Exercises for numerical differentiation

Øyvind Ryan

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1. Mark each of the following statements as true or false.

a. When we use the approximation $f'(a) \approx (f(a+h) - f(a))/h$ on a computer, we can always obtain higher accuracy by choosing a smaller value for h.

b. If we increase the number of bits for storing floating-point numbers (e.g.128-bit precision), we can obtain better numerical approximations to derivatives.

c. We are using Newton's difference quotient method to approximate the derivative of the function $f(x) = e^x$ at the point $x = 1$ with a step value of $h = 0.1$ (with 64-bit precission). If we change the step length to $h = 0.01$ then the error will be reduced by approximately a factor of 10.

d. The approximation $f'(a) \approx (f(a+h) - f(a))/h$ will give the exact answer (ignoring numerical round-off errors) if the function f is linear.

e. Since we cannot know exactly how well the values of $f(a+h)$ and $f(a)$ are represented on a computer, it is difficult to estimate accurately what the error will be in numerical differentiation.

2. **a.** (Exam 2010) We are to calculate an approximation to the derivative $f'(a)$ to the function $f(x) = \cos(x)$ by the approximation

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}.$$

Then the absolute error for any $h > 0$ is bounded by (we do not take round off errors into account)

☐ $h^2/2$

☐ $h^2 \cos(1)$

☐ $h \cos(a)/4$

☐ $h/2$

b. (Exam 2008) We are going to calculate an approximation to the derivative $f'(a)$ of the function f by the approximation

$$f'(a) \approx \frac{f(a+h) - f(a)}{h}.$$

If we are using floating point numbers the total error is bounded by (In the two last alternatives ϵ^* depends on the type of floating point numbers used):

☐ $\frac{h^2}{2}\max_{x\in[a,a+h]}\left|f''(x)\right|$

☐ $\frac{h^3}{6}\max_{x\in[a,a+h]}\left|f'''(x)\right|$

☐ $\frac{h^2}{6}\max_{x\in[a,a+h]}\left|f'''(x)\right|+\frac{6\epsilon^*}{h^3}\max_{x\in[a,a+h]}\left|f(x)\right|$

☐ $\frac{h}{2}\max_{x\in[a,a+h]}\left|f''(x)\right|+\frac{2\epsilon^*}{h}\max_{x\in[a,a+h]}\left|f(x)\right|$

3. In this exercise we are going to numerically compute the derivative of $f(x) = e^x$ at $a = 1$ using Newton's quotient as described in observation **??**. The exact derivative to 20 digits is

$$f'(1) \approx 2.71828182845904523 54.$$

a. Compute the approximation $\big(f(1+h)-f(1)\big)/h$ to $f'(1)$. Start with $h = 10^{-4}$, and then gradually reduce h. Also compute the error, and determine an h that gives close to minimal error.
Solution: On my computer 10^{-8} is the power of 10 which gives the least error in the approximation. This can be btained by running the following program:

```
from math import *

for p in range(15):
  h=10.0**(-p)
  print p, abs((exp(1+h)-exp(1))/h-exp(1))
```

b. Determine the optimal h as described in Lemma **??** and compare with the value you found in (a).
Answer: $h^* \approx 8.4\times10^{-9}$.
Solution: If we use the values $\epsilon^* = 7\times10^{-17}$ from Example **??**, then Lemma **??** gives the optimal h $h^* = 2\sqrt{\epsilon^*} \approx 1.6733\times10^{-8}$ (terms cancel since $f(a) = f''(a)$).

4. Mark each of the following statements as true or false.

a. If we ignore round-off errors, the symmetric Newton's quotient method is exact for polynomials of degree 2 or lower.

b. Even though the symmetric Newton differentiation scheme gives better accuracy, there is a trade-off as it is much more computationally demanding (i.e. it requires many more calculations) than the non-symmetric method.

5. In this exercise we are going to check the symmetric Newton's quotient and numerically compute the derivative of $f(x) = e^x$ at $a = 1$, see exercise 11.1.**??**. Recall that the exact derivative with 20 correct digits is

$$f'(1) \approx 2.7182818284590452354.$$

a. Compute the approximation $\big(f(1+h) - f(1-h)\big)/(2h)$ to $f'(1)$. Start with $h = 10^{-3}$, and then gradually reduce h. Also compute the error, and determine an h that gives close to minimal error.

b. Determine the optimal h given by (**??**) and compare with the value you found in (a).
Answer: $h^* \approx 5.9 \times 10^{-6}$.

6. Determine $f'(a)$ numerically using the two asymmetric Newton's quotients

$$f_r(x) = \frac{f(a+h) - f(a)}{h}, \qquad f_l(x) = \frac{f(a) - f(a-h)}{h}$$

as well as the symmetric Newton's quotient. Also compute and compare the relative errors in each case.

a. $f(x) = x^2$; $a = 2$; $h = 0.01$.

b. $f(x) = \sin x$; $a = \pi/3$; $h = 0.1$.
Answer: With 6 digits:
$(f(a+h) - f(a))/h = 0.455902$, relative error: 0.0440981.
$(f(a) - f(a-h))/h = 0.542432$, relative error: 0.0424323.
$(f(a+h) - f(a-h))/(2h) = 0.499167$, relative error: 0.000832917.

c. $f(x) = \sin x$; $a = \pi/3$; $h = 0.001$.

d. $f(x) = \sin x$; $a = \pi/3$; $h = 0.00001$.

e. $f(x) = 2^x$; $a = 1$; $h = 0.0001$.

f. $f(x) = x\cos x$; $a = \pi/3$; $h = 0.0001$.

7. **a.** Show that the approximation to $f'(a)$ given by the symmetric Newton's quotient is the average of the two asymmetric quotients

$$f_r(x) = \frac{f(a+h)-f(a)}{h}, \qquad f_l(x) = \frac{f(a)-f(a-h)}{h}.$$

b. Sketch the graph of the function

$$f(x) = \frac{-x^2+10x-5}{4}$$

on the interval $[0,6]$ together with the three secants associated with the three approximations to the derivative in (a) (use $a=3$ and $h=2$). Can you from this judge which approximation is best?

Solution: We can plot the cuve together with the secants as follows with Python:

```
from numpy import *
from scitools.easyviz import *

x=arange(0,6,0.05,float)
plot(x,(-x**2+10*x-5)/4)
hold('on')
plot([1,3],[(-1**2+10*1-5)/4,(-3**2+10*3-5)/4])
plot([1,5],[(-1**2+10*1-5)/4,(-5**2+10*5-5)/4])
plot([3,5],[(-3**2+10*3-5)/4,(-5**2+10*5-5)/4])
```

c. Determine the three difference quotients in (a) numerically for the function $f(x)$ using $a=3$ and $h_1=0.1$ and $h_2=0.001$. What are the relative errors?

Answer: With 6 digits:
$(f(a+h)-f(a))/h = 0.975$, relative error: 0.025.
$(f(a)-f(a-h))/h = 1.025$, relative error: 0.025.
$(f(a+h)-f(a-h))/(2h) = 1$, relative error: 8.88178×10^{-16}.

d. Show that the symmetric Newton's quotient at $x=a$ for a quadratic function $f(x)=ax^2+bx+c$ is equal to the derivative $f'(a)$.

8. Use the symmetric Newton's quotient and determine an approximation to the derivative $f'(a)$ in each case below. Use the values of h given by $h=10^{-k}$ $k=4,5,\dots,12$ and compare the relative errors. Which of these values of h gives the smallest error? Compare with the optimal h predicted by (**??**).

a. The function $f(x) = 1/(1+\cos(x^2))$ at the point $a = \pi/4$.
Answer: Optimal h: 2.9×10^{-6}.

b. The function $f(x) = x^3 + x + 1$ at the point $a = 0$.
Answer: Optimal h: 3.3×10^{-6}

9. Mark each of the following statements as true or false.

a. The 4-point method with a step length of $h = 0.2$ will usually have a smaller error than the symmetric Newton's quotient method with $h = 0.1$.

b. If we ignore round-off, the 4-point method is exact for all polynomials.

10. In this exercise we are going to check the 4-point method and numerically compute the derivative of $f(x) = e^x$ at $a = 1$. For comparison, the exact derivative to 20 digits is

$$f'(1) \approx 2.7182818284590452354.$$

a. Compute the approximation

$$\frac{f(a-2h) - 8f(a-h) + 8f(a+h) - f(a+2h)}{12h}$$

to $f'(1)$. Start with $h = 10^{-3}$, and then gradually reduce h. Also compute the error, and determine an h that gives close to minimal error.
Solution: On my computer 10^{-3} is the power of 10 which gives the least error in the approximation. This can be tested by running the following program:

```
from math import *

for p in range(15):
  h=10.0**(-p)
  print p, abs((exp(1-2*h)-8*exp(1-h)+8*exp(1+h)-exp(1+2*h))/(12*h)-exp(1))
```

b. Determine the optimal h given by (**??**) and compare with the experimental value you found in (a).
Answer: Opitmal h: 9.9×10^{-4}.
Solution: If we use the value $\epsilon^* = 7\times 10^{-17}$ from Example **??** then (**??**) gives the optimal h $h^* = \sqrt[5]{\frac{27\epsilon^*}{2}} \approx 9.8875\times 10^{-4}$ (terms cancel since $f(a) = f^{(5)}(a)$)

11. **a.** (Exam 2009) We use the expression $(f(h)-2f(0)+f(h))/h^2$ to calculate approximations to $f''(0)$ (we do the calculations exact, without round off errors). Then the result will always be correct if $f(x)$ is

☐ a trigonometric function

☐ a logarithmic function

☐ a polynomial of degree 4

☐ a polynomial of degree 3

b. (Exam 2007) We approximate the second derivative of the function $f(x)$ at $x=0$, by the approximation

$$D_2 f(0) = \frac{f(h)-2f(0)+f(-h)}{h^2}$$

We assume that f is differentiable an infinite number of times, and we do not take round off errors into account. Then the error

$$\left|f''(0)-D_2 f(0)\right|$$

is bounded by

☐ $\frac{h^2}{12}\max_{x\in[-h,h]}\left|f''(x)\right|$

☐ $\frac{h^2}{48}\max_{x\in[-h,h]}\left|f^{(4)}(x)\right|$

☐ $\frac{h}{4}\max_{x\in[-h,h]}\left|f''(x)\right|$

☐ $\frac{h^2}{12}\max_{x\in[-h,h]}\left|f^{(4)}(x)\right|$

12. We use our standard example $f(x)=e^x$ and $a=1$ to check the 3-point approximation to the second derivative given in (**??**). For comparison recall that the exact second derivative to 20 digits is

$$f''(1) \approx 2.7182818284590452354.$$

a. Compute the approximation $\big(f(a-h)-2f(a)+f(a+h)\big)/h^2$ to $f''(1)$. Start with $h=10^{-3}$, and then gradually reduce h. Also compute the actual error, and determine an h that gives close to minimal error.
Solution: On my computer 10^{-4} is the power of 10 which gives the least error in the approximation. This can be tested by running the following program:

```
from math import *

for p in range(15):
  h=10.0**(-p)
  print p, abs((exp(1-h)-2*exp(1)+exp(1+h))/h**2-exp(1))
```

b. Determine the optimal h given by (**??**) and compare with the value you determined in (a).
Answer: Optimal h: 2.24×10^{-4}.
Solution: If we use the value $\epsilon^* = 7 \times 10^{-17}$ from Example **??** then Observation **??** gives the optimal choice of h $h^* = \sqrt[4]{36\epsilon^*} \approx 2.2405 \times 10^{-4}$ (terms cancel since $f(a) = f^{(4)}(a)$).

13. This exercise illustrates a different approach to designing numerical differentiation methods.

a. Suppose that we want to derive a method for approximating the derivative of f at a which has the form

$$f'(a) \approx c_1 f(a-h) + c_2 f(a+h), \quad c_1, c_2 \in \mathbb{R}.$$

We want the method to be exact when $f(x) = 1$ and $f(x) = x$. Use these conditions to determine c_1 and c_2.
Answer: $c_1 = -1/(2h)$, $c_2 = 1/(2h)$.
Solution: If the approximation method $f'(a) \approx c_1 f(a-h) + c_2 f(a+h)$ is to be exact for $f(x) = 1$, we must have that $0 = c_1 + c_2$, since $f(a-h) = f(a+h) = 1$, and since $f'(x) = 0$. Therefore we must have that $c_2 = -c_1$.

If the method is to be exact for $f(x) = x$ we must in the same way have that

$$1 = c_1(a-h) + c_2(a+h) = c_1(a-h) - c_1(a+h) = -2c_1 h,$$

so that $c_1 = -\frac{1}{2h}$,so that also $c_2 = \frac{1}{2h}$. The method therefore becomes $-\frac{1}{2h} f(a-h) + \frac{1}{2h} f(a+h) = \frac{f(a+h)-f(a-h)}{2h}$

b. Show that the method in (a) is exact for all polynomials of degree 1, and compare it to the methods we have discussed in this chapter.
Solution: If $f(x) = cx + d$ we have that $f'(x) = c$, and the method takes the form

$$\frac{f(a+h) - f(a-h)}{2h} = \frac{c(a+h) + d - (c(a-h) + d)}{2h} = \frac{2ch}{2h} = c,$$

so that the method is exact for all polynomials of degree ≤ 1.We see that the method coincides with the symmetric Newton-method for differentiation, and it therefore has an error of order $\frac{1}{h^2}$, which is better than the Newton's quotient (which has an error of order $\frac{1}{h}$). It is worse than the four point method for numerical differentiation,which has order $\frac{1}{h^4}$.

Here it also should have been mentioned that the method also is exact for polynomials of degree ≤ 2 (also see **??**). There are several ways to see this. First, the error estimate from Section **??** uses $f^{(3)}(x)$, and since all second degree polynomials have a third derivative equal to 0, the error must be zero. One could also as above substitute $f(x) = x^2$ into the formula:

$$\frac{f(a+h)-f(a-h)}{2h} = \frac{(a+h)^2-(a-h)^2}{2h} = \frac{4ah}{2h} = 2a,$$

which also is $f'(a)$. Finally, the symmetric Newton quotient was defined as the derivativee at a of the unique parabola interpolating f at $a-h, a$, and $a+h$. If f itself is a parabola it is equal to this interpolant since it is unique, so that the symmetric Newton quotient must return the derivative.

c. Use the procedure in (a) and (b) to derive a method for approximating the second derivative of f,

$$f''(a) \approx c_1 f(a-h) + c_2 f(a) + c_3 f(a+h), \quad c_1, c_2, c_3 \in \mathbb{R},$$

by requiring that the method should be exact when $f(x) = 1$, x and x^2. Do you recognise the method?

Answer: $c_1 = -1/h^2$, $c_2 = 2/h^2$, $c_3 = -1/h^2$.

Solution: If the approximation method $f''(a) \approx c_1 f(a-h) + c_2 f(a) + c_3 f(a+h)$ is exact for $f(x) = 1$, we must have that $0 = c_1 + c_2 + c_3$. If it is exact for $f(x) = x$ we must have that

$$0 = c_1(a-h) + c_2 a + c_3(a+h) = a(c_1+c_2+c_3) + h(-c_1+c_3) = h(-c_1+c_3),$$

which gives that $c_1 = c_3$. If it is exact for $f(x) = x^2$ we must have that

$$\begin{aligned} 2 &= c_1(a-h)^2 + c_2 a^2 + c_3(a+h)^2 \\ &= a^2(c_1+c_2+c_3) - 2ahc_1 + 2ahc_3 + h^2(c_1+c_3) = 2c_1 h^2, \end{aligned}$$

which gives that $c_1 = \frac{1}{h^2}$. We therefore also get that $c_3 = \frac{1}{h^2}$, and that $c_2 = -c_1 - c_2 = -\frac{2}{h^2}$, so that the method becomes

$$\frac{1}{2h} f(a-h) - \frac{1}{h} f(a) + \frac{1}{2h} f(a+h) = \frac{f(a-h) - 2f(a) + f(a+h)}{h^2}.$$

We see that this coincides with the already seen three point method to compute the second derivative in this section.

d. Show that the method in (c) is exact for all cubic polynomials.
Solution: All third degree polynomials have a fourth derivative equal to 0, and therefore the truncation error becomes 0 ($M_1 = 0$ in Theorem **??**). Alternatively we can substitute $f(x) = x^3$ into the formula:

$$\begin{aligned}
&\frac{f(a-h) - 2f(a) + f(a+h)}{2h} \\
&= \frac{(a-h)^3 - 2a^3 + (a+h)^3}{h^2} \\
&= \frac{a^3 - 3a^2h + 3ah^2 - h^3 - 2a^3 + a^3 + 3a^2h + 3ah^2 + h^3}{h^2} \\
&= \frac{6ah^2}{h^2} = 6a,
\end{aligned}$$

which coincides with the second derivative of f in a.

14. Previously we saw the that the Newton difference quotient could be applied reduce bass in digital sound. What will happen to the sound if we instead apply the numerical approximation of the second derivative to it?
Solution: We see that the coefficients in the new approximation are taken from row 2 of Pascal's triangle with alternating sign. This means that also this approximation reduces bass. Since the values are taken from a higher row in Pascal's triangle, one is lead to believe that it reduces more bass than the Newton difference quotient.

15. Assume that $x_0, x_1, \ldots, x_k$ is a uniform partition of $[a, b]$. It is possible to show that the divided difference $f[x_0, x_1, \ldots, x_k]$ can be written on the form $a\sum_{r=0}^{k} c_r(-1)^r f(x_r)$, where a is a constant and c_r are taken from row $k-1$ in Pascal's triangle. By following the same reasoning as in this section, or appealing to Theorem **??**, it is also clear that higher order divided differences are approximations to the higher order derivatives. Explain why this means that applying approximations to the higher order derivatives to sound samples in a sound will typically reduce bass in sound.

16. Mark each of the following statements as true or false.

a. Numerical integration methods are usually constructed by dividing the interval of integration into many subintervals and using some sort of approximation to the area under the function on each subinterval.

17. In this exercise we are going to study the definition of the integral for the function $f(x) = e^x$ on the interval $[0,1]$.

a. Determine lower and upper sums for a uniform partition consisting of 10 subintervals.
Answer: $\underline{I} \approx 1.63378$, $\overline{I} \approx 1.805628$.

b. Determine the absolute and relative errors of the sums in (a) compared to the exact value $e-1 = 1.718281828$ of the integral.
Answer: $\left|I - \underline{I}\right| \approx 0.085$, $\frac{|I-\underline{I}|}{|I|} = 0.0491781$.
$\left|I - \overline{I}\right| \approx 0.087$, $\frac{\left|I-\overline{I}\right|}{|I|} = 0.051$.

c. Write a program for calculating the lower and upper sums in this example. How many subintervals are needed to achieve an absolute error less than 3×10^{-3}?

18. Compute the velocities at all points in the orbit for Jupiter, Mars, and Earth, for the orbital data files used in Example **??**, and plot them against each other. Which planet has highest velocity, and lowest? The speed should be in units per second. Note that the time difference between different samples is one day.
Solution: It is straightforward to write a function which computes the speeds for the orbit data in a given file. The following code can be used for this:

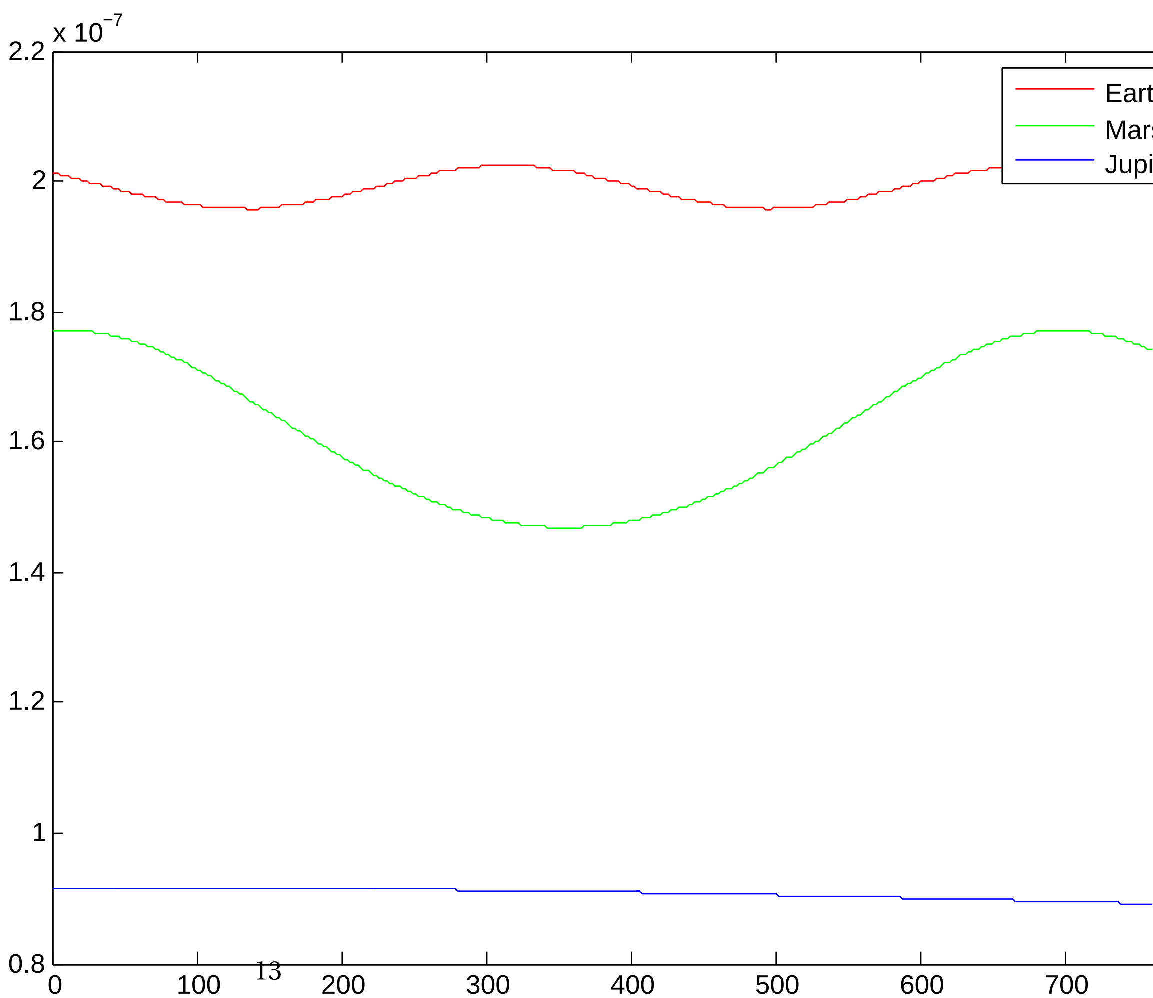
```
function speeds=findspeeds(filename)
  coords=findcoords(filename);
  N=size(coords,2);
  lengths=zeros(1,N-1);
  for k=1:(N-1)
    lengths(k)=norm(coords(:,k)-coords(:,k+1));
  end
  speeds=lengths/(60*60*24); % Numerical derivative
```

The speeds for the three different orbit files can then be plotted together as follows:

```
speeds=findspeeds('earth.txt');
plot(speeds,  'r');
hold on;
speeds=findspeeds('mars.txt');
plot(speeds,'g');
speeds=findspeeds('jupiter.txt');
```

```
plot(speeds,'b');
legend('Earth','Mars','Jupiter');
```

The result is shown in Figure **??**. As expected from Kepler's laws, we see that the orbital velocities are biggest for the planets closest to the sun. We see also that the velocities display a periodic pattern, and that the period is shorter for planets closer to the sun. The explanation is that the orbits are elliptic, not circular, and that the velocities are bigger at points in the orbit which are closer to the sun.


x 10^-7
2.2
2
1.8
1.6
1.4
1.2
1
0.8
0
100
200
300
400
500
600
700
Eart
Mars
Jupi