_{k=1}^{m} (2k-1)\,k = \mathcal{O}(m^3/6)$.

6. Determine the condition number of the algorithm

$$x \rightarrow \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Solution. Assume $f\colon \mathbb{R} \rightarrow \mathbb{R}$, $f \in C^3(\mathbb{R})$. The (relative) condition number is defined as

$$\kappa = \frac{|\delta F|}{|\delta x|} \frac{|x|}{|F(x)|}$$

with

$$F(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Compute

$$\delta F = F(x+\delta x) - F(x) = \frac{f(x+\delta x+h) - 2f(x+\delta x) + f(x+\delta x-h)}{h^2} - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Taylor series expand and keep $\mathcal{O}(\delta x)$ terms

$$\delta F = \frac{f'(x+h) - 2f'(x) + f'(x-h)}{h^2}\,\delta x,$$

to obtain condition number

$$\kappa = \left| \frac{f'(x+h) - 2f'(x) + f'(x-h)}{f(x+h) - 2f(x) + f(x-h)} \right| |x|.$$

For small h, $\kappa = |x\,f'''(x)/f''(x)|$.