NTNU

Kunnskap for en bedre verden

Institutt for matematiske fag

# Eksamensoppgave i
# **TMA4320 Introduksjon til vitenskapelige beregninger**

**Faglig kontakt under eksamen:** Anton Evgrafov

**Tlf:** 4503 0163

**Eksamensdato:** 30. mai 2017

**Eksamenstid (fra–til):** 09:00–13:00

**Hjelpemiddelkode/Tillatte hjelpemidler:** B: Spesifiserte trykte hjelpemidler tillatt:

- K. Rottmann: Matematisk formelsamling

Bestemt, enkel kalkulator tillatt.

**Målform/språk:** bokmål

**Antall sider:** 9

**Antall sider vedlegg:** 0

**Kontrollert av:**

Dato Sign

## Oppgave 1

**a)** Vi betrakter en likning

$$f(x) = (x-2)(x-1) = 0. \tag{1}$$

Konstruer en fikspunkt iterasjon fra (1), med røttene til $f$ som fikspunkter. Bestem om denne iterasjonen konvergerer lokalt (i nærheten av fikspunkter) mot røttene av $f$. Hvis ja, bestem også konvergensraten for hver av røttene.

**Solution:** there are infinitely many possibilities here. For example we could isolate the term $3x$ in $f(x) = (x-2)(x-1) = x^2 - 3x + 2 = 0$ to obtain a fixed-point iteration

$$x = g(x) = \frac{x^2+2}{3}.$$

By construction $1 = g(1)$ and $2 = g(2)$. The absolute values of the derivative $|g'(x)| = |2x/3|$ at the fixed point determine the convergence and its speed. Here we have $|g'(1)| = 2/3 < 1$, while $|g'(2)| = 4/3 > 1$. Thus this iteration converges in the vicinity of $x = 1$ with the rate $2/3$, whereas it diverges in the vicinity of $x = 2$.

The following Python snippet:

```python
from __future__ import division, print_function

g = lambda x: (x*x+2)/3

print('Testing near x = 1.0\n')
x  = 1.0
x0 = 1.3
for i in range(12):
    x1 = g(x0)
    print('i = %3d, xi = %e, |(x{i}-x)/(x{i-1}-x)| = %e' % \
          (i, x1, abs((x1-x)/(x0-x))))
    x0 = x1

print('dg/dx(x) = %e' % (2*x/3))


print('\nTesting near x = 2.0\n')
x  = 2.0
x0 = 2.3
```

```
for i in range(6):
    x1 = g(x0)
    print('i = %3d, xi = %e, |(x{i}-x)/(x{i-1}-x)| = %e' % \
              (i, x1, abs((x1-x)/(x0-x))))
    x0 = x1
```

produces the output:

```
Testing near x = 1.0

i =   0, xi = 1.230000e+00, |(x{i}-x)/(x{i-1}-x)| = 7.666667e-01
i =   1, xi = 1.170967e+00, |(x{i}-x)/(x{i-1}-x)| = 7.433333e-01
i =   2, xi = 1.123721e+00, |(x{i}-x)/(x{i-1}-x)| = 7.236556e-01
i =   3, xi = 1.087583e+00, |(x{i}-x)/(x{i-1}-x)| = 7.079070e-01
i =   4, xi = 1.060946e+00, |(x{i}-x)/(x{i-1}-x)| = 6.958610e-01
i =   5, xi = 1.041868e+00, |(x{i}-x)/(x{i-1}-x)| = 6.869819e-01
i =   6, xi = 1.028497e+00, |(x{i}-x)/(x{i-1}-x)| = 6.806228e-01
i =   7, xi = 1.019268e+00, |(x{i}-x)/(x{i-1}-x)| = 6.761656e-01
i =   8, xi = 1.012969e+00, |(x{i}-x)/(x{i-1}-x)| = 6.730895e-01
i =   9, xi = 1.008702e+00, |(x{i}-x)/(x{i-1}-x)| = 6.709898e-01
i =  10, xi = 1.005827e+00, |(x{i}-x)/(x{i-1}-x)| = 6.695674e-01
i =  11, xi = 1.003896e+00, |(x{i}-x)/(x{i-1}-x)| = 6.686089e-01
dg/dx(x) = 6.666667e-01

Testing near x = 2.0

i =   0, xi = 2.430000e+00, |(x{i}-x)/(x{i-1}-x)| = 1.433333e+00
i =   1, xi = 2.634967e+00, |(x{i}-x)/(x{i-1}-x)| = 1.476667e+00
i =   2, xi = 2.981016e+00, |(x{i}-x)/(x{i-1}-x)| = 1.544989e+00
i =   3, xi = 3.628820e+00, |(x{i}-x)/(x{i-1}-x)| = 1.660339e+00
i =   4, xi = 5.056111e+00, |(x{i}-x)/(x{i-1}-x)| = 1.876273e+00
i =   5, xi = 9.188085e+00, |(x{i}-x)/(x{i-1}-x)| = 2.352037e+00
```

## Oppgave 2

**a)** Finn polynomene $p_1(x)$, $p_2(x)$ av *lavest mulig grad* som interpolerer funksjonen $f(x) = \sin(\pi x/6)$ i punktene

- $p_1$: $x_1 = 0$, $x_2 = 3$;
- $p_2$: $x_1 = 0$, $x_2 = 3$, og $x_3 = 1$.

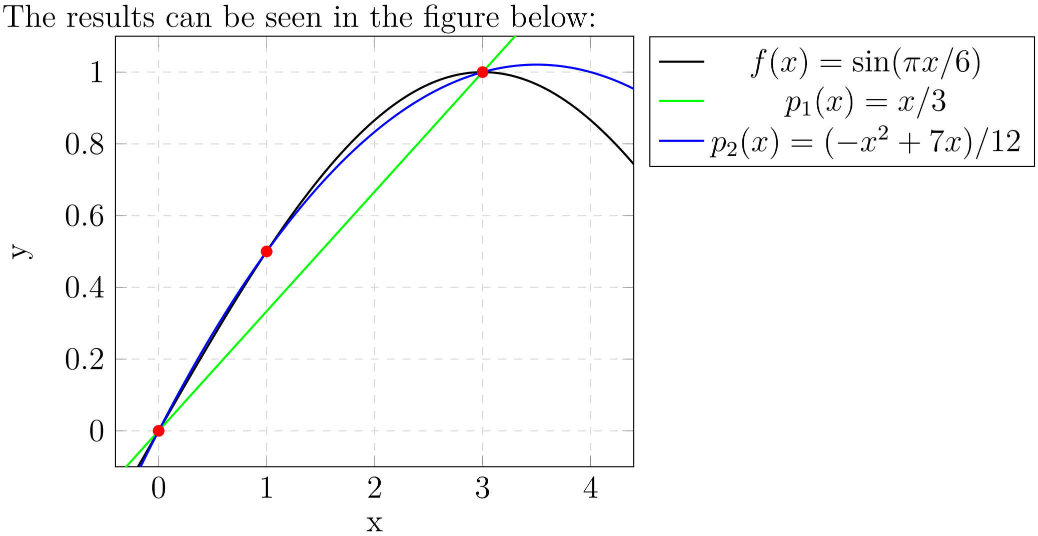
**Solution:** since we are essentially adding a new interpolation point to obtain $p_2$, we could use Newton's divided differences representation of the interpolation polynomial. Thus

$$\begin{aligned} f[x_1] = 0, \quad f[x_2] = 1, \quad f[x_3] = 1/2,\\ f[x_1,x_2] = \frac{1-0}{3-0} = 1/3, \quad f[x_2,x_3] = \frac{1/2-1}{1-3} = 1/4,\\ f[x_1,x_2,x_3] = \frac{1/4-1/3}{1-0} = -1/12. \end{aligned}$$

As a result we have

$$\begin{aligned} p_1(x) &= 0 + 1/3(x-0) = x/3,\\ p_2(x) &= p_1(x) - 1/12(x-0)(x-3) = -x^2/12 + 7/12x. \end{aligned}$$

The results can be seen in the figure below:




Polynomet $P(x)$ av lavest mulig grad som interpolerer en glatt funksjon $F(x)$ i punktene $x_1, \ldots, x_n$ oppfyller følgende feilestimat:

$$F(x) - P(x) = \frac{(x-x_1)\ldots(x-x_n)}{n!} F^{(n)}(c), \tag{2}$$

med $c \in [\min\{x, x_1, \ldots, x_n\}, \max\{x, x_1, \ldots, x_n\}]$.

**b)** *Vurder* feilen $e = \max_{x\in[0,3]} |f(x) - p_2(x)|$ ut fra (2), hvor $f$ og $p_2$ er som i **a)**. Du trenger ikke å finne den nøyaktige verdi av $e$! Bare finn *en passende rimelig øverste grense* og forklar svaret.

**Solution:** again, there are many ways of answering this question. In my opinion the simplest estimate is like this:

$$e = \max_{x\in[0,3]} |f(x) - p_2(x)| \le \max_{x\in[0,3]} \frac{|(x-0)(x-3)(x-1)|}{3!} \frac{\pi^3}{6^3} \max_{c\in[0,3]} |-\cos(\pi c/6)|$$
$$\le \frac{3\cdot 3\cdot 2}{6}\frac{\pi^3}{6^3} \le 0.431,$$

where I have simply replaced each term $|x - x_i|$ with its largest value on the interval $[0, 3]$, and used the fact that $|\cos(\cdot)| \le 1$. This estimate can be further sharpened in several ways[1], but this is not required.

[1]For example, $\max_{x\in[0,3]} |(x-0)(x-3)(x-1)|$ is only $\approx 2.113$ and not $3\cdot 3\cdot 2 = 18$, as we "computed".

## Oppgave 3

**a)** Beregn en tilnærmelse til integral

$$i = \int_{-1}^{1} \frac{\mathrm{d}x}{x^2+1} \tag{3}$$

ved hjelp av trapesregelen basert på 1 og 2 "paneler".

**Solution:** direct computation. Using one panel, we get

$$i \approx \frac{1-(-1)}{2}(f(-1)+f(1)) = 1,$$

while for two manels we have

$$i \approx \frac{0-(-1)}{2}(f(-1)+f(0)) + \frac{1-0}{2}(f(0)+f(1)) = 3/2,$$

which seems to get closer to the analytical value $i = \arctan(1) - \arctan(-1) = \pi/2 \approx 1.571$.

**b)** Feilestimatet for trapesregelen $Q_{[a,b]}f$ med ett panel er gitt av

$$\int_a^b f(x)\,\mathrm{d}x = Q_{[a,b]}f - \frac{h^3}{12}f''(c),$$

der $c$ er et punkt mellom $a$ og $b$, og $h = b - a$.

Bruk nå adaptive kvadraturer til å estimere forskjellen $i - Q_{[-1,1]}f$, for $f(x) = 1/(x^2+1)$ og $i$ er gitt av (3). Du kan gjenbruke de numeriske beregningene fra **a)**.

**Solution:** this is a standard technique explained in section 5.4 in the book. Indeed:

$$\begin{aligned}\int_{-1}^{1} f(x)\,\mathrm{d}x &= Q_{[-1,1]}f - \frac{h^3}{12}f''(c)\\ &\approx Q_{[-1,0]}f + Q_{[0,1]}f - 2\frac{(h/2)^3}{12}f''(c),\end{aligned}$$

where $h = 2$. Thus

$$\frac{3}{4}\frac{h^3}{12}f''(c) \approx Q_{[-1,1]}f - (Q_{[-1,0]}f + Q_{[0,1]}f) = 1.0 - 1.5 = -\frac{1}{2},$$

and the error

$$i - Q_{[-1,1]}f = -\frac{h^3}{12}f''(c) \approx \frac{4}{3}\frac{1}{2} = \frac{2}{3} \approx 0.67.$$

This estimate is not too far from the real error $i - Q_{[-1,1]}f = \pi/2 - 1 \approx 0.57$.

**Oppgave 4** I prosjekt 3 har vi løst en andregrads differensiallikning av type

$$\begin{aligned} y''(t) &= \frac{\alpha}{m}(v(t, y(t)) - y'(t)), \\ y(0) &= \hat{y}_0, \\ y'(0) &= \hat{y}_1. \end{aligned} \tag{4}$$

hvor $\alpha$, $m$ er positive konstanter, $v$ er et gitt funksjon, og $\hat{y}_0$ og $\hat{y}_1$ er kjente begynnelsesverdier. For enkelhets skyld antar vi i denne oppgave at $y$ er en skalar funksjon (og ikke en posisjon med to koordinater, som i prosjektet). Vi definerer også en konstant $k = \alpha/m$.

**a)** Skriv om likning (4) til et system av to førsteordens differensiallikninger.

**Solution:** We put $z = y'$, then

$$\begin{pmatrix} y \\ z \end{pmatrix}'(t) = \begin{pmatrix} z(t) \\ k(v(t, y(t)) - z(t)) \end{pmatrix}$$

and

$$\begin{pmatrix} y \\ z \end{pmatrix}(0) = \begin{pmatrix} \hat{y}_0 \\ \hat{y}_1 \end{pmatrix}$$

Vi skal bruke den *implisitte* Euler metoden for å finne den numeriske løsningen til systemet du har funnet i **a)**.

**b)** La $v(t, y) = \sin(y)$, $\hat{y}_0 = \pi/2$, $\hat{y}_1 = 0$, $k = 2$, $h = 0.1$. Skriv ned et system av ikke-lineære likninger, som må løses for å finne en tilnærmelse til $(y(h), y'(h))$.

**Solution:** The basic idea of the implicit Euler method for solwing an ODE $y' = f(t, y)$ is $(w_{k+1} - w_k)/h = f(t_{k+1}, w_{k+1})$, or $w_{k+1} - hf(t_{k+1}, w_{k+1}) = w_k$. Substituting the right hand side of the system computed in **a)** and other given data we get:

$$\begin{pmatrix} y_1 \\ z_1 \end{pmatrix} - 0.1 \begin{pmatrix} z_1 \\ 2\sin(y_1) - 2z_1 \end{pmatrix} = \begin{pmatrix} y_0 \\ z_0 \end{pmatrix} = \begin{pmatrix} \hat{y}_0 \\ \hat{y}_1 \end{pmatrix}$$

The final system is thus

$$\begin{cases} y_1 - 0.1z_1 = \pi/2 \\ 1.2z_1 - 0.2\sin(y_1) = 0 \end{cases}$$

**c)** Gjør en iterasjon med Newtons metode for systemet du har fått i **b)**. Bruk begynnelsesverdiene $\hat{y}_0 = \pi/2$, $\hat{y}_1 = 0$ som start verdi for Newton iterasjonen.

**Solution:** Newtons iterasjonen kan skrives som $r_k + J_k(s_{k+1} - s_k) = 0$, where $J_k$ is the Jacobian of the non-linear system evaluated at $s_k$, and $r_k$ is its residual.

We insert the numbers now:

$$
\begin{aligned}
s_0 &= \begin{pmatrix} \pi/2 \\ 0 \end{pmatrix}, \\
r_0 &= \begin{pmatrix} \pi/2 - 0.1 \cdot 0 - \pi/2 \\ 1.2 \cdot 0 - 0.2\sin(\pi/2) - 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -0.2 \end{pmatrix} \\
J_0 &= \begin{pmatrix} 1 & -0.1 \\ -0.2\cos(\pi/2) & 1.2 \end{pmatrix} = \begin{pmatrix} 1 & -0.1 \\ 0 & 1.2 \end{pmatrix}
\end{aligned}
$$

Solving a small $2 \times 2$ system we that after one step of Newton's iteration the approximation to the solution is

$$
s_1 = \begin{pmatrix} \pi/2 + 1/60 \\ +1/6 \end{pmatrix}
$$

**Oppgave 5**

**a)** Beregn LU faktoriseringen (med delvis pivotering) av matrisen

$$A = \begin{pmatrix} 1 & 4 & 4 \\ 1 & 3 & 1 \\ 2 & 6 & 3 \end{pmatrix}$$

**Solution:**

$$LU = A = \begin{pmatrix} 1 & 4 & 4 \\ 1 & 3 & 1 \\ 2 & 6 & 3 \end{pmatrix}, \quad P = I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Exchange rows 1 and 3 ($|2|>|1|$):

$$LU = \begin{pmatrix} 2 & 6 & 3 \\ 1 & 3 & 1 \\ 1 & 4 & 4 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Subtract 1/2 of the row 1 from rows 2 and 3:

$$LU = \begin{pmatrix} 2 & 6 & 3 \\ 0.5 & 0 & -0.5 \\ 0.5 & 1 & 2.5 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

Exchange rows 2 and 3 ($|1|>|0|$):

$$LU = \begin{pmatrix} 2 & 6 & 3 \\ 0.5 & 1 & 2.5 \\ 0.5 & 0 & -0.5 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

And we are done:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0.5 & 0 & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 2 & 6 & 3 \\ 0 & 1 & 2.5 \\ 0 & 0 & -0.5 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

It is always a good idea to verify the computation: $LU = PA$.

**b)** Ved hjelp av beregningene i **a)**, bestem $x \in \mathbb{R}^3$ slik at $Ax = b = [-3, 2, 2]^{\mathrm{T}}$.

**Solution:** We know that $PAx = LUx = Pb = [2, -3, 2]^{\mathrm{T}}$. Let us put $Ux = y$, then $Ly = Pb$. We find $y$ by solving the lower-triangular system:

$$\begin{aligned} y_1 &= 2 \\ y_2 &= -3 - 0.5y_1 = -4 \\ y_3 &= 2 - 0.5y_1 = 1 \end{aligned}$$

Finally, we find $x$ by solving an upper-triangular system $Ux = y$:

$$\begin{aligned} x_3 &= y_3/(-0.5) = -2 \\ x_2 &= y_2 - 2.5x_3 = -4 + 5 = 1 \\ x_1 &= (y_1 - 6x_2 - 3x_3)/2 = (2 - 6 + 6)/2 = 1. \end{aligned}$$

It is always a good idea to verify the computation: $Ax = b$.

**c)** Gitt att $\|A^{-1}\|_\infty = 23$, beregn kondisjonstallet (i $\infty$-norm) $\kappa_\infty(A)$. Ved hjelp av denne informasjon, beregn en øvre grense på

$$\frac{\|x - \tilde{x}\|_\infty}{\|x\|_\infty},$$

hvor $A\tilde{x} = \tilde{b} = [-3, 2, 2.5]^{\mathrm{T}}$.

**Solution:** The condition number $\kappa_\infty(A) = \|A\|_\infty \|A^{-1}\|_\infty = \|A^{-1}\|_\infty \max_i \sum_j |A_{ij}| = 23 \max\{9, 5, 11\} = 23 \cdot 11 = 253$.

The condition number tells us how the relative perturbation in the problem data in the worst case can propagate into the relative perturbation of the solution to the problem; namely

$$\frac{\|x - \tilde{x}\|_\infty}{\|x\|_\infty} \leq \kappa_\infty(A) \frac{\|b - \tilde{b}\|_\infty}{\|b\|_\infty} = 253 \frac{0.5}{3} \approx 42.1667.$$

In reality, nothing close to this upper bound happens in this case: indeed

$$\frac{\|x - \tilde{x}\|_\infty}{\|x\|_\infty} = 2.$$

How can one derive the upper bound if one does not remember it? We would like to estimate $\|x - \tilde{s}\|_\infty$ from above, and $\|x\|_\infty$ from below (because it is in the denominator):

$$\begin{aligned} x - \tilde{x} &= A^{-1}(b - \tilde{b}) &\implies&\quad \|x - \tilde{x}\|_\infty \leq \|A^{-1}\|_\infty \|b - \tilde{b}\|_\infty, \\ b &= Ax &\implies&\quad \|b\|_\infty \leq \|A\|_\infty \|x\|_\infty. \end{aligned}$$

Combining these two inequalities we get

$$\frac{\|x - \tilde{x}\|_\infty}{\|x\|_\infty} \leq \|A^{-1}\|_\infty \|A\|_\infty \frac{\|b - \tilde{b}\|_\infty}{\|b\|_\infty}.$$