Solutions to Exercises to

Programming Methods in Scientific Computing

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Letzte Änderung: 22. November 2017

Chapter 3 Python, the Fundamentals

Exercise 3.1

Exercise 3.2

Wir weitern die gegeben 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.

```
class Polynomial:
    def __init__(self, coeff):
        self.coeff = coeff

    def __str__(self):
        s = ""
        if self.coeff == []:
            s = "0"
        else:
            s += "{} x^0".format(self.coeff[0])
        for i in range(1,len(self.coeff)):
            s += " + {} x^{}".format(self.coeff[i], i)
        return s

    def __repr__(self):
        return str(s)

    def __call__(self, x):
        s = 0
        for i in range(len(self.coeff)):
            s += self.coeff[i]*x**i
        return s

    def __add__(self, other):
        l = []
        if len(self.coeff) > len(other.coeff):
            l += self.coeff
            for i in range(len(other.coeff)):
                l[i] += other.coeff[i]
        else:
            l += other.coeff
            for i in range(len(self.coeff)):
                l[i] += self.coeff[i]
        return Polynomial(l)

    def __eq__(self, other):
```

```
        return self.coeff == other.coeff

    def derivative(self):
        coeff = []
        for i in range(1,len(self.coeff)):
            coeff.append(i * self.coeff[i])
        return Polynomial(coeff)

    def antiderivative(self):
        coeff = [0]
        for i in range(len(self.coeff)):
            coeff.append(self.coeff[i]/(i+1))
        return Polynomial(coeff)
```

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

```
p = Polynomial([1,2,3])
print("The given polynmial p:")
print(p)
print("The derivative of p:")
print( p.derivative() )
print("The antiderivative of p:")
print( p.antiderivative() )
print("Taking antiderivative and then derivative:")
print( p.antiderivative().derivative() )
```

Dabei erhalten wir den folgenden Output:

```
$ python exercise_03_02.py
The given polynmial 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.

```
class Matrix():
    def __init__(self, entries):
        m = len(entries)
        if m == 0:
            raise ValueError("height must be positive")
        n = len(entries[0])
        if n == 0:
            raise ValueError("width must be positive")
        for i in range(1, m):
```

```
            if len(entries[i]) != n:
                raise ValueError("rows must have the same width")
        self.height = m
        self.width = n
        self.entries = entries

    def __getitem__(self, i):       # allows to get the rows via A[i]
        return self.entries[i]

    def __setitem__(self, i, k):    # allows to set rows via A[i]
        self.entries[i] = k

    def __str__(self):              # allows print(A) for a Matrix A
        rows = ["["]*self.height
        for j in range(self.width): # construct output columnwise, align left
            numbers = []            # numbers to appear in column j
            maxlen = 0              # maximal length of a number in column j
            for i in range(self.height):
                s = str(self[i][j])
                numbers.append(s)
                if len(s) > maxlen:
                    maxlen = len(s)
            for i in range(self.height):
                # pad the entries if they are too short
                rows[i] += numbers[i] + " "*(maxlen-len(numbers[i])) + " "
        s = ""
        for r in rows:
            s += r[:-1] + "]\n" # remove white space at the end of ech line
        s = s[:-1]              # remove empty line at the end
        return s

    def __repr__(self):
        return str(self)

    def __mul__(self, other):
        if self.width != other.height:
            raise TypeError('matrix dimensions do not match')
        newentries = []
        for i in range(self.height):
            row = []
            for j in range(other.width):
                s = self[i][0] * other[0][j]    # makes s have the right type
                for k in range(1, self.width):
                    s += self[i][k] * other[k][j]
                row.append(s)
            newentries.append(row)
        return Matrix(newentries)

    def __eq__(self, other):
        if self.height != other.height or self.width != other.width:
                return False
        for i in range(self.height):
            for j in range(self.width):
                if self[i][j] != other[i][j]:
                    return False
        return True
```

```

    def mapentries(self, f):        # applies a function to all entries
        A = zeromatrix(self.height, self.width) # zeromatrix is defined below
        for i in range(self.height):
            for j in range(self.width):
                A[i][j] = f(self[i][j])
        return A

    def addrow(self, i, j, c):      # add c times row j to row i
        for k in range(self.width):
            self[i][k] =  c * self[j][k] + self[i][k]
            # makes c responsible for implementing the operations

    def addcolumn(self, i, j, c):   # add c times column j to column i
        for k in range(self.height):
            self[k][i] = c * self[k][j] + self[k][i]

    def multrow(self, i, c):        # multiply row i with c
        for j in range(self.width):
            self[i][j] = c * self[i][j]

    def multcolumn(self, j, c):     # multiply row j with c
        for i in range(self.height):
            self[i][j] = c * self[i][j]

    def swaprows(self, i, j):       # swap rows i and j
        if i > self.height or j > self.height:
            raise ValueError("swap nonexistent rows")
        l = self[i]
        self[i] = self[j]
        self[j] = l

    def transpose(self):
        T = zeromatrix(self.width, self.height)
        for i in range(self.height):
            for j in range(self.width):
                T[j][i] = self[i][j]
        return T
```

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

```
def zeromatrix(height, width):  # creates a zero matrix
    entries = []
    for i in range(height):
        entries.append([0]*width)
    return Matrix(entries)

def identitymatrix(size):       # creates an identiy matrix
    E = zeromatrix(size, size)
    for i in range(size):
        E[i][i] = 1
    return E
```

Die Assoziativität der Matrixmultiplikation testen wir mit dem folgenden Code:

```
A = Matrix([[0,1],[1,0],[1,1]])
print("A:")
```

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

```
class Rational():
    def __init__(self, num, denum = 1):   # default denumerator is 1
        if type(num) == Rational:
            p = num/Rational(denum)
            self.num = p.num
            self.denum = p.denum
        elif type(num) != int:
            raise TypeError("numerator is no integer")
        elif type(denum) != int:
            raise TypeError("denumerater is no integer")
        elif denum == 0:
            raise ZeroDivisionError("denumerator is zero")
        else:
            self.num = num
            self.denum = denum

    def __str__(self):    # allows print(x) for Rational x
        return "{}/{}".format(self.num, self.denum)

    def __repr__(self):
        return str(self)
```

```
    def __add__(self, other):
        if type(other) == int:
            return self + Rational(other)
        elif type(other) == Rational:
            return Rational( self.num * other.denum + self.denum * other.num,
                 self.denum * other.denum )
        raise TypeError("unsupported operand type(s) for + or add(): '
            Rational' and '{}'".format(type(other).__name__))

    def __sub__(self, other):
        if type(other) == int:
            return self - Rational(other)
        elif type(other) == Rational:
            return Rational( self.num * other.denum - self.denum * other.num,
                 self.denum * other.num )
        raise TypeError("unsupported operand type(s) for - or sub(): '
            Rational' and '{}'".format(type(other).__name__))

    def __mul__(self, other):
        if type(other) == int:
            return self * Rational(other)
        elif type(other) == Rational:
            return Rational( self.num * other.num, self.denum * other.denum )
        raise TypeError("unsupported operand type(s) for * or mul(): '
            Rational' and '{}'".format(type(other).__name__))

    def __truediv__(self, other):
        if type(other) == int:
            return self / Rational(other)
        elif type(other) == Rational:
            if other.num == 0:
                raise ZeroDivisionError("division by zero")
            return Rational( self.num * other.denum, self.denum * other.num)
        raise TypeError("unsupported operand type(s) for / or truediv(): '
            Rational' and '{}'".format(type(other).__name__))

    def __pow__(self, n):   # supports only integer powers
        if not type(n) == int:
            raise TypeError("unsupported operand type(s) for ** or pow(): '
                Rational' and '{}'".format(type(n).__name__))
        if n >= 0:
            return Rational(self.num**n, self.denum**n)
        return Rational(self.denum, self.num)**(-n)

    def __pos__(self):
        return Rational( self.num, self.denum )

    def __neg__(self):
        return Rational( -self.num, self.denum )

    def __abs__(self):
        if self.num <= 0 and self.denum > 0:
            return Rational(-self.num, self.denum)
        elif self.num >= 0 and self.denum < 0:
            return Rational(self.num, -self.denum)
```

```
        return Rational(self.num, self.denum)

    def __eq__(self, other):
        if type(other) == int:  # allows comparison to int, used for x == 0
            return (self == Rational(other))
        return (self.num * other.denum == self.denum * other.num)

    def __float__(self):
        return self.num / self.denum
```

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

```
from copy import deepcopy

# expects the matrix entries to be comparable to 0 in a sensible way
def naive_lu(A):
    if A.height != A.width:
        raise ValueError("matrix is not square")
    U = deepcopy(A)   # circumvent pass by reference
    n = U.height
    L = identitymatrix(n)
    # bring U in upper triangular form, change L such that always LU = A
    for j in range(n):
        if U[j][j] == 0:
            raise ValueError("algorithm does not work for this matrix")
        for i in range(j+1,n):
            L.addcolumn(j, i,  U[i][j]/U[j][j]) # important: change L first
            U.addrow(i, j, -U[i][j]/U[j][j])
    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:

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

Als Output erhalten wir das Folgende:

```
$ 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.

```python
from copy import deepcopy
from math import sqrt

# expects int or float as matrix entries
def cholesky(A):
    if A.height != A.width:
        raise ValueError("matrix is not square")
    B = deepcopy(A)
    n = B.height
    L = zeromatrix(n,n)
    for i in range(n):
        rowsum = 0
        for j in range(i):
            s = 0
            for k in range(j):
                s += L[i][k] * L[j][k]
            L[i][j] = (B[i][j] - s)/L[j][j]
            rowsum += L[i][j]**2
        L[i][i] = sqrt( B[i][i] - rowsum )
    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:

```
A = Matrix([[1,2,1],[2,5,2],[1,2,10]])
print("A:")
print(A)
L = cholesky(A)
print("L:")
print(L)
print("L * L^T:")
print(L * L.transpose())
B = Matrix([[1.01E-2, 0.705, 1.42E-2],[0.705,49.5,1],[1.42E-2,1,1]])
print("B:")
print(B)
L = cholesky(B)
print("L:")
print(L)
print("L * L^T:")
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.

```
from copy import deepcopy

# expects the matrix entries to be comparable to 0 in a sensible way
def invert(A):
    if A.height != A.width:
        raise ValueError("matrix is not square")
    B = deepcopy(A)   # circumvent pass by reference
    n = B.height
    Inv = identitymatrix(n)
    B = B.mapentries(Rational)      # make all
    Inv = Inv.mapentries(Rational)  # entries rational
    # bring B in lower triangular form
    for j in range(n):
        p = -1
        for i in range(j,n):
            if B[i][j] != 0:
                p = i
                break
        if p == -1:
            raise ZeroDivisionError("matrix is not invertible")
        for i in range(p+1,n):
            Inv.addrow(i, p, -B[i][j]/B[p][j])  # import: change inverse first
            B.addrow(i, p, -B[i][j]/B[p][j])
    # norm the diagonal entries
    for i in range(n):
        Inv.multrow(i, B[i][i]**(-1))   # **(-1) also works for Rational
        B.multrow(i, B[i][i]**(-1))
    # bring B into identity form
    for j in range(n):
        for i in range(j):
            Inv.addrow(i, j, -B[i][j])
            B.addrow(i, j, -B[i][j])
    return Inv
```

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:

```
A = Matrix([[3,-1,2],[-3,4,-1],[-6,5,-2]])
print("A:")
print(A)
B = invert(A)
print("A^(-1) with rationals:")
print(B)
print("A^(-1) with floats:")
```

```
print(B.mapentries(float))
print("Checking if A*B == I (using rationals):")
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 3.7

Wir Berechnen die QR-Zerlegung einer nicht-singulären Matrix A durch Anwenden des Gram-Schmidt-Verfahrens auf die Spalten von A, von links nach rechts:

```
from copy import deepcopy
from math import sqrt

# assumes the matrix to have integer or float values
# and to be nonsingular
def qrdecomp(A):
    if A.height != A.width:
        return ValueError("only square matrices are supported")
    n = A.height
    Q = deepcopy(A)
    R = identitymatrix(n)
    for j in range(n):
        # make the j-th column of Q orthogonal to the next columns
        for k in range(j):
            s = 0   # inner product of j-th and k-th columns
            for i in range(n):
                s += Q[i][j] * Q[i][k]
            Q.addcolumn(j, k, -s)
            R.addrow(k, j, s)
        sn = 0   # squared norm of the j-th column
        for i in range(n):
            sn += Q[i][j]**2
        Q.multcolumn(j, sqrt(sn)**(-1))
        R.multrow(j, sqrt(sn))
    return (Q,R)
```

Für die gegebene Matrix

$$A = \begin{pmatrix} 12 & -51 & 4 \\ 6 & 167 & -68 \\ -4 & 24 & -41 \end{pmatrix}$$

testen wir das Programm mithilfe des folgenden Codes:

```
A = Matrix([[12,-51,4],[6,167,-68],[-4,24,-41]])
print("A:")
print(A)
(Q,R) = qrdecomp(A)
print("Q:")
print(Q)
print("Q * Q^T:")
print(Q * Q.transpose())
print("R:")
print(R)
print("Q*R:")
print(Q*R)
```

Wir erhalten den folgenden Output:

```
$ python exercise_03_07.py
A:
[12 -51 4  ]
[6  167 -68]
[-4 24  -41]
Q:
[0.8571428571428571  -0.3942857142857143 -0.33142857142857124]
[0.42857142857142855 0.9028571428571428  0.03428571428571376 ]
[-0.2857142857142857 0.17142857142857143 -0.9428571428571428 ]
Q * Q^T:
[0.9999999999999998      1.474514954580286e-16 -1.6653345369377348e-16]
[1.474514954580286e-16   0.9999999999999998    4.996003610813204e-16  ]
[-1.6653345369377348e-16 4.996003610813204e-16 1.0                    ]
R:
[14.0 20.999999999999996 -14.000000000000002]
[0.0  175.0              -69.99999999999999 ]
[0.0  0.0                35.0               ]
Q*R:
[12.0 -51.0 4.000000000000002]
[6.0  167.0 -68.0            ]
[-4.0 24.0  -41.0            ]
```

Exercise 3.8

(1)

Alle notwendigen Funktionswerte werden zunächst berechnet und in einer Liste gespeichert, um das mehrfache Berechnen gleicher Funktionswerte zu umgehen.

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

(2)

Wir testen unser Programm anhand des gegebenen Integrals $\int_0^\pi \sin(x)\,\mathrm{d}x$ mit dem folgenden Code:

```python
from math import sin, pi
n = 1
s = 0
while 2 - s >= 1.E-6:   # sin is concave on [0,pi] -> estimate too small
    n += 1              # can skip n = 1 because it results in 0
    s = trapeze(sin, 0, pi, n)

print("Estimate for integral of sin from 0 to pi using trapeze:")
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:

```python
def powertrapeze(f, a, b, mmax):
    integrals = []              # list of the approximations
    values = [f(a), f(b)]       # list of the calculated values
    for m in range(1,mmax+1):
        n = 2**m
        for k in range(1,n,2):
            values.insert(k, f(a + (k/n)*(b-a)))    # add new values
        integral = 0
        for i in range(len(values)-1):
            integral += values[i] + values[i+1]
        integral = (b-a)*integral/n/2
        integrals.append(integral)                  # add new approx.
    return integrals
```

Hiermit berechnen die Approximationen für $\int_0^\pi \sin(x)\,\mathrm{d}x$ für $m = 1, \ldots, 10$ mit dem folgenden Code:

```
from math import sin, pi
m = 10
results = powertrapeze(sin, 0, pi, m)
print("Calculate trapeze estimate for int. of sin from 0 to pi, 2^m intervals:")
print(" m \testimate \t\terror")
for i in range(m):
    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 $a_0 \leq a_1 \leq \cdots \leq a_n$, da sin auf $[0, \pi]$ konkav ist. Deshalb ist die Vermutung 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:

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

Es fällt auf, dass das Verhältnis sogar gegen 4 zu gehen scheint.

(3)

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

```python
m = 10
f = (lambda x : 3**(3*x-1))
results = powertrapeze( f, 0, 2, m)
print("Calculate trapeze estimate for int. of 3^(3x-1) from 0 to 2, 2^m intervals:")
print(" m \testimate")
for i in range(m):
    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. Hierfür nutzen wir (erneut) den folgenden Code:

```python
print("Quotients of any two subsequent differences of estimates:")
for i in range(m-2):
    q = (results[i] - results[i+1])/(results[i+1] - results[i+2])
    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 $0 \le a \le b \le 1$, dass

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

Für alle $n \ge 1$ und $0 \le k \le n-1$ gilt deshalb

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

Der gesamte Fehler bei einer Unterteilung von $[0,1]$ in n Intervalle lässt sich deshalb durch

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

abschätzen. Dabei gilt

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

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

```
from math import exp
f = (lambda x: exp(x**2))
m = 11
results = powertrapeze(f, 0, 1, m)
print("Calculate trapeze estimate for int. of e^(x^2) from 0 to 1, 2^m
    intervals:")
for i in range(m):
    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 $f(x) = e^x$ an der Entwicklungsstelle 0, so gilt für das Restglied $R_n(x) \coloneqq e^x - T_n(x)$, dass es für jedes $x \in \mathbb{R}$ ein ξ zwschen 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

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

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:

```
def exp_approx(x):
    y = 1       # current approx
    d = 6       # number of digits
    n = 1
    fac = 1     # n!
    if x >= 0:
        while fac < (3**x) * (x**(n+1)) * 10**d:
            y += x**n / fac
            n += 1
            fac *= n
    if x < 0:
        while fac < ((-x)**(n+1)) * 10**d:
            y += x**n / fac
            n += 1
            fac *= n
    return y
```

Wir testen die Genauigkeit des Programms mit dem folgenden Code:

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

Wir erhalten den folgenden (gekürzten) Output:

```
Comparison of exp_approx(x) and exp(x) up to 7 digits.
  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 die gewünschten Genauigkeit, da die aufzuaddierenden Summanden $x^n/n!$ dann zu klein werden.

Exercise 3.12

(1)

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

```python
class TimeOutError(Exception):
    pass
```

Wir implementieren das Newton-Verfahren mit der gewünschten Genauigkeit:

```python
def newton(f, f_prime, x):
    n = 1
    xold = x
    xnew = x
    while n <= 100:
        d = f_prime(xold)
        if d == 0:
            raise ZeroDivisionError("derivative vanishes at {}".format(xold))
        xnew = xold - f(xold)/d
        if 0 <= xnew - xold <= 1.E-7 or 0 <= xold - xnew <= 1.E-7:
            return xnew
        xold = xnew
        n += 1
    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:

```
f = (lambda x: x**2 - 2)
fprime = (lambda x: 2*x)
print("Calculating an approximation of sqrt(2):")
print( newton(f, fprime, 1) )
```

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.