

Solutions to Exercises to

**Programming Methods
in Scientific Computing**

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Chapter 3 Python, the Fundamentals

Exercise 3.2

Wir erweitern die gegebene Klasse `Polynomial` um eine Methode `derivative` zum Ableiten, sowie eine Methode `antiderivative` zum Bilden einer Stammfunktion. Dabei wählen wir die „Integrationskonstante“ als 0. Wir definieren außerdem Funktionen zum Ausgeben von Polynomen durch die `print`-Funktion.

```
1 class Polynomial:
2     def __init__(self, coeff):
3         self.coeff = coeff
4
5     def __str__(self):
6         s = ""
7         if self.coeff == []:
8             s = "0"
9         else:
10            s += "{} x^0".format(self.coeff[0])
11            for i in range(1, len(self.coeff)):
12                s += " + {} x^{}".format(self.coeff[i], i)
13            return s
14
15     def __repr__(self):
16         return str(s)
17
18     def __call__(self, x):
19         s = 0
20         for i in range(len(self.coeff)):
21             s += self.coeff[i]*x**i
22         return s
23
24     def __add__(self, other):
25         l = []
26         if len(self.coeff) > len(other.coeff):
27             l += self.coeff
28             for i in range(len(other.coeff)):
29                 l[i] += other.coeff[i]
30         else:
31             l += other.coeff
32             for i in range(len(self.coeff)):
33                 l[i] += self.coeff[i]
34         return Polynomial(l)
35
36     def __eq__(self, other):
```

Für das gegebene Polynom $p(x) = 3x^2 + 2x + 1$ testen wir unser Programm mit dem folgenden Code:

```

1 p = Polynomial([1,2,3])
2 print("The given polynomial p:")
3 print(p)
4 print("The derivative of p:")
5 print( p.derivative() )
6 print("The antiderivative of p:")
7 print( p.antiderivative() )
8 print("Taking antiderivative and then derivative:")

```

Dabei erhalten wir den folgenden Output:

```

$ python exercise_03_02.py
The given polynomial p:
1 x^0 + 2 x^1 + 3 x^2
The derivative of p:
2 x^0 + 6 x^1
The antiderivative of p:
0 x^0 + 1.0 x^1 + 1.0 x^2 + 1.0 x^3
Taking antiderivative and then derivative:
1.0 x^0 + 2.0 x^1 + 3.0 x^2

```

Exercise 3.3

Wir definieren direkt Klasse `Matrix`, die über alle Methoden verfügt, die wir in diesem und den späteren Aufgabenteilen nutzen werden.

```

1 class Matrix():
2     def __init__(self, entries):
3         m = len(entries)
4         if m == 0:
5             raise ValueError("height must be positive")
6         n = len(entries[0])
7         if n == 0:
8             raise ValueError("width must be positive")
9         for i in range(1, m):
10            if len(entries[i]) != n:
11                raise ValueError("rows must have the same width")
12        self.height = m
13        self.width = n
14        self.entries = entries
15
16    def __getitem__(self, i):      # allows to get the rows via A[i]
17        return self.entries[i]
18
19    def __setitem__(self, i, k):   # allows to set rows via A[i]
20        self.entries[i] = k
21
22    def __str__(self):            # allows print(A) for a Matrix A
23        rows = ["["]*self.height
24        for j in range(self.width): # construct output columnwise, align left
25            numbers = []           # numbers to appear in column j
26            maxlen = 0             # maximal length of a number in column j
27            for i in range(self.height):

```

```

28         s = str(self[i][j])
29         numbers.append(s)
30         if len(s) > maxlen:
31             maxlen = len(s)
32     for i in range(self.height):
33         # pad the entries if they are too short
34         rows[i] += numbers[i] + " "*(maxlen-len(numbers[i])) + " "
35     s = ""
36     for r in rows:
37         s += r[:-1] + "\n" # remove white space at the end of ech line
38     s = s[:-1] # remove empty line at the end
39     return s
40
41 def __repr__(self):
42     return str(self)
43
44 def __mul__(self, other):
45     if self.width != other.height:
46         raise TypeError('matrix dimensions do not match')
47     newentries = []
48     for i in range(self.height):
49         row = []
50         for j in range(other.width):
51             s = self[i][0] * other[0][j] # makes s have the right type
52             for k in range(1, self.width):
53                 s += self[i][k] * other[k][j]
54             row.append(s)
55         newentries.append(row)
56     return Matrix(newentries)
57
58 def __eq__(self, other):
59     if self.height != other.height or self.width != other.width:
60         return False
61     for i in range(self.height):
62         for j in range(self.width):
63             if self[i][j] != other[i][j]:
64                 return False
65     return True
66
67 def mapentries(self, f): # applies a function to all entries
68     A = zeromatrix(self.height, self.width) # zeromatrix is defined below
69     for i in range(self.height):
70         for j in range(self.width):
71             A[i][j] = f(self[i][j])
72     return A
73
74 def addrow(self, i, j, c): # add c times row j to row i
75     for k in range(self.width):
76         self[i][k] = c * self[j][k] + self[i][k]
77     # makes c responsible for implementing the operations
78
79 def addcolumn(self, i, j, c): # add c times column j from column i
80     for k in range(self.height):
81         self[k][i] = c * self[k][j] + self[k][i]
82
83 def multrow(self, i, c): # multiply row i with c

```

```

84         for j in range(self.width):
85             self[i][j] = c * self[i][j]
86
87     def swaprows(self, i, j):          # swap rows i and j
88         if i > self.height or j > self.height:
89             raise ValueError("swap nonexistent rows")
90         l = self[i]
91         self[i] = self[j]
92         self[j] = l
93
94     def transpose(self):
95         T = zeromatrix(self.width, self.height)
96         for i in range(self.height):
97             for j in range(self.width):
98                 T[j][i] = self[i][j]
99         return T

```

Wir definieren zudem Hilfsfunktionen, die wir im Weiteren nutzen werden:

```

1  def zeromatrix(height, width): # creates a zero matrix
2      entries = []
3      for i in range(height):
4          entries.append([0]*width)
5      return Matrix(entries)
6
7  def identitymatrix(size):      # creates an identity matrix
8      E = zeromatrix(size, size)
9      for i in range(size):
10         E[i][i] = 1
11     return E
12
13  def copymatrix(A):            # forcefully copies a matrix
14      B = zeromatrix(A.height, A.width)
15      for i in range(A.height):
16         for j in range(A.width):
17             B[i][j] = A[i][j]
18     return B

```

Die Assoziativität der Matrixmultiplikation testen wir mit dem folgenden Code:

```

1  A = Matrix([[0,1],[1,0],[1,1]])
2  print("A:")
3  print(A)
4  B = Matrix([[1,2,3,4],[5,6,7,8]])
5  print("B:")
6  print(B)
7  C = Matrix([[1,0],[0,1],[1,0],[0,1]])
8  print("C:")
9  print(C)
10 print("Checking if A(BC) == (AB)C:")
11 print(A * (B * C) == (A * B) * C)

```

Wir erhalten wir (durch Ausführen in der Konsole) den folgenden Output:

```

$ python exercise_03_03.py
A:
[0 1]

```

```

[1 0]
[1 1]
B:
[1 2 3 4]
[5 6 7 8]
C:
[1 0]
[0 1]
[1 0]
[0 1]
Checking if A(BC) == (AB)C:
True

```

Exercise 3.4

Wir schreiben zunächst eine Klasse `Rational`, die ein genaues Rechnen mit rationalen Zahlen erlaubt.

```

1 class Rational():
2     def __init__(self, num, denum = 1): # default denominator is 1
3         if type(num) == Rational:
4             p = num/Rational(denum)
5             self.num = p.num
6             self.denum = p.denum
7         elif type(num) != int:
8             raise TypeError("numerator is no integer")
9         elif type(denum) != int:
10            raise TypeError("denumerater is no integer")
11        elif denum == 0:
12            raise ZeroDivisionError("denominator is zero")
13        else:
14            self.num = num
15            self.denum = denum
16
17    def __str__(self): # allows print(x) for Rational x
18        return "{}/{ {}".format(self.num, self.denum)
19
20    def __repr__(self):
21        return str(self)
22
23    def __add__(self, other):
24        if type(other) == int:
25            return self + Rational(other)
26        elif type(other) == Rational:
27            return Rational( self.num * other.denum + self.denum * other.num,
28                             self.denum * other.denum )
29        raise TypeError("unsupported operand type(s) for + or add(): '
30            Rational' and '{}'.format(type(other).__name__)
31
32    def __sub__(self, other):
33        if type(other) == int:
34            return self - Rational(other)
35        elif type(other) == Rational:

```

```

34         return Rational( self.num * other.denum - self.denum * other.num,
35                           self.denum * other.num )
36     raise TypeError("unsupported operand type(s) for - or sub(): '
37                     Rational' and '{}'.format(type(other).__name__))
38
39 def __mul__(self, other):
40     if type(other) == int:
41         return self * Rational(other)
42     elif type(other) == Rational:
43         return Rational( self.num * other.num, self.denum * other.denum )
44     raise TypeError("unsupported operand type(s) for * or mul(): '
45                     Rational' and '{}'.format(type(other).__name__))
46
47 def __truediv__(self, other):
48     if type(other) == int:
49         return self / Rational(other)
50     elif type(other) == Rational:
51         if other.num == 0:
52             raise ZeroDivisionError("division by zero")
53         return Rational( self.num * other.denum, self.denum * other.num )
54     raise TypeError("unsupported operand type(s) for / or truediv(): '
55                     Rational' and '{}'.format(type(other).__name__))
56
57 def __pow__(self, n): # supports only integer powers
58     if not type(n) == int:
59         raise TypeError("unsupported operand type(s) for ** or pow(): '
60                         Rational' and '{}'.format(type(n).__name__))
61     if n >= 0:
62         return Rational(self.num**n, self.denum**n)
63     return Rational(self.denum, self.num)**(-n)
64
65 def __pos__(self):
66     return Rational( self.num, self.denum )
67
68 def __neg__(self):
69     return Rational( -self.num, self.denum )
70
71 def __abs__(self):
72     if self.num <= 0 and self.denum > 0:
73         return Rational(-self.num, self.denum)
74     elif self.num >= 0 and self.denum < 0:
75         return Rational(self.num, -self.denum)
76     return Rational(self.num, self.denum)
77
78 def __eq__(self, other):
79     if type(other) == int: # allows comparison to int, used for x == 0
80         return (self == Rational(other))
81     return (self.num * other.denum == self.denum * other.num)
82
83 def __float__(self):
84     return self.num / self.denum

```

Die LU-Zerlegung von passenden Matrix mit ganzzahligen Einträgen kann nun dem folgenden naiven Algorithmus berechnet werden:

```

1 def naive_lu(A): # expects a Rational valued matrix as input

```

```

2   if A.height != A.width:
3       raise ValueError("matrix is not square")
4   U = copymatrix(A)  # circumvent pass by reference
5   n = U.height
6   L = identitymatrix(n)
7   # bring U in upper triangular form, change L such that always LU = A
8   for j in range(n):
9       if U[j][j] == 0:
10          raise ValueError("algorithm does not work for this matrix")
11       for i in range(j+1,n):
12          L.addcolumn(j, i, U[i][j]/U[j][j]) # important: change L first
13          U.addrow(i, j, -U[i][j]/U[j][j])
14   return (L,U)

```

Wir testen das Program anhand der gegebenen Matrizen

$$A = \begin{pmatrix} 3 & 2 & 1 \\ 6 & 6 & 3 \\ 9 & 10 & 6 \end{pmatrix} \quad \text{und} \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

mit dem folgenden Code:

```

1 A = Matrix([[3,2,1],[6,6,3],[9,10,6]])
2 print("A:")
3 print(A)
4 (L,U) = naive_lu(A.mapentries(Rational))
5 print("L:")
6 print(L)
7 print("U:")
8 print(U)
9 B = Matrix([[0,1],[1,0]])
10 print("B:")
11 print(B)
12 print("Trying to calculate the LU decomposition of B:")
13 (L,U) == naive_lu(B)

```

Als Output erhalten wir folgendes:

```

$ python exercise_03_04.py
A:
[3 2 1]
[6 6 3]
[9 10 6]
L:
[9/9  0/18  0]
[18/9 18/18 0]
[27/9 36/18 1]
U:
[3/1  2/1  1/1  ]
[0/3  6/3  3/3  ]
[0/162 0/162 162/162]
Check if L*U == A:
True
B:
[0 1]
[1 0]

```



```

Trying to calculate the LU decomposition of B:
Traceback (most recent call last):
  File "exercise_03_04.py", line 62, in <module>
    (L,U) == naive_lu(B)
  File "exercise_03_04.py", line 15, in naive_lu
    raise ValueError("algorithm does not work for this matrix")
ValueError: algorithm does not work for this matrix

```

Da die Matrix B keine LU-Zerlegung besitzt, ist es okay, dass unser Algorithmus diese nicht findet.

Exercise 3.5

Wir bestimmen die Cholesky-Zerlegung eintragsweise.

```

1 def cholesky(A):    # expects int or float as matrix entries
2     if A.height != A.width:
3         raise ValueError("matrix is not square")
4     B = copymatrix(A)
5     n = B.height
6     L = zeromatrix(n,n)
7     for i in range(n):
8         rowsum = 0
9         for j in range(i):
10            s = 0
11            for k in range(j):
12                s += L[i][k] * L[j][k]
13            L[i][j] = (B[i][j] - s)/L[j][j]
14            rowsum += L[i][j]**2
15     L[i][i] = sqrt( B[i][i] - rowsum )
16     return L

```

Für die gegebenen Matrizen

$$A = \begin{pmatrix} 1 & 2 & 1 \\ 2 & 5 & 2 \\ 1 & 2 & 10 \end{pmatrix} \quad \text{und} \quad B = \begin{pmatrix} 1.01 \cdot 10^{-2} & 0.705 & 1.42 \cdot 10^{-2} \\ 0.705 & 49.5 & 1 \\ 1.42 \cdot 10^{-2} & 1 & 1 \end{pmatrix}$$

testen wir unser Programm mit dem folgenden Code:

```

1 A = Matrix([[1,2,1],[2,5,2],[1,2,10]])
2 print("A:")
3 print(A)
4 L = cholesky(A)
5 print("L:")
6 print(L)
7 print("L * L^T:")
8 print(L * L.transpose())
9 B = Matrix([[1.01E-2, 0.705, 1.42E-2],[0.705,49.5,1],[1.42E-2,1,1]])
10 print("B:")
11 print(B)
12 L = cholesky(B)
13 print("L:")

```

```

14 print(L)
15 print("L * L^T:")
16 print(L * L.transpose())

```

Wir erhalten den folgenden Output:

```

$ python exercise_03_05.py
A:
[1 2 1 ]
[2 5 2 ]
[1 2 10]
L:
[1.0 0 0 ]
[2.0 1.0 0 ]
[1.0 0.0 3.0]
L * L^T:
[1.0 2.0 1.0 ]
[2.0 5.0 2.0 ]
[1.0 2.0 10.0]
B:
[0.0101 0.705 0.0142]
[0.705 49.5 1 ]
[0.0142 1 1 ]
L:
[0.1004987562112089 0 0 ]
[7.015012190980423 0.5381486415443629 0 ]
[0.14129528100981847 0.016374437298272527 0.9898320672556135]
L * L^T:
[0.010100000000000001 0.705 0.014200000000000003]
[0.705 49.5 1.0 ]
[0.014200000000000003 1.0 1.0 ]

```

Exercise 3.6

Mithilfe elementarer Zeilenumformungen, die in der Klasse `Matrix` implementiert sind, lässt sich nun der Gauß-Algorithmus zum Invertieren von Matrizen implementieren.

```

1 # we assume that the input matrix is well-behaved
2 # i.e. entries allow a reasonable comparison to 0
3 def invert(A):
4     if A.height != A.width:
5         raise ValueError("matrix is not square")
6     B = copymatrix(A) # circumvent pass by reference
7     n = B.height
8     Inv = identitymatrix(n)
9     B = B.mapentries(Rational) # make all
10    Inv = Inv.mapentries(Rational) # entries rational
11    # bring B in lower triangular form
12    for j in range(n):
13        p = -1
14        for i in range(j,n):
15            if B[i][j] != 0:
16                p = i
17                break

```

```

18         if p == -1:
19             raise ZeroDivisionError("matrix is not invertible")
20         for i in range(p+1,n):
21             Inv.addrow(i, p, -B[i][j]/B[p][j]) # import: change inverse
22             first
23             B.addrow(i, p, -B[i][j]/B[p][j])

```

Wir testen unser Programm anhand der gegebenen Matrix

$$A = \begin{pmatrix} 3 & -1 & 2 \\ -3 & 4 & -1 \\ -6 & 5 & -2 \end{pmatrix}$$

mit dem folgenden Code:

```

1 A = Matrix([[3,-1,2],[-3,4,-1],[-6,5,-2]])
2 print("A:")
3 print(A)
4 B = invert(A)
5 print("A^(-1) with rationals:")
6 print(B)
7 print("A^(-1) with floats:")
8 print(B.mapentries(float))
9 print("Checking if A*B = I (using rationals):")
10 print(A.mapentries(Rational) * B == identitymatrix(3))

```

Dabei nutzen wir erneut die Klasse `Rational`, um ein genaues Rechnen zu erlauben. Wir erhalten den folgenden Output:

```

python exercise_03_06.py
A:
[3  -1  2 ]
[-3  4  -1]
[-6  5  -2]
A^(-1) with rationals:
[-1162261467/3486784401  3099363912/3486784401  -2711943423/3486784401]
[0/43046721             28697814/43046721  -14348907/43046721 ]
[59049/59049            -59049/59049      59049/59049       ]
A^(-1) with floats:
[-0.3333333333333333  0.8888888888888888  -0.7777777777777778]
[0.0                0.6666666666666666  -0.3333333333333333]
[1.0                -1.0                1.0                ]
Checking if A*B = I (using rationals):
True

```

Exercise 3.8

(1)

Alle notwendigen Funktionswerte werden zunächst berechnet und in einer Liste gespeichert, um mehrfaches Berechnen des gleichen Funktionswertes zu umgehen.

```

1 def trapeze(f,a,b,n):
2     values = [f(a + (k/n)*(b-a)) for k in range(n+1)]
3     integral = 0
4     for i in range(len(values)-1):
5         integral += values[i] + values[i+1]
6     integral = (b-a)*integral/n/2
7     return integral

```

(2)

Wir testen unser Programm anhand des gegebenen Integrals $\int_0^\pi \sin(x) dx$ mit dem folgenden Code:

```

1 from math import sin, pi
2 n = 1
3 s = 0
4 while 2 - s >= 1.E-6: # sin is concave on [0,pi] -> estimate too small
5     n += 1           # can skip n = 1 because it results in 0
6     s = trapeze(sin, 0, pi, n)
7
8 print("Estimate for integral of sin from 0 to pi using trapeze:")
9 print(s)

```

Wir erhalten den folgenden Output:

```

$ python exercise_03_08.py
Estimate for integral of sin from 0 to pi using trapeze:
1.9999990007015205

```

Exercise 3.9

(1)

Wir definieren eine neue Funktion `powertrapeze`, welche das angegebene Verfahren implementiert:

```

1 def powertrapeze(f, a, b, mmax):
2     integrals = [] # list of the approximations
3     values = [f(a), f(b)] # list of the calculated values
4     for m in range(1,mmax+1):
5         n = 2**m
6         for k in range(1,n,2):
7             values.insert(k, f(a + (k/n)*(b-a))) # add new values
8         integral = 0
9         for i in range(len(values)-1):
10             integral += values[i] + values[i+1]
11         integral = (b-a)*integral/n/2
12         integrals.append(integral) # add new approx.
13     return integrals

```

Hiermit berechnen die Approximationen für $\int_0^\pi \sin(x) dx$ für $m = 1, \dots, 10$ mit dem folgenden Code:

```

1 from math import sin, pi
2 m = 10
3 results = powertrapeze(sin, 0, pi, m)
4 print("Calculate trapeze estimate for int. of sin from 0 to pi, 2^m intervals
   :")
5 print(" m \testimate \t\terror")
6 for i in range(m):
7     print("{:2d}\t{}\t{: .20f}".format(i+1, results[i], 2-results[i]))

```

Wir erhalten den folgenden Output:

```

Calculate trapeze estimate for int. of sin from 0 to pi, 2^m intervals:
m      estimate      error
1      1.5707963267948966    0.42920367320510344200
2      1.8961188979370398    0.10388110206296019555
3      1.9742316019455508    0.02576839805444919307
4      1.9935703437723395    0.00642965622766045186
5      1.9983933609701445    0.00160663902985547224
6      1.9995983886400386    0.00040161135996141795
7      1.9998996001842035    0.00010039981579645918
8      1.9999749002350518    0.00002509976494824429
9      1.9999937250705773    0.00000627492942273378
10     1.9999984312683816    0.00000156873161838433

```

(2)

Es fällt auf, dass sich der Fehler in jedem Schritt etwa geviertelt wird. Bezeichnet a_n die n -te Approximation, so gilt $a_0 \leq a_1 \leq \dots \leq a_n$; deshalb ist diese Beobachtung äquivalent dazu, dass die Quotienten $(a_i - a_{i+1}) / (a_{i+1} - a_{i+2})$ ungefähr 4 sind.

Dies testen wir mit dem folgenden weiteren Code:

```

1 print("Quotients of any two subsequent differences of estimates:")
2 for i in range(m-2):
3     q = (results[i] - results[i+1]) / (results[i+1] - results[i+2])
4     print(q)

```

Wir erhalten den folgenden Output:

```

Quotients of any two subsequent differences of estimates:
4.164784400584785
4.039182316416593
4.009677144752887
4.002411992937073
4.00060254408483
4.000150607761501
4.000037649528035
4.000009414842847

```

(3)

Wir berechnen die Approximationen für $\int_0^2 3^{3x-1} dx$ für $m = 1, \dots, 10$ mit dem folgenden Code:

```
1 m = 10
2 f = (lambda x : 3**(3*x-1))
3 results = powertrapeze( f, 0, 2, m)
4 print("Calculate trapeze estimate for int. of 3^(3x-1) from 0 to 2, 2^m
      intervals:")
5 print(" m \testimate")
6 for i in range(m):
7     print("{:2d}\t{:24.20f}".format(i+1, results[i]))
```

Wir erhalten den folgenden Output:

```
Calculate trapeze estimate for int. of 3^(3x-1) from 0 to 2, 2^m intervals:
m      estimate
1      130.66666666666665719276
2      89.58204463929762084717
3      77.74742639121230070032
4      74.66669853961546721166
5      73.88840395800384897029
6      73.69331521665949935596
7      73.64451070980437918934
8      73.63230756098684537392
9      73.62925664736960129630
10     73.62849391106399821183
```

Da f konvex ist, sind die Approximationen b_n monoton fallend. Die Vermutung lässt sich erneut durch das Betrachten der Quotienten $(b_i - b_{i+1})/(b_{i+1} - b_{i+2})$ überprüfen. Wir nutzen den folgenden Code:

```
1 print("Quotients of any two subsequent differences of estimates:")
2 for i in range(m-2):
3     q = (results[i] - results[i+1])/(results[i+1] - results[i+2])
4     print(q)
```

Wir erhalten den folgenden Output:

```
Quotients of any two subsequent differences of estimates:
3.471562932248868
3.841500716121706
3.958305665211694
3.9894387356667425
3.9973509398114637
3.9993371862347957
3.9998342622879792
3.999958563440565
```

Unsere Vermutung scheint sich zu bestätigen.

Exercise 3.10

Für die Funktion $f(x) = e^{x^2}$ gilt $f''(x) = (4x^2 + 2)e^{x^2}$. Da $f''(x) > 0$ auf $[0, 1]$ monoton steigend ist, gilt für alle $0 \leq a \leq b \leq 1$, dass

$$|E(f, a, b)| \leq \frac{(b-a)^3}{12} \max_{a \leq x \leq b} |f''(x)| \leq \frac{(b-a)^3}{12} f''(b).$$

Für alle $n \geq 1$ und $0 \leq k \leq n-1$ gilt deshalb

$$\left| E\left(f, \frac{k}{n}, \frac{k+1}{n}\right) \right| \leq \frac{1}{12n^3} \left(4 \left(\frac{k+1}{n} \right)^2 + 2 \right) \underbrace{e^{((k+1)/n)^2}}_{\leq e \leq 4} \leq \frac{1}{12n^3} (4+2) \cdot 4 \leq \frac{2}{n^3}.$$

Der gesamte Fehler für eine Unterteilung von $[0, 1]$ in n Intervalle lässt sich deshalb insgesamt durch

$$n \cdot \frac{2}{n^3} = \frac{2}{n^2}$$

abschätzen. Dabei gilt

$$\frac{2}{n^2} < 10^{-6} \iff n^2 > 2 \cdot 10^6 \iff n > \sqrt{2} \cdot 10^3 \iff n > 1500.$$

Für das verbesserte Trapezverfahren aus Exercise 3.9 gilt mit $n = 2^m$, dass $n > 1500$ für $m \geq 11$. Wir nutzen nun den folgenden Code, um die entsprechenden Approximationen für $m = 1, \dots, 11$ zu bestimmen:

```

1 from math import exp
2 f = (lambda x: exp(x**2))
3 m = 11
4 results = powertrapeze(f, 0, 1, m)
5 print("Calculate trapeze estimate for int. of e^(x^2) from 0 to 1, 2^m
    intervals:")
6 for i in range(m):
7     print("m={:2d}\t{:24.20f}".format(i+1, results[i]))

```

Wir erhalten den folgenden Output:

```

$ python exercise_03_10.py
Calculate trapeze estimate for int. of e^(x^2) from 0 to 1, 2^m intervals:
m= 1      1.57158316545863208091
m= 2      1.49067886169885532865
m= 3      1.46971227642966528748
m= 4      1.46442031014948170764
m= 5      1.46309410260642858148
m= 6      1.46276234857772702291
m= 7      1.46267939741858832292
m= 8      1.46265865883777390621
m= 9      1.46265347414312651964
m=10     1.46265217796637525538
m=11     1.46265185392199392744

```

Exercise 3.11

Ist $T_n(x) = \sum_{k=0}^n x^k/k!$ das k -te Taylorpolynom für f an der Entwicklungsstelle 0, so gilt für das Restglied $R_n(x) := e^x - T_n(x)$, dass es für jedes $x \in \mathbb{R}$ ein ξ zwischen 0 und x gibt, so dass

$$R_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \xi^n = \frac{e^\xi \xi^n}{(n+1)!}.$$

Für alle $x \geq 0$ gilt $e^\xi \leq e^x \leq 3^x$, und somit gilt

$$|R_n(x)| \leq \frac{3^x x^n}{(n+1)!} \quad \text{für alle } x \geq 0.$$

Für alle $x \leq 0$ gilt $e^\xi \leq e^0 = 1$, und somit

$$|R_n(x)| \leq \frac{(-x)^n}{(n+1)!}.$$

Dies führt zu dem folgenden Code:

```

1 def exp_approx(x):
2     y = 1          # current approx
3     d = 6          # number of digits
4     n = 1
5     fac = 1        # n!
6     if x >= 0:
7         while fac < (3**x) * (x**(n+1)) * 10**d:
8             y += x**n / fac
9             n += 1
10            fac *= n
11    if x < 0:
12        while fac < ((-x)**(n+1)) * 10**d:
13            y += x**n / fac
14            n += 1
15            fac *= n
16    return y

```

Wir testen die Genauigkeit des Programms mit dem folgenden Code:

```

1 from math import exp
2 print("Comparison of exp_approx(x) and exp(x) up to 7 digits.")
3 print("{:>3s}   {:>22s}   {:>22s}   {:>13s}".format("x", "approximation", "exact",
4     "difference (10 digits)"))
5 for x in range(-30,31):
6     approx = exp_approx(x)
7     exact = exp(x)          # not really exact, but better than the above
8     print("{:3d}   {:22.7f}   {:22.7f}   {:13.10f}".format(x, approx, exact,
9         exact-approx))

```

Wir erhalten den folgenden (gekürzten) Output:

x	approximation	exact	difference (10 digits)
-30	-0.0000855	0.0000000	0.0000855145

-29	0.0000551	0.0000000	-0.0000550745
-28	0.0000050	0.0000000	-0.0000050079
-27	-0.0000045	0.0000000	0.0000044619
-26	-0.0000014	0.0000000	0.0000013633
-25	-0.0000006	0.0000000	0.0000006464
-24	-0.0000003	0.0000000	0.0000002671
-23	-0.0000000	0.0000000	0.0000000403
-22	-0.0000000	0.0000000	0.0000000071
-21	-0.0000000	0.0000000	0.0000000192
[...]			
21	1318815734.4832141	1318815734.4832146	0.0000004768
22	3584912846.1315928	3584912846.1315918	-0.0000009537
23	9744803446.2489052	9744803446.2489033	-0.0000019073
24	26489122129.8434715	26489122129.8434715	0.0000000000
25	72004899337.3858795	72004899337.3858795	0.0000000000
26	195729609428.8387451	195729609428.8387756	0.0000305176
27	532048240601.7988281	532048240601.7986450	-0.0001831055
28	1446257064291.4738770	1446257064291.4750977	0.0012207031
29	3931334297144.0424805	3931334297144.0419922	-0.0004882812
30	10686474581524.4667969	10686474581524.4628906	-0.0039062500

Für etwa $x \geq 23$ und $x \leq -26$ hat unsere Approximation nicht mehr mit der gewünschten Genauigkeit, da die aufzuaddierenden Summanden $x^n/n!$ dann betragsmäßig zu klein werden.

Exercise 3.12

(1)

Wir definieren zunächst eine Klasse `TimeoutError`, um ggf. eine passende Fehlermeldung ausgeben zu können.

```
1 class TimeoutError(Exception):
2     pass
```

Wir implementieren das Newton-Verfahren für mit der gewünschten Genauigkeit:

```
1 def newton(f, f_prime, x):
2     n = 1
3     xold = x
4     xnew = x
5     while n <= 100:
6         d = f_prime(xold)
7         if d == 0:
8             raise ZeroDivisionError("derivative vanishes at {}".format(xold))
9         xnew = xold - f(xold)/d
10        if 0 <= xnew - xold <= 1.E-7 or 0 <= xold - xnew <= 1.E-7:
11            return xnew
12        xold = xnew
13        n += 1
14    raise TimeoutError("the calculation takes too long")
```

(2)

Wir testen unser Programm anhand der gegebenen Funktion $f(x) = x^2 - 2$ mit dem folgenden Code:

```
1 f = (lambda x: x**2 - 2)
2 fprime = (lambda x: 2*x)
3 print("Calculating an approximation of sqrt(2):")
4 print( newton(f, fprime, 1) )
5 #   Calculating an approximation of sqrt(2):
6 #   1.4142135623730951
```

Wir erhalten den folgenden Output:

```
$ python exercise_03_12.py
Calculating an approximation of sqrt(2):
1.4142135623730951
```

Dabei stimmen die ersten 15 Nachkommestellen mit dem exakten Ergebnis überein.