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Written Exam on Basic Numerical Methods, 1DV519, 7,5 hp
Saturday 30th of November 2019, 12.00–17.00.

The solutions should be complete, correct, motivated, well structured and easy to follow.
Aids: Calculator (you may use a scientific calculator but *not* with internet connection).
Please begin each question on a new paper.
Preliminary grades: 15p-17p⇒E; 18p-20p⇒D; 21p-23p⇒C; 24p-26p⇒B; 27p-30p⇒A.

1. Given the following set of points $(x, y) : (-2.0, 0.8), (-1.0, 1.0), (0.0, 0.5), (1.0, 0.2), (2.0, 0.1)$; fit the data with a polynomial of degree **one** using the least square method. Draw a figure with the given data set together with your resulting polynomial. (5p)

We want $y \approx kx + m$ and put up the system

$$\underbrace{\begin{pmatrix} 1 & -2 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} m \\ k \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} 0.8 \\ 1.0 \\ 0.5 \\ 0.2 \\ 0.1 \end{pmatrix}}_{b}$$

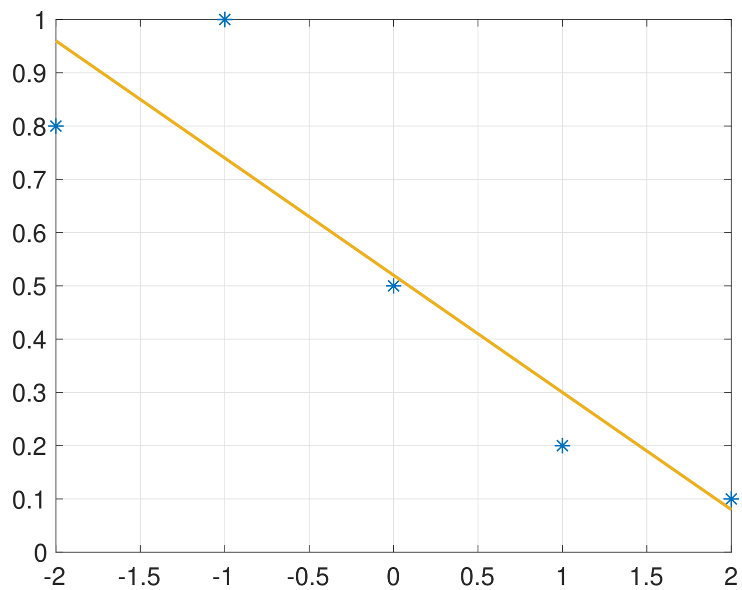
which is overdetermined. We put up the normal equations as $A^T Ax = A^T b$ with

$$A^T A = \begin{pmatrix} 5 & 0 \\ 0 & 10 \end{pmatrix} \qquad A^T b = \begin{pmatrix} 2.6 \\ -2.2 \end{pmatrix}.$$

Solving this leads to

$$\begin{pmatrix} m \\ k \end{pmatrix} = \begin{pmatrix} 0.52 \\ -0.22 \end{pmatrix}$$

that is $y \approx -0.22x + 0.52$.



2. (a) Given the following set of points (x, y);

x	1	2	3	4
y	1	1	1	1

determine the corresponding interpolating polynomial (of lowest possible degree).
Hint: Think rather than compute.

(b) For high degree interpolating polynomials, a certain phenomenon can often be observed. What is this phenomenon called?

(c) Next, consider the points

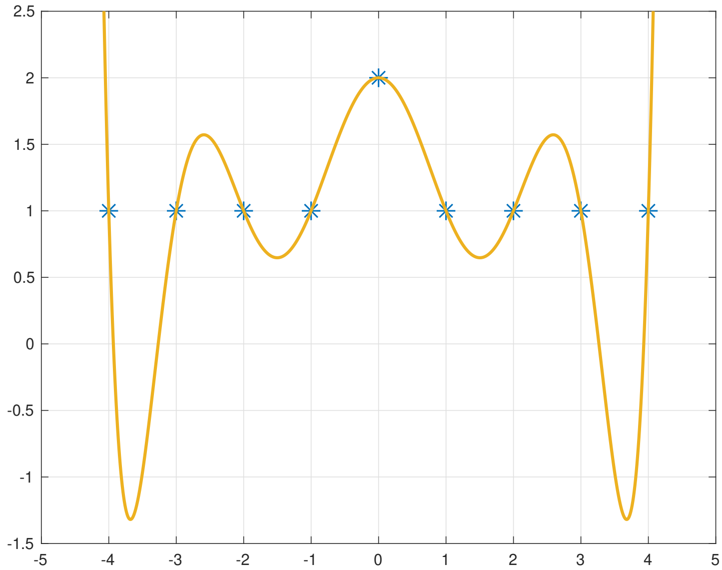
x	-4	-3	-2	-1	0	1	2	3	4
y	1	1	1	1	2	1	1	1	1

Without doing any actual computations, make a sketch of the corresponding interpolating polynomial (together with the given points).
The scales on the axes do not need to be very exact, but the behaviour of the polynomial including the above-mentioned phenomenon should be clearly demonstrated. (5p)

(a) The polynomial $y = 1$ passes through all points and according to the *main theorem of polynomial interpolation* an interpolating polynomial of degree smaller than $n - 1$ (in this case a third degree polynomial or less) is unique.

(b) Runge phenomenon.

(c)



3. The equation $\ln x = \sin x$ has one (and only one) root for $x > 0$.

(a) Solve the equation using the Bisection method using some appropriate starting data (three iterations are enough). Give the answer together with the estimated error.

(b) How many iterations would you have to do in order to get four correct decimals? (5p)

(a) To use the bisection method we first have to rewrite the equation as $f(x) = \ln x - \sin x$ and seek x such that $f(x) = 0$.

Starting with e.g. the interval $[a,\ b] = [0.35,\ 2.75]$ we have

$$f(a) = -1.3927 < 0 \qquad\qquad f(b) = 0.6299 > 0$$

Compute $c = (a + b)/2 = 1.55$ and $f(c) = -0.5615 < 0$. We thus put $a = c$, i.e $[a,\ b] = [1.55,\ 2.75]$.

Compute $c = (a + b)/2 = 2.15$ and $f(c) = -0.0714 < 0$. We thus put $a = c$, i.e $[a,\ b] = [2.15,\ 2.75]$.

Compute $c = (a + b)/2 = 2.45$ and $f(c) = 0.2583 > 0$. We thus put $b = c$, i.e $[a,\ b] = [2.15,\ 2.45]$.

<u>Answer:</u> $x = 2.3 \pm 0.15$

(b) Four correct decimals means an error less than $0.5 \cdot 10^{-4}$. For every iteration the error becomes half as big, where we after 3 iterations had 0.15. After n iterations more the error is $0.15/2^n$. Solving $0.15/2^n = 0.5 \cdot 10^{-4}$ we get $n = \log_2(3 \cdot 10^3) = 11.55$. Thus we need 12 more iterations, in total 15.

4. What is the result when calculating

   (a) $(1+2^{-26})-1$ (b) $3+10^{-18}$ (c) $10^{-20}-10^{-16}$ (d) 2^{-52} (e) 2^{-53}

   in floating point arithmetics (IEEE double precision)?

   (f) Analytically, $f'(x) = \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$, and this can be used to approximate $f'(x)$ by calculating $D_{x,h} = \frac{f(x+h)-f(x)}{h}$ in a computer with a small $h \neq 0$.

   Sketch the resulting error $\text{abs}\,(D_{x,h} - f'(x))$, as a function of h. It should be a log-log plot (logarithmic scaling on both x-axis and y-axis) for values of h ranging from 10^{-20} to 1. *You may assume that $x \sim \mathcal{O}(1)$, that $f(x)$ and $f'(x)$ are well-defined in a neighbourhood around x and that $f''(x) \neq 0$.* (5p)

   (a) 2^{-26} (b) 3 (c) $10^{-20}-10^{-16} = -9.999 \cdot 10^{-17}$ (d) 2^{-52} (e) 2^{-53}

   (f) See LectureNotes10

5. The function values y are given for a few points according to

x	0	0.2	0.4	0.6	0.8
$y(x)$	0.10000	0.66800	0.82200	0.45900	−0.13000

a) Compute an approximation to the integral $\int_0^{0.8} y(x)dx$ using Simpson's method. All available function values must be used.

b) Assume that the truncation error in the above computation can be estimated to 0.002. How large would the error be (approximately) if the number of function values would be increased such that the step length is halved. Motivate your answer.

c) Use Richardson extrapolation on the value obtained in a) in order to find an improved approximation of the integral $\int_0^{0.8} y(x)dx$. (5p)

Answer:

(a) $S(h = 0.2) = \frac{0.2}{3}(0.10000 + 4 * 0.66800 + 2 * 0.82200 + 4 * 0.45900 - 0.13000)$
$= 0.40813333\ldots \approx 0.40813$

(b) Simpson's method is 4th order accurate. This means that if we make h 2 times smaller the error will be $2^4 = 16$ times smaller. $0.002/16 = 1.25 \cdot 10^{-4}$.

(c) We first need $S(h = 0.4) = \frac{0.4}{3}(0.10000 + 4 * 0.82200 - 0.13000) = 0.43440$.

Richardson extrapolation is given by

$Q = F(h) + kh^n + \mathcal{O}(h^{n+1})$, $\qquad Q = \frac{2^n F(h/2) - F(h)}{2^n - 1} + \mathcal{O}(h^{n+1})$

Here $n = 4$ and we obtain the extrapolation

$\frac{16S(h=0.2) - S(h=0.4)}{15} = \frac{16*0.40813333\ldots - 0.4344}{15} = 0.40638222\ldots$

Answer: 0.40638

6. (a) Derive a finite difference formula that uses the values $f(x+h)$, $f(x)$ and $f(x-2h)$ to approximate $f'(x)$. The formula should be as accurate as possible.

(b) Find the error term and the order for the approximation formula obtained in (a). (5p)

(a) Using Taylor expansions we have

$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \dots$

and

$f(x-2h) = f(x) - 2hf'(x) + 4\frac{h^2}{2} f''(x) - 8\frac{h^3}{6} f'''(x) + \dots.$

Make the ansatz $D_h = \frac{af(x+h)+bf(x)+cf(x-2h)}{h}$. Inserting the Taylor expansions, leads to

$$\begin{aligned}
D_h &= \frac{af(x+h) + bf(x) + cf(x-2h)}{h} \\
&= \frac{a(f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \dots) + bf(x)}{h} \\
&+ \frac{c(f(x) - 2hf'(x) + 4\frac{h^2}{2} f''(x) - 8\frac{h^3}{6} f'''(x) + \dots)}{h} \\
&= \frac{(a+b+c)f(x) + (a-2c)hf'(x) + (a+4c)\frac{h^2}{2} f''(x) + (a-8c)\frac{h^3}{6} f'''(x) + \dots}{h} \qquad (1)
\end{aligned}$$

Demand for consistency: $a+b+c=0$ and $a-2c=1$. We can make one more demand and demanding $a+4c=0$ me maximize the accuracy. We have

$$\begin{aligned} a+b+c &= 0 \\ a-2c &= 1 \\ a+4c &= 0 \end{aligned} \qquad \Longrightarrow \qquad a = 4/6, b = -3/6, c = -1/6$$

Thus the formula $\frac{4f(x+h)-3f(x)-f(x-2h)}{6h}$ is the most accurate approximation of $f'(x)$ given the values $f(x+h)$, $f(x)$ and $f(x-2h)$.

(b) Inserting a, b, c above into (**??**) gives

$$D_h = f'(x) + \frac{h^2}{3} f'''(x) + \dots$$

The error term is $\frac{h^2}{3} f'''(x) + \mathcal{O}(h^3)$ (or $\frac{h^2}{3} f'''(c)$ for some c between $x-2h$ and $x+h$) and the approximation formula is thus second order accurate.

Good luck!

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List of formulas for the exam in Basic Numerical Methods, 2019

These formulas will be attached to the exam. The list is not guaranteed to be complete, and the use, meaning, conditions and assumptions of the formulas are purposely left out.

- **Taylor's formula**

$$f(x) = f(a) + \tfrac{f'(a)}{1!}(x-a) + \tfrac{f''(a)}{2!}(x-a)^2 + \ldots + \tfrac{f^{(n)}(a)}{n!}(x-a)^n + \tfrac{f^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}$$

(ξ between x and a)

- **Absolute and relative error**

$$\Delta_x = \tilde{x} - x, \qquad \frac{\Delta_x}{x} \approx \frac{\Delta_x}{\tilde{x}}, \qquad \Delta_{x+y} = \Delta_x + \Delta_y, \qquad \frac{\Delta_{xy}}{xy} \approx \frac{\Delta_x}{x} + \frac{\Delta_y}{y}$$

- **Error propagation formulas, condition number (1D)**

$$\Delta f \approx f'(x)\Delta x, \qquad \left|\frac{\Delta f/f}{\Delta x/x}\right| \approx \left|\frac{xf'(x)}{f(x)}\right|$$

$$\Delta f \approx f''(x)\frac{\Delta x^2}{2}$$

- **Correct decimals**
  $|\Delta x| \leq 0.5 \cdot 10^{-t}$

- **Numbers in base B**
  $x = x_m B^m + x_{m-1}B^{m-1} + \ldots + x_0 B_0 + x_{-1}B^{-1} + \ldots = (x_m x_{m-1} \ldots x_0.x_{-1} \ldots)_B$

- **Iterative methods**

Bisection method:

```
c=(a+b)/2;
while (b-a)>2*tol
    if f(c)*f(a)>0
        a=c;
    else
        b=c;
    end
    c=(a+b)/2;
end
```

Newton-Raphson: $$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}, \qquad J(\mathbf{x}_n)(\mathbf{x}_{n+1} - \mathbf{x}_n) + \mathbf{f}(\mathbf{x}_n) = 0$$

The secant method: $$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})},$$

$$e_n = x_n - x^*, \qquad |x_{n+1} - x^*| < \bar{c}|x_n - x^*|^p, \qquad \lim_{n\to\infty} \tfrac{|e_{n+1}|}{|e_n|^p} = c$$

• **Equation systems**

$A\mathbf{x} = \mathbf{b}$, residual $\mathbf{r} = \mathbf{b} - A\widetilde{\mathbf{x}}$

LU-factorization:	$A = LU, \quad PA = LU$
QR-factorization:	$A = QR, \quad Q^TQ = I$
(Iterative methods)	$A = D + L + U$
Jacobi methods:	$\mathbf{x}^{(k)} = -D^{-1}(L+U)\mathbf{x}^{(k-1)} + D^{-1}\mathbf{b}$
Gauss-Seidel:	$\mathbf{x}^{(k)} = -(D+L)^{-1}U\mathbf{x}^{(k-1)} + (D+L)^{-1}\mathbf{b}$

Backward: $\|\mathbf{r}\|_\infty$, forward: $\|\mathbf{x} - \widetilde{\mathbf{x}}\|_\infty$

• **Norms and condition numbers**

Let $\mathbf{x} = (x_1, \ldots, x_n)$ be a vector:

$$\|\mathbf{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p\right)^{1/p}, \quad \|\boldsymbol{x}\|_1 = \sum_{i=1}^{n} |x_i|, \quad \|\boldsymbol{x}\|_2 = \sqrt{x_1^2 + \cdots + x_n^2}, \quad \|\mathbf{x}\|_\infty = \max_i |x_i|.$$

Let A be a $n \times n$ matrix:

$$\|A\| = \sup_{\mathbf{x}\neq 0} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|}, \qquad \|A\mathbf{x}\| \leq \|A\| \cdot \|\mathbf{x}\|, \qquad \kappa(A) = \|A\| \cdot \|A^{-1}\|$$

$A(\mathbf{x} + \delta\mathbf{x}) = \mathbf{b} + \delta\mathbf{b}$

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(A)\frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|}, \qquad econd(A) = \frac{\|\delta\mathbf{x}\|/\|\mathbf{x}\|}{\|\delta\mathbf{b}\|/\|\mathbf{b}\|} \leq \kappa(A),$$

• **Interpolation**

Let $(x_0, y_0), \ldots, (x_n, y_n)$ be $n+1$ points in the xy-plane.

Monomial:	$P(x) = a_0 + a_1x + \ldots + a_nx^n$
Lagrangre:	$P(x) = \sum_{j=0}^{n} y_j\ell_j(x), \qquad \ell_j(x) = \prod_{\substack{0\leq m\leq n \\ m\neq j}} \frac{x - x_m}{x_j - x_m}$

Newton's divided differences:

$$P(x) = [y_0] + [y_0, y_1](x - x_0) + \cdots + [y_0, \ldots, y_k](x - x_0)(x - x_1)\cdots(x - x_{n-1}).$$

$$[y_0] = f(x_0), \quad [y_0, y_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}, \quad [y_0, y_1, y_2] = \frac{[y_1, y_2] - [y_0, y_1]}{x_2 - x_0}, \ldots$$

Interpolation errors:

$$R(x) = f(x) - P(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{f^{n+1}(\xi)}{(n+1)!}, \qquad x_0 < \xi < x_n,$$

• **Least squares, normal equations** $A^TA\mathbf{x} = A^T\mathbf{b}$, residual $\mathbf{r} = \mathbf{b} - A\mathbf{x}$

• **Finite differences**

$$\frac{f(x+h) - f(x)}{h} = f'(x) + f''(\xi)\frac{h}{2} \qquad \xi \in [x, x+h]$$

$$\frac{f(x) - f(x-h)}{h} = f'(x) - f''(\xi)\frac{h}{2} \qquad \xi \in [x-h, x]$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + f^{(3)}(\xi)\frac{h^2}{6} \qquad \xi \in [x-h, x+h]$$

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + f^{(4)}(\xi)\frac{h^2}{12} \qquad \xi \in [x-h, x+h]$$

- **Trapezoidal rule, Simpson's rule**

$$\int_a^b f(x)dx = \tfrac{h}{2}\left(f(x_0) + 2\textstyle\sum_{k=1}^{n-1} f(x_k) + f(x_n)\right) - \tfrac{(b-a)h^2}{12} f''(\xi), \qquad h = \frac{b-a}{n}$$

$$\int_a^b f(x)dx = \tfrac{h}{3}\left(f(x_0) + 4\textstyle\sum_{k=1}^{n} f(x_{2k-1}) + 2\textstyle\sum_{k=1}^{n-1} f(x_{2k}) + f(x_{2n})\right) - \tfrac{(b-a)h^4}{180} f^{(4)}(\xi), \qquad h = \frac{b-a}{2n}$$

$a < \xi < b$

- **Richardson extrapolation**

$$Q = F(h) + kh^n + \mathcal{O}(h^{n+1}), \qquad Q = \tfrac{2^n F(h/2) - F(h)}{2^n - 1} + \mathcal{O}(h^{n+1})$$

- **Romberg** $R_{i,1} = T(h/2^{i-1})$, $R_{ij} = \frac{4^{j-1}R_{i,j-1} - R_{i-1,j-1}}{4^{j-1}-1}$

- **Numerical solutions of differential equations**

Differential equation $y' = f(x, y)$ with initial condition $y(x_0) = y_0$

Euler forward ($g_i \sim \mathcal{O}(h)$): $\quad y_{n+1} = y_n + hf(x_n, y_n)$

Euler backward ($g_i \sim \mathcal{O}(h)$): $\quad y_{n+1} = y_n + hf(x_{n+1}, y_{n+1})$

Heun's method ($g_i \sim \mathcal{O}(h^2)$): $\quad \begin{cases} y_{n+1} = y_n + \frac{1}{2}(k_1 + k_2) \\ k_1 = hf(x_n, y_n) \\ k_2 = hf(x_n + h, y_n + k_1) \end{cases}$

RK4 ($g_i \sim \mathcal{O}(h^4)$): $\quad \begin{cases} y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \\ k_1 = hf(x_n, y_n) \\ k_2 = hf(x_n + h/2, y_n + k_1/2) \\ k_3 = hf(x_n + h/2, y_n + k_2/2) \\ k_4 = hf(x_n + h, y_n + k_3) \end{cases}$

where $x_{n+1} = x_n + h$.