Final Honour School of Mathematics Part A

A7 Numerical Analysis
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1. Let $f \in C^{n+1}([x_0, x_n], \mathbb{R})$ be a function with $(n+1)$ continuous derivatives and with given function values $f(x_i) = f_i$ at $n+1$ points $x_0 < x_1 < \cdots < x_n$.

   (a) [6 marks] Write down the Lagrange interpolating polynomial $p_n(x)$ of degree n for f at the given nodes x_i, and prove that for each $x \in [x_0, x_n]$ there exists $\xi(x) \in (x_0, x_n)$ such that the following error formula holds,

$$e_n(x) := f(x) - p_n(x) = (x - x_0)(x - x_1)\dots(x - x_n)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}.$$

Answer: [Book work] $p_n(x) = \sum_{k=0}^{n} f_k L_{n,k}(x)$, where

$$L_{n,k}(x) = \frac{(x - x_0)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)}{(x_k - x_0)\cdots(x_k - x_{k-1})(x_k - x_{k+1})\cdots(x_k - x_n)} \quad \text{[1 mark]}.$$

The error formula is trivial for $x = x_i$, as $e_n(x) = 0$ by construction. Let $x \notin \{x_0, \dots, x_n\}$, and define

$$\phi(t) := e_n(t) - \frac{e_n(x)}{\pi(x)}\pi(t),$$

where

$$\begin{aligned}\pi(t) &:= (t - x_0)(t - x_1)\cdots(t - x_n) \\ &= t^{n+1} - \left(\sum_{i=0}^{n} x_i\right) t^n + \dots (-1)^{n+1} x_0 x_1 \dots x_n \in \Pi_{n+1} \quad \text{[2 marks]}.\end{aligned}$$

By construction, ϕ vanishes at the $n+2$ points x and x_i $(i = 0, \dots, n)$. Therefore, ϕ' vanishes at $n+1$ points $\xi_0, \dots, \xi_n$ between these points, ϕ'' vanishes at n points between these new points, and so on until $\phi^{(n+1)}$ vanishes at an (unknown) point $\xi = \xi(x)$ in (x_0, x_n) [1 mark]. But

$$\phi^{(n+1)}(t) = e_n^{(n+1)}(t) - \frac{e_n(x)}{\pi(x)}\pi^{(n+1)}(t) = f^{(n+1)}(t) - \frac{e_n(x)}{\pi(x)}(n+1)!,$$

since $p_n^{(n+1)}(t) \equiv 0$ and because $\pi(t)$ is a monic polynomial of degree $n+1$. The result follows immediately from this identity since $\phi^{(n+1)}(\xi) = 0$ [2 marks].

   (b) [6 marks] Derive Simpsons Rule as a special case of Newton-Cotes quadrature.

Answer: [Adaptation of a known technique to a new example] Let x_0, x_1, x_2 be equally spaced points, i.e., $x_0 = x_1 - h$ and $x_2 = x_1 + h$, and let

$$\begin{aligned}p_2(x) &= \sum_{k=0}^{2} f(x_k) L_{2,k}(x) \\ &= f(x_0)\frac{(x - x_1)(x - x_1 - h)}{2h^2} - f(x_1)\frac{(x - x_1 + h)(x - x_1 - h)}{h^2} + f(x_2)\frac{(x - x_1 + h)(x - x_1)}{2h^2}\end{aligned}$$

be the Lagrange interpolating polynomial of degree 2 [2 marks]. Newton-Cotes approximates the integral $\int_{x_0}^{x_2} f(x)\mathrm{d}x$ by

$$
\begin{aligned}
\int_{x_0}^{x_2} p_2(x)\mathrm{d}x &= \sum_{k=0}^{2} f(x_k)\int_{x_0}^{x_2} L_{2,k}\mathrm{d}x \\
&= \frac{1}{2h^2}\left(f(x_0)\int_{-h}^{h} x(x-h)\mathrm{d}x - 2f(x_1)\int_{-h}^{h}(x+h)(x-h)\mathrm{d}x + f(x_2)\int_{-h}^{h}(x+h)x\mathrm{d}x\right) \\
&= \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right) \quad \text{[4 marks]}.
\end{aligned}
$$

(c) [6 marks] Derive an error estimate of Simpsons Rule from the approximation error of the Lagrange interpolating polynomial of degree 2. What is the degree of accuracy of Simpsons Rule?

Answer: [Adaptation of book work]

$$
\begin{aligned}
\left|\int_{x_0}^{x_2} f(x)\mathrm{d}x - \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right)\right| &= \left|\int_{x_0}^{x_2} f(x)-p_2(x)\mathrm{d}x\right| \\
&\leqslant \int_{x_0}^{x_2} |e_2(x)|\,\mathrm{d}x = \int_{-h}^{h}\left|(x+h)x(x-h)\frac{f^{(3)}(\xi(x))}{3!}\right|\mathrm{d}x \\
&= \left|\frac{f^{(3)}(\xi)}{6}\right|\frac{h^4}{2}, \quad \text{[4 marks]}
\end{aligned}
$$

for some $\xi \in (x_0, x_2)$, by the Integral Mean Value Theorem, which shows that Simpson's Rule is exact for polynomials of degree 2, as their third derivative vanishes [1 mark]. However, the refined theory developed in lectures shows that the degree of accuracy of Newton-Cotes integration is in fact $n+1$, that is, Simpson's rule is exact for polynomials of degree 3 [1 mark].

(d) [7 marks] Recall that Gauss-Chebychev Quadrature is defined with respect to Chebychev polynomials, which are orthogonal with respect to inner product defined on $L^2_w(-1,1)$ with weight function $w(x) = 1/\sqrt{1-x^2}$. Derive the Gauss-Chebychev Quadrature rule for the Chebychev polynomial of degree 3,

$$\phi_3(x) = 4x^3 - 3x.$$

What is the degree of accuracy of this formula? [*Hint: You may use the fact that* $\mathrm{d}/\mathrm{d}x \arcsin x = 1/\sqrt{1-x^2}$].

Answer: [New, though application of a known technique] The roots of ϕ_3 are $x_0 = -\sqrt{3}/2$, $x_1 = 0$, $x_2 = \sqrt{3}/2$ [1 mark]. The Gauss-Chebychev quadrature formula is

$$\int_{-1}^{1}\frac{f(x)}{\sqrt{1-x^2}}\mathrm{d}x \approx \sum_{k=0}^{2} w_k f(x_k),$$

where

$$w_k = \int_{-1}^{1}\frac{L_{2,k}(x)}{\sqrt{1-x^2}}\mathrm{d}x. \quad \text{[1 mark]}$$

Thus, the quadrature formula is given by

$$\begin{aligned}\int_{-1}^{1} \frac{f(x)}{\sqrt{1-x^2}}\mathrm{d}x \approx &= \frac{2}{3}\Big(f(x_0)\left[\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\mathrm{d}x - \frac{\sqrt{3}}{2}\int_{-1}^{1}\frac{x}{\sqrt{1-x^2}}\mathrm{d}x\right] \\ &\quad - 2f(x_1)\left[\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\mathrm{d}x - \frac{3}{4}\int_{-1}^{1}\frac{1}{\sqrt{1-x^2}}\mathrm{d}x\right] + f(x_2)\left[\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\mathrm{d}x + \frac{\sqrt{3}}{2}\int_{-1}^{1}\frac{x}{\sqrt{1-x^2}}\mathrm{d}x\right]\Big) \\ &= \frac{2}{3}\left(f(x_0)\frac{\pi}{2} - 2f(x_1)\left[\frac{\pi}{2} - \frac{3\pi}{2}\right] + f(x_2)\frac{\pi}{2}\right) \\ &= \frac{\pi}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right),\end{aligned}$$

where we used

$$\begin{aligned}\int_{-1}^{1} \frac{x^2}{\sqrt{1-x^2}}\mathrm{d}x &\overset{\text{(integration by parts)}}{=} 0 + \int_{-1}^{1}\sqrt{1-x^2}\mathrm{d}x \overset{\text{(substitute } x=\sin t)}{=} \frac{\pi}{2}, \\ \int_{-1}^{1} \frac{x}{\sqrt{1-x^2}}\mathrm{d}x &\overset{\text{(by symmetry)}}{=} 0, \\ \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}}\mathrm{d}x &\overset{\text{(use hint)}}{=} \arcsin x\Big|_{-1}^{1} = \pi.\end{aligned}$$ [4 marks]

In lectures we proved that the degree of accuracy of Gauss Quadature is $2n+1$ when a $(n+1)$-th degree orthogonal polynomial is used, that is the degree of accuracy is 5 in our case. In other words, if f is a polynomial of degree 5, then the Gauss-Chebychev formula is exact [1 mark].

2. (a) [5 marks] Define the notion of a norm $\|\cdot\|$ on a real vector space V. Define the notion of an inner product $\langle\cdot,\cdot\rangle$ on V, and prove that $\|u\| := \langle u,u\rangle^{1/2}$ defines a norm on V, the *inner product norm*. If you use the Cauchy-Schwartz inequality, you need to prove its validity.

Answer: [Book work] A mapping $\|\cdot\| : V \to \mathbb{R}$ is a norm on V if it satisfies

i) $\|u\| \geqslant 0$ for all $u \in V$, with $\|u\| = 0$ if and only if $u = 0 \in V$,

ii) $\|\lambda u\| = |\lambda|\|u\|$ for all $\lambda \in \mathbb{R}$ and all $u \in V$,

iii) $\|u+v\| \leqslant \|u\| + \|v\|$ for all $u, v \in V$. [1 mark]

A mapping $\langle\cdot,\cdot\rangle : V \times V \to \mathbb{R}$ is an inner product if it satisfies

I) $\langle u,u\rangle \geqslant 0$ for all $u \in V$ and $\langle u,u\rangle = 0$ if, and only if $u = 0$,

II) $\langle u,v\rangle = \langle v,u\rangle$ for all $u, v \in V$,

III) $\langle \alpha u + \beta v, z\rangle = \alpha\langle u,z\rangle + \beta\langle v,z\rangle$ for all $u,v,z \in V$ and all $\alpha,\beta \in \mathbb{R}$. [1 mark]

Now let $\|u\| := \langle u,u\rangle^{1/2}$. Then I) implies property i), and

$$\|\lambda u\|^2 \overset{\text{III)}}{=} \lambda\langle u, \lambda u\rangle \overset{\text{II)}}{=} \lambda\langle \lambda u, u\rangle \overset{\text{III)}}{=} \lambda^2\|u\|^2$$

implies property ii) [1 mark]. Finally,

$$\|u+v\|^2 = \langle u+v, u+v\rangle \overset{\text{II),III)}}{=} \|u\|^2 + 2\langle u,v\rangle + \|v\|^2 \overset{\text{C.S.}}{\leqslant} \|u\|^2 + 2\|u\|\|v\| + \|v\|^2 = (\|u\|+\|v\|)^2$$

implies property iii) [1 mark], where the Cauchy-Schwartz Inequality (C.S.) is proven as follows: For every $\lambda > 0$,

$$0 \leqslant \langle u - \lambda v, u - \lambda v\rangle = \|u\|^2 - 2\lambda\langle u,v\rangle + \lambda^2\|v\|^2 =: \phi(\lambda),$$

which is a quadratic function in λ and takes its minimiser at $\lambda^* = \langle u,v\rangle/\|v\|^2$. The C.S.-Inequality now follows from $\phi(\lambda^*) \geqslant 0$ [1 mark].

(b) [5 marks] Prove that any inner product norm $\|u\| := \langle u, u\rangle^{1/2}$ satisfies the *parallelogram law*

$$2\|u\|^2 + 2\|v\|^2 = \|u+v\|^2 + \|u-v\|^2, \qquad \forall\, u, v \in V. \tag{1}$$

Hence, or otherwise, prove that the L_1 norm on $V = C([0,1])$ is not an inner product norm.

Answer: [New but elementary]

$$\begin{aligned}\|u+v\|^2 + \|u-v\|^2 &= \langle u+v, u+v\rangle + \langle u-v, u-v\rangle \\ &= \langle u,u\rangle + 2\langle u,v\rangle + \langle v,v\rangle + \langle u,u\rangle - 2\langle u,v\rangle + \langle v,v\rangle \\ &= 2\|u\|^2 + 2\|v\|^2. \quad \text{[3 marks]}\end{aligned}$$

Let

$$f(x) = \begin{cases} 1, & (x \in [0,1/2]), \\ 0, & (x \in (1/2,1]) \end{cases} \qquad g(x) = \begin{cases} 0, & (x \in [0,1/2]), \\ 1, & (x \in (1/2,1]). \end{cases}$$

Then $h(x) := f(x) + g(x) \equiv 1$ and $\ell(x) := f(x) - g(x) = 1$ for $x \in [0,1/2]$ and $\ell(x) = -1$ for $x \in (1/2,1]$. We have

$$\begin{aligned}\|f+g\|_{L_1}^2 + \|f-g\|_{L_1}^2 &= \|h\|_{L_1}^2 + \|\ell\|_{L_1}^2 = 1 + 1 \\ &\neq \frac{1}{2} + \frac{1}{2} = 2\|f\|_{L_1}^2 + 2\|g\|_{L_1}^2.\end{aligned}$$

The L_1-norm does not satisfy the parallelogram law, and hence it cannot be induced by an inner product [2 marks].

(c) [7 marks] Let $\{\phi_0, \phi_1, \dots\}$ be a set of orthogonal polynomials with respect to some inner product $\langle\cdot,\cdot\rangle$, and such that $\phi_k(x)$ is of exact degree k ($k = 0, 1, \dots$). Prove that there exist sequences of real numbers $(\alpha_k)_{k=1}^\infty$, $(\beta_k)_{k=1}^\infty$ and $(\gamma_k)_{k=1}^\infty$ such that the following three-term recursion holds,

$$\phi_{k+1}(x) = \alpha_k(x - \beta_k)\phi_k(x) - \gamma_k\phi_{k-1}(x), \quad (k = 1, 2, \dots). \tag{2}$$

Answer: [Book work] Since $x\phi_k \in \Pi_{k+1}$ and $\{\phi_0, \phi_1, \dots, \phi_{k+1}\}$ is a basis for Π_{k+1}, there exist $\sigma_{k,0}, \sigma_{k,1}, \dots, \sigma_{k,k+1}$ in $\mathbb{R}$ such that

$$x\phi_k(x) = \sum_{i=0}^{k+1} \sigma_{k,i}\phi_i(x). \quad \text{[1 mark]} \tag{3}$$

Using $x\phi_j \in \Pi_{k-1}$ for $j \leqslant k-2$, which implies $\langle x\phi_k, \phi_j\rangle = \langle \phi_k(x), x\phi_j(x)\rangle = 0$ [1 mark], we take inner products on both sides of (3) with ϕ_j and find that for $j \leqslant k-2$,

$$0 = \langle x\phi_k, \phi_j\rangle = \left\langle \sum_{i=0}^{k+1} \sigma_{k,i}\phi_i, \phi_j \right\rangle = \sum_{i=0}^{k+1} \sigma_{k,i}\langle \phi_i, \phi_j\rangle = \sigma_{k,j}\langle \phi_j, \phi_j\rangle. \quad \text{[2 mark]}$$

Hence, $\sigma_{k,j} = 0$ for $j \leqslant k-2$, so that (3) becomes

$$x\phi_k(x) = \sigma_{k,k+1}\phi_{k+1}(x) + \sigma_{k,k}\phi_k(x) + \sigma_{k,k-1}\phi_{k-1}(x). \quad \text{[2 marks]}$$

Since $x\phi_k$ is of exact degree $k+1$, we must have $\sigma_{k,k+1} \neq 0$, which makes it possible to solve for ϕ_{k+1} as an expression of the form (2) [1 mark].

(d) [8 marks] Recall that the Laguerre polynomials are orthogonal with respect to the inner product $\langle f, g\rangle = \int_0^\infty \mathrm{e}^{-x} f(x)g(x)\mathrm{d}x$. For $k = 1$ compute the parameters β_k and γ_k/α_k in the three-term recursion (2) that relates the degree 2 Laguerre polynomial $\phi_2(x)$ to the Laguerre polynomials of degrees 1 and 0, $\phi_1(x) = 1 - x$ and $\phi_0(x) = 1$.

Answer: [New] By the previous part, we know that $\alpha_k, \beta_k, \gamma_k$ exist. We may also assume that the ϕ_j are scaled so that $\langle \phi_j, \phi_j\rangle = 1$, which is easily checked for ϕ_0 and ϕ_1 [1 mark]. Since we must ensure that ϕ_{k+1} is orthogonal to ϕ_j ($j \leqslant k$), we must force this condition in particular for $j = k-1, k$, which yields two constraints [1 mark] on the parameters $\alpha_k, \beta_k, \gamma_k$: Orthogonality with ϕ_k yields

$$0 = \langle \phi_{k+1}, \phi_k\rangle = \alpha_k\langle (x-\beta_k)\phi_k, \phi_k\rangle - \gamma_k\langle \phi_{k-1}, \phi_k\rangle = \alpha_k\left(\langle x\phi_k, \phi_k\rangle - \beta_k\right),$$

where we have used $\langle \phi_k, \phi_k\rangle = 1$ and $\langle \phi_k, \phi_{k-1}\rangle = 0$, hence,

$$\beta_k = \int_0^\infty \mathrm{e}^{-x}\, x\phi_k^2(x)\mathrm{d}x. \quad \text{[2 marks]}$$

Orthogonality with ϕ_{k-1} implies

$$0 = \langle \phi_{k+1}, \phi_{k-1}\rangle = \alpha_k\langle (x-\beta_k)\phi_k, \phi_{k-1}\rangle - \gamma_k\langle \phi_{k-1}, \phi_{k-1}\rangle = \alpha_k\langle x\phi_k, \phi_{k-1}\rangle - \gamma_k,$$

where we have used $\langle \phi_{k-1}, \phi_{k-1}\rangle = 1$ and $\langle \phi_k, \phi_{k-1}\rangle = 0$, hence,

$$\frac{\gamma_k}{\alpha_k} = \int_0^\infty \mathrm{e}^{-x}\, x\phi_k(x)\phi_{k-1}(x)\mathrm{d}x. \quad \text{[1 mark]}$$

In the case $k = 1$ this yields

$$\begin{aligned}\beta_1 &= \int_0^\infty \mathrm{e}^{-x}\, x(1-x)^2\mathrm{d}x = 1 - 2\cdot 2! + 3! = 3,\\ \frac{\gamma_1}{\alpha_1} &= \int_0^\infty \mathrm{e}^{-x}\, x(1-x)\mathrm{d}x = 1! - 2! = -1,\end{aligned}$$

where we used

$$\int_0^\infty x^k\, \mathrm{e}^{-x}\,\mathrm{d}x = -x^k\,\mathrm{e}^{-x}\Big|_0^\infty + k\int_0^\infty x^{k-1}\,\mathrm{e}^{-x}\,\mathrm{d}x = \cdots = k! \quad \text{[3 marks]}$$

3. Let $n \geqslant 2$ be an integer.

(a) [6 marks] Define the notion of an *orthogonal matrix* $Q \in \mathbb{R}^{n\times n}$. Prove that for any given vector $u \in \mathbb{R}^n$ there exists a vector $w \in \mathbb{R}^n$ such that $H(w)u = v$, where $v^{\mathrm{T}} = \left(\sqrt{u^{\mathrm{T}}u}\ 0\ \dots\ 0\right)$ and $H(w)$ is the *Householder reflection*

$$H(w) = \mathrm{I} - \frac{2}{w^{\mathrm{T}}w}ww^{\mathrm{T}}.$$

Express w explicitly in terms of u, and show that $H(w)$ is an orthogonal matrix.

Answer: [Book work] Q is orthogonal if $Q^{\mathrm{T}}Q = \mathrm{I}$, that is, $Q^{\mathrm{T}} = Q^{-1}$ [1 mark]. If $u = 0$, we may choose $w \neq 0$ arbitrarily, as $H(w)0 = 0$ [1 mark]. If $u \neq 0$, choose $w = (u - v)$ (which is explicit in u, since v is defined in terms of u), so that $H(w)$ is well defined and

$$H(w)u = \mathrm{I}\,u - \frac{2(u-v)^{\mathrm{T}}u}{(u-v)^{\mathrm{T}}(u-v)}(u-v) = u - (u-v), \quad \text{[2 marks]}$$

where the last equality follows from

$$(u-v)^{\mathrm{T}}(u-v) = u^{\mathrm{T}}u - 2u^{\mathrm{T}}v + v^{\mathrm{T}}v = u^{\mathrm{T}}u - 2u^{\mathrm{T}}v + u^{\mathrm{T}}u = 2(u-v)^{\mathrm{T}}u. \quad \text{[1 mark]}$$

$H(w)$ is orthogonal, because

$$H(w)^{\mathrm{T}}H(w) = \mathrm{I} - \frac{4}{w^{\mathrm{T}}w}ww^{\mathrm{T}} + \frac{4w^{\mathrm{T}}w}{(w^{\mathrm{T}}w)^2}ww^{\mathrm{T}} = \mathrm{I}. \quad \text{[1 mark]}$$

(b) [7 marks] Define the notion of QR-factorisation of a matrix $A \in \mathbb{R}^{n\times m}$ and show how this factorisation can be computed via Householder reflections. Show how the QR-factorisation can, alternatively, be computed via Gram-Schmidt orthogonalisation and compare the flop count of both algorithms.

Answer: [First part is book work. Alternative method is new, though students have seen Gram-Schmidt orthogonalisation.] A QR factorisation of a $n \times n$ matrix A is the splitting of A into a product $A = QR$ of an orthogonal matrix Q and an upper triangular matrix $R = (r_{ij})$, that is, $r_{ij} = 0$ if $i > j$ [1 mark]. Let us recursively construct Householder matrices $H(w_i)$ $(i = 1, \dots, n-1)$ such that

$$H(w_{n-1}) \cdot H(w_{n-2}) \dots H(w_1)A = R$$

is upper triangular, so that $Q = H(w_1)H(w_2)\dots H(w_{n-1})$ satisfies $A = QR$. Inductively, let $B^0 = A$ and

$$B^{k-1} = H(w_{k-1}) \cdot H(w_{n-2}) \cdot \dots \cdot H(w_1)A,$$

which is of block form

$$B^{k-1} = \left(b_{ij}^{k-1}\right) = \begin{bmatrix} R^{k-1} & C^{k-1} \\ 0 & D^{k-1} \end{bmatrix} \tag{4}$$

with R^{k-1} a $(k-1)\times(k-1)$ upper triangular matrix. Define

$$u_k = \begin{bmatrix} b_{kk}^{k-1} \\ \vdots \\ b_{nk}^{k-1} \end{bmatrix} \in \mathbb{R}^{n-k+1}, \quad v_k = \begin{bmatrix} \sqrt{u_k^{\mathrm{T}}u_k} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \in \mathbb{R}^{n-k+1}, \quad w_k = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ u_k - v_k \end{bmatrix} \in \mathbb{R}^n.$$

Then

$$H(w_k)\begin{bmatrix} R^{k-1} \\ 0 \end{bmatrix} = \begin{bmatrix} R^{k-1} \\ 0 \end{bmatrix}$$

and the last $n-k$ entries of the first column of

$$H(w_k)\begin{bmatrix} C^{k-1} \\ D^{k-1} \end{bmatrix}$$

are zero, so that B^k is also of the required (partially triangularised) block form (4). The claim thus follows by induction [3 marks]. The complexity is $\sum_{k=0}^{n-1}(n-k)^2 = n^3/3 + n^2/2 + n/6$ flops, plus $O(n^2)$ flops for the construction of the w_k [1 mark]. A QR factorisation can also be computed via Gram-Schmidt orthogonalisation, in which the k-th column q_k of Q is inductively defined from the k-th column a_k of A as follows,

$$h_k = a_k - \sum_{j=1}^{k-1}(q_j^{\mathrm{T}}a_k)q_k,$$

$$q_k = \frac{1}{\sqrt{h_k^{\mathrm{T}}h_k}}h_k,$$

and setting $R = (r_{ij})$, where $r_{ij} = q_i^{\mathrm{T}} a_j$ for $i < j$ and $r_{jj} = \sqrt{h_j^{\mathrm{T}} h_j}$, a calculation that takes $\sum_{k=1}^{n} 2nk = n^2(n+1) = n^3 + n^2$ flops. This procedure is 3 times more costly, but the columns of Q become available one by one, while the method with Householder matrices can compute these columns only at the end [2 marks].

(c) [5 marks] Prove that for any vector $x \in \mathbb{R}^n$ there exists an $n \times n$ orthogonal *Givens rotation* matrix $J(i,j)$ such that $y = J(i,j)x$ has entries $y_j = 0$, $y_k = x_k$ $(k \notin \{i,j\})$. Determine y_i and the entries of $J(i,j)$ as a function of the entries of x.

Answer: [Book work and adaptation of seen material] If $x_i = x_j = 0$, then $J = \mathrm{I}$ will do and there is nothing to prove [1 mark]. If $(x_i, x_j) \neq (0,0)$, let

$$J = (g_{ij}) = \begin{bmatrix} 1 & & & & & & \\ & \cdot & & & & & \\ & & c & & s & & \\ & & & \cdot & & & \\ & & -s & & c & & \\ & & & & & \cdot & \\ & & & & & & 1 \end{bmatrix}$$

with $g_{ii} = g_{jj} = c := x_i / \sqrt{x_i^2 + x_j^2}$, $g_{ij} = -g_{ji} = s := x_j / \sqrt{x_i^2 + x_j^2}$, and $g_{k\ell} = \delta_{k,\ell}$ if $(k,\ell) \notin \{i,j\}^2$ [2 marks]. Then $J^{\mathrm{T}} J = \mathrm{I}$ and $y = Jx$ satisifes $y_k = x_k$ for $k \notin \{i,j\}$, $y_i = cx_i + sx_j = \sqrt{x_i^2 + y_i^2}$, and $y_j = -sx_i + cx_j = 0$. Thus, $J(i,j) := J$ satisfies the requirements [2 marks].

(d) [7 marks] Show how, for any given symmetric $n \times n$ matrix A, Householder reflections may be used to construct an orthogonal matrix Q such that $B = Q^{\mathrm{T}} A Q$ is a tri-diagonal matrix, and compute the number of floating point operations this reduction requires. Show how the eigenvalues and eigenvectors of A can be obtained from the eigenvalues and eigenvectors of B. Show how Givens rotations may be used to compute a QR factorisation of B, and explain the advantage of applying the symmetric QR algorithm to B instead of A for the purposes of computing the eigenvalues and eigenvectors of A.

Answer: [Book work and adaptation of seen material] Let A be symmetric, and let

$$H(w_{n-1}) \cdot H(w_{n-2}) \cdot \ldots \cdot H(w_1) A = Q^{\mathrm{T}} A = R$$

be the upper triangularisation of A under the construction of Part (b). Then $Q^{\mathrm{T}} A Q = RQ$ is symmetric, and since right multiplication by $H(w_k)$ only operates on columns $k, \ldots, n$,

$$RQ = RH(w_1) H(w_2) \ldots H(w_{n-1})$$

has only one lower nonzero subdiagonal. By symmetry, it also has only one upper nonzero superdiagonal, hence $B := Q^{\mathrm{T}} A Q$ is tri-diagonal [2 marks]. The cost is twice the cost we computed in Part (b) (except that v does not have to be computed, that is, $(2/3)n^3 + O(n^2)$ [1 mark].

Since B is similar to A, it has the same eigenvalues, and the eigenvectors of A can easily be found from the eigenvectors of B by left multiplication with Q [1 mark]. In each step of the symmetric QR factorisation applied to B, we need to compute a QR-factorisation $B = \tilde{Q}\tilde{R}$ of B and form $B_+ := \tilde{R}\tilde{Q}$. If this were applied to A this would involve a cubic cost. However, since B is tri-diagonal, the QR factorisation is achieved by the following procedure, at a total cost of $(16 + c_1)(n-1)$ flops [1 mark] for a small constant c_1:

$\tilde{R} := B$;
for $i = 1, \ldots, n-1$
$x := \tilde{R}(:, i)$ (i-th column);
form $J(i, i+1)$ as in Part (c) (4 flops, plus constant c_1 flops for square root);
$\tilde{R} \leftarrow J(i, i+1)\tilde{R}$ (12 flops);
end.

Since, due to the action of the rotations $J(i, j)$, the factor $\tilde{R}$ has only two nonzero superdiagonals, the formation of $B_+ = \tilde{R}\tilde{Q} = \tilde{R}J(1,2)^{\mathrm{T}}J(2,3)^{\mathrm{T}} \ldots J(n-1,n)^{\mathrm{T}}$ also only takes $12(n-1)$ flops and results in a symmetric matrix with only one non-zero subdiagonal, i.e., a tri-diagonal matrix. Thus, each iteration of the symmetric QR algorithm takes only linear instead of cubic time [2 marks].

