## Homework Problem Sheet 10

For some problems, parts of the solution are already given. Fill in the gaps and complete the proofs where you see a red band at the left margin.
Introduction. Quadrature, fixed point iterations

## Problem 10.1 Error of Simpson's Rule and Gaussian Quadrature

(10.1a) Show that the following holds for the error of Simpson's rule for $f \in \mathcal{C}^{4}([a, b])$ :

$$
\int_{a}^{b} f(x) \mathrm{d} x-\frac{b-a}{6}\left[f(a)+4 f\left(\frac{1}{2} a+\frac{1}{2} b\right)+f(b)\right]=-\frac{1}{90}\left(\frac{b-a}{2}\right)^{5} f^{(4)}(\xi)
$$

where $\xi \in[a, b]$ is a suitable intermediate value. For this purpose follow the idea of the proof of the second part of [NMI, Thm. 4.2] and give detailed reasons on why every step is correct.
Solution: Just as in the script we use the Newtonian description of the error of interpolation and obtain:

$$
\mathrm{I}_{[a, b]}[f]-Q_{[a, b]}^{(2)}[f]=
$$

Next we will replace the divided differences of the sampling point that occurs twice $(a+b) / 2$ as in [NMI, Cor. 3.12]:

$$
\mathrm{I}_{[a, b]}[f]-Q_{[a, b]}^{(2)}[f]=
$$

where the point $\widehat{\xi}_{x}$ in general depends on $x$. Since the polynomial term in the integral does not switch sign we can use the first intermediate value theorem of integration:
(10.1b) Prove [NMI, Thm. 4.18]: For any $f \in \mathcal{C}^{2 n+2}([-1,1])$ there exists a $\xi \in(-1,1)$ such that

$$
\int_{-1}^{1} f(x) \mathrm{d} x-Q^{(n)}[f]=\frac{f^{(2 n+2)}(\xi)}{(2 n+2)!} \int_{-1}^{1} \prod_{j=0}^{n}\left(x-x_{j}\right)^{2} \mathrm{~d} x
$$

## Solution:

Since $Q^{(n)} p=I p$ for all $p \in \mathbb{P}_{2 n+1}$, where I denotes the integral operator $\mathrm{I}[f]:=\int_{a}^{b} f \mathrm{~d} x$ we can chose the Hermite interpolation polynomial for the data
and we get:

$$
\int_{-1}^{1} f(x) \mathrm{d} x-Q^{(n)}[f]=
$$

| To estimate the error of interpolation we use [NMI, Thm. 3.6]:

## Problem 10.2 Gauss-Hermite Quadrature

Quadrature formulas can also be used to approximate the values of improper integrals. This problem discusses an example.
Let $f: \mathbb{R} \rightarrow \mathbb{R}$ be integrable, we define $I_{w}[f]:=\int_{-\infty}^{\infty} f(t) w(t) \mathrm{d} t$ for the weight function $w(t):=\mathrm{e}^{-t^{2}}$. For $n \in \mathbb{N}$, let $f_{n}$ denote the monomial $f_{n}(t):=t^{n}$.
(10.2a) From the Analysis course we know $I_{w}\left[f_{0}\right]=I_{w}[1]=\sqrt{\pi}$. Using integration by parts, prove that

$$
I_{w}\left[t^{n}\right]= \begin{cases}0 & n=1,3, \ldots \\ 2^{-n / 2} \sqrt{\pi}(1 \cdot 3 \cdot 5 \cdot \ldots \cdot(n-1)) & n=2,4, \ldots\end{cases}
$$

Solution: For $n$ odd, the integrand is an odd function, so the integral is zero. For $n$ even, $n=0,2,4, \ldots$, it follows from integration by parts that

$$
\int_{-\infty}^{\infty} t^{n} \mathrm{e}^{-t^{2}} \mathrm{~d} t=
$$

Rewriting this for $n=2,4, \ldots$ and applying it inductively, results in
(10.2b) Determine a polynomial $H_{2}$ of degree 2 that satisfies $I_{w}\left[t^{n} H_{2}\right]=0$ for $n=0,1$ and $I_{w}\left[H_{2}^{2}\right]=1$, and $H_{2}(t) \xrightarrow{t \rightarrow \infty} \infty$. This polynomial $H_{2}$ is called the Hermite polynomial of degree 2.

Solution: We set $H_{2}(t)=a_{0}+a_{1} t+a_{2} t^{2}$ with unknown coefficients $a_{i}, i=0,1,2$. Then we must have
(10.2c) Find the zeros $t_{0}, t_{1}$ of $H_{2}$ with $t_{0}<t_{1}$.

Solution: The two zeros of $\mathrm{H}_{2}$ are
(10.2d) Let $\left\{\ell_{0}, \ell_{1}\right\}$ be the Lagrange interpolation polynomials associated to the points $\left\{t_{0}, t_{1}\right\}$ (the roots of $H_{2}$ from subproblem (10.2c)). Approximate the integral $I_{w}[f]$ for $f(t)=\cos (t)$ using the Gauss-Hermite quadrature formula given by

$$
Q_{w}^{(1)}[f]:=\sum_{i=0}^{1} f\left(x_{i}\right) \alpha_{i} \approx I_{w}[f],
$$

where the weights are defined by $\alpha_{i}:=I_{w}\left[\ell_{i}\right], i=0,1$. Compare the result to the exact value

$$
\int_{-\infty}^{\infty} \cos (t) \mathrm{e}^{-t^{2}} \mathrm{~d} t=\frac{\sqrt{\pi}}{\mathrm{e}^{1 / 4}}
$$

Solution: The quadrature weights are
and $\alpha_{1}=\alpha_{0}$ for symmetry reasons. Hence

$$
1.3804 \approx \frac{\sqrt{\pi}}{\mathrm{e}^{1 / 4}}=\int_{-\infty}^{\infty} f(t) \mathrm{e}^{-t^{2}} \mathrm{~d} t \approx \sum_{i=0}^{1} f\left(t_{i}\right) \alpha_{i}=\sqrt{\pi} \cos \left(\frac{1}{\sqrt{2}}\right) \approx 1.3475
$$

## Problem 10.3 Fixed-point Iteration in 1D

Consider the fixed-point iteration $\Phi(x)=x, n=0,1, \ldots$ for $\Phi: \mathbb{R} \rightarrow \mathbb{R}$ given by

$$
\Phi(x)=\arctan \left(\frac{x}{2}\right) .
$$

(10.3a) Show that there exists a unique solution $x^{*}$ for the fixed-point interation of $\Phi(x)$ and that for $x^{(0)} \in \mathbb{R}$ the iterative method $x^{(k+1)}=\Phi\left(x^{k}\right), k=0,1,2, \ldots$ converges to $x^{*}$.

Hint: Apply [NMI, Thm. 5.10].

## Solution:

(10.3b) Determine an a priori error estimate for $k=25$ iterations when $x^{(0)}=\pi$.

Solution: Noting that $x^{(1)}=\arctan \left(\frac{\pi}{2}\right)$ and applying the appropriate error estimate from [NMI, Thm. 5.10] we have with $L:=\sup _{x \in \mathbb{R}}\left|\Phi^{\prime}(x)\right|=\frac{1}{2}$
(10.3c) What is the order/speed of convergence of the fixed-point interation? Write a MatLAB function FPIteration.m that simulates $n=25$ steps of the fixed-point iteration $\Phi(x)=x$, and then plot the error convergence in a semi logarithmic plot (type help semilogy). You'll observe that your plot shows a straight line. Explain why.

## Solution:

Listing 10.1: Solution for subproblem (10.3c)

```
function FPIteration
% Function to calculate the solution to arctan(x/2) = x using
% fixed-point iteration
x = pi;
nIterations = 25;
f = @(x) atan(x/2);
y = zeros(nIterations, 1);
y(1) = x;
for i = 1:25
    y(i+1) = f(y(i));
    fprintf('iteration: %d, x = %f\n', i, y(i+1));
end
err = y - y(nIterations+1);
figure(1);
grid on
semilogy (1:nIterations+1, err, '. -b');
title ('Convergence 1-D fixed-point iteration');
```

```
xlabel('k');
ylabel('Rel. error');
end
```



Figure 10.1: Fixed-point iteration for $\Phi(x)=\arctan \left(\frac{x}{2}\right)$.

## Problem 10.4 Gauss Quadrature Over General Interval

(10.4a) Implement a MATLAB function GaussLegendre.m, that takes as input the limits of integration a and $b$, the number points to use $n \in \mathbb{N}$ and the function handle $f$, and calculates the approximation $Q_{[a, b]}^{(n)}[f]$ to $\int_{a}^{b} f(x) \mathrm{d} x$ where $Q_{[a, b]}^{(n)}[f]$ denotes Gauss-Legendre quadrature. You may use the function gaussQuad.m given on the course website, to compute the quadrature points and weights for the interval $[-1,1]$.
(10.4b) Plot the error convergence for $[a, b]=[-2,2]$,

$$
f_{1}(x):=\frac{|x|^{2.5}}{\sqrt{x^{3}+10}} \quad \text { and } \quad f_{2}(x):=\frac{x^{2}}{\sqrt{x^{3}+10}}
$$

and $n=1, \ldots, 80$. Explain.

## Problem 10.5 Fixed-point Iteration in 2D

Consider the fixed-point iteration $\mathbf{z}=\Phi(\mathbf{z})$ for $\Phi: \mathbb{R}^{2} \rightarrow \mathbb{R}^{2}$ given by

$$
\begin{equation*}
\Phi(\mathbf{z})=\binom{\frac{1}{2} x^{2}+\frac{1}{4} x+\frac{1}{2} y}{\frac{2}{3} y}, \quad \text { where } \quad \mathbf{z}=\binom{x}{y} . \tag{10.5.1}
\end{equation*}
$$

(10.5a) Calculate the Jacobian $\mathbf{J}$ of $\Phi$ and its inverse $\mathbf{J}^{-1}$.
(10.5b) Show that the fixed-point iteration of $\Phi(\mathbf{z})$ has a unique solution $\mathbf{z}^{\star}$ on

$$
E=\left\{\mathbf{z} \in \mathbb{R}^{2} \mid x \in[-2 / 3,1 / 5], y \in[-3 / 4,1 / 4]\right\}
$$

and that it converges in the $\infty$-norm for all initial values $\mathbf{z}^{(0)} \in E$.
Hint: Use Banach's fixed-point theorem.
(10.5c) Show that $\Phi$ is not a contraction on $E$ in the 1-norm.
(10.5d) Let

$$
\tilde{\Phi}(\mathbf{z}):=\frac{1}{7}\binom{6 \cos (x)-2 y}{2 \sin (x)-\frac{2 y}{1+y^{2}}}, \quad \text { where } \quad \mathbf{z}=\binom{x}{y} .
$$

Give a maximal set $\tilde{E} \subseteq \mathbb{R}^{2}$ s.t. the fixed point iteration $\tilde{\Phi}\left(\mathbf{z}^{(k)}\right)=\mathbf{z}^{(k+1)}$ converges for all initial values $\mathbf{z}^{(0)} \in \tilde{E}$.

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Matlab: Submit all files in the online system. Include the files that generate the plots. Label all your plots. Include commands to run your functions. Comment on your results.

## References

[NMI] Lecture Notes for the course "Numerische Mathematik I".

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