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Chapter 10

Introduction to Scientific Computation

Symbolic Computation with SymPy

Symbolic computation is an important tool for scientists, mathematicians and engineers. Some of the most well-developed systems are Mathematica and Maple. These commercial products are not free. A good alternative is SymPy, a Python library for symbolic computation. This chapter shows, by way of example, some basic capabilities of SymPy.

SymPy is well suited for the Jupyter notebook environment. The examples below are shown as they would appear in a jupyter notebook.¹

10.1 Basic SymPy commands

Import SymPy and define variables:

```
import sympy as sp
                                                  # import sympy
                                                  # define variables
           x,y,z,b = sp.symbols('x y z beta')
           x,y,z,b
Out [1]:
           (x, y, z, \beta)
```

Define functions:

```
# define an explicit function
Out [2]:
```

¹In newer versions of jupyter notebook, the words "In" and "Out" that preced the cell numbers are omitted. For clarity of presentation, "In" and "Out" are used here.

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In [3]:
$$g = x*(y + z)$$
 # another explicit function g # print g

Out [3]: x(y+z)

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Factor, expand and simplify:

Out [4]:
$$(x - y)(x + y)$$

Out [5]:
$$xy + xz$$

Out [6]:
$$x(y+z) + \frac{x^2 - y^2}{x - y}$$

Out [7]:
$$xy + xz + x + y$$

Collect, substitute and coefficients:

In [8]:
$$p = sp.expand((x + z)*(y + z)**2)$$
 # define p

Out [8]:
$$xy^2 + 2xyz + xz^2 + y^2z + 2yz^2 + z^3$$

In
$$[9]$$
: sp.collect(p,z) # collect terms in powers of z

Out [9]:
$$xy^2 + z^3 + z^2(x+2y) + z(2xy+y^2)$$

Out [10]:
$$y^2z + 3y^2 + 2yz^2 + 6yz + z^3 + 3z^2$$

In [11]:
$$p.subs(z,2*y)$$
 # substitute 2*y in place of z

Out [11]:
$$9xy^2 + 18y^3$$

Out [12]:
$$z^3 + 5z^2 + 8z + 4$$

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```
In [13]:
          p.coeff(z,2)
                               # coefficient of z^2
```

Out [13]: x + 2y

Equations and solutions:

Out [14]: $x^2 - 5x + 6$

Out [15]: $x^2 - 5x + 6 = 0$

Out [16]: [2, 3]

Out [17]:

In
$$[18]$$
: solns $[1]$ # print second solution (index = 1)

Out [18]:

Out [19]: True

Out [20]: True

Systems of equations:

In [21]:
$$g = 3*x + 2*y$$
 # define function g eq1 = $sp.Eq(g,7)$ # define equation g = 7 eq1 # print eq1

Out [21]: 3x + 2y = 7

```
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```

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```
In [22]:
            h = 2*x - y
                                 # Define function h
                                 # Define equation h = 4
            eq2 = sp.Eq(h,4)
            eq2
                                 # print eq2
            2x - y = 4
Out [22]:
 In [23]:
            solns = sp.solve((eq1,eq2),(x,y)) # solve equations
            solns
                                                 # print solns
Out [23]:
            \{x: 15/7, y: 2/7\}
 In [24]:
            # The solution is given as a dictionary.
            solns[x] # print dictionary value for x
            \frac{15}{7}
Out [24]:
 In [25]:
            solns[y]
                        # print dictionary value for y
Out [25]:
 In [26]:
            eq1.subs(((x,solns[x]),(y,solns[y]))) # check eq1
Out [26]:
            True
 In [27]:
            eq2.subs(((x,solns[x]),(y,solns[y]))) # check eq2
Out [27]:
            True
 In [28]:
            # Another example
            # Define equations and solve
            solns = solve((Eq(x**2 - y**2,0),Eq(x + 2*y,1)),(x,y))
                          # print solutions
            solns
Out [28]:
            [(-1, 1), (1/3, 1/3)]
 In [29]:
            # The solution is given as a list of tuples
            solns[0]
                       # print first solution
Out [29]:
            (-1, 1)
 In [30]:
            solns[1][0] # print first element of second solution
Out [30]:
            \bar{3}
```

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Built-in functions:

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```
In [31]:
          myroot = sp.sqrt(x*y)
                                     # square roots
          myroot
                                     # print
```

Out [31]:

Out [32]: $-\cos(2x)$

Out [33]:

Out [34]: $\log(x) + \log(y)$

Assumptions:

Out [36]: $v\sqrt{u^2}$

Out [37]: [0, -I, I]

In [38]: eq2 = sp.Eq(
$$w*(w**2 + 1),0$$
) # same polynomial in w sp.solve(eq2,w) # solve eq2

Out [38]: [0]

Working with numbers:

```
In [39]:
           sp.pi
                                      # pi
```

Out [39]: π ws-book9x6

In [40]:	<pre>sp.pi.evalf()</pre>	# pi to	15 significant	figures
Out [40]:	3.14159265358979			
In [41]:	sp.pi.evalf(30)	# pi to	30 significant	figures
Out [41]:	3.1415926535897932384626	64338328		
In [42]:	1/3	#	regular Python	calculation
Out [42]:	0.3333333333333333			
In [43]:	sp.Integer(1)/sp.Intege	er(3) #	symbolic 1/3	
Out [43]:	$\frac{1}{3}$			
In [44]:	sp.Rational(1,3)	#	symbolic 1/3	
Out [44]:	$\frac{1}{3}$			
In [45]:	<pre># evaluate 1/3 to 12 st sp.Rational(1,3).evalf</pre>	0	nt figures	

Out [45]:

Define the polynomial

$$p = (x+y)(x^2 - y)(ax + y)$$

using SymPy.

- \bullet Expand p.
- Find the coefficient of x^3 .

0.3333333333333

- \bullet Find the coefficient of a.
- Evaluate p at x = 7, y = 3.

Exercise 10.1b

Use SymPy to compute the following.

- Simplify the function x xz/y. Factor the polynomial $x^3 2x^2 + x 2$.
- Evaluate $\sin(e^x)$ at $x = \pi$ to 30 significant figures.

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Exercise 10.1c

Solve the system of equations

$$2x^2 - 9y^2 = 1 ,$$

$$3y - x^2 = 0 ,$$

using SymPy. Check that the equations are satisfied by each solution

10.2 Calculus with SymPy

Out [1]:
$$x\cos(y) - y$$

Derivatives:

In
$$[2]$$
: sp.diff(f,y) # differentiate f with respect to (wrt) y

Out [2]:
$$-x\sin(y) - 1$$

In
$$[3]$$
: sp.diff(f,x,y) # differentiate f wrt x and y

Out [3]:
$$-\sin(y)$$

$$\begin{array}{ll} \text{In [4]:} & \text{myder = sp.Derivative(f,x) \# symbolic derivative df/dx} \\ & \text{myder} & \text{\# print} \end{array}$$

Out [4]:
$$\frac{\partial}{\partial x}(x\cos(y) - y)$$

Out [5]: $\cos(y)$

Integrals:

Out [6]:
$$\frac{x^2 \cos(y)}{2} - xy$$

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In
$$[7]$$
: sp.integrate(f,x,y) # integrate f wrt x and y

Out [7]:
$$\frac{x^2 \sin(y)}{2} - \frac{xy^2}{2}$$

In
$$[8]$$
: sp.integrate(f,(y,-2,3)) # integrate f wrt y from -2 to 3

Out [8]:
$$x \sin(3) + x \sin(2) - \frac{5}{2}$$

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Out
$$[9]$$
: -5

Out [10]:
$$\int (x\cos(y) - y) \, dy$$

Out [11]:
$$x \sin(y) - \frac{y^2}{2}$$

Out [12]:
$$\int_{-1}^{1} (x \cos(y) - y) dy$$

Out [13]: $2x\sin(1)$

Differential equations:

Out [15]:
$$\frac{d}{dt}F(t)$$

Out [16]:
$$-F(t) + \frac{d^2}{dt^2}F(t) = e^t$$

Out [17]:
$$F(t) = C_2 e^{-t} + \left(C_1 + \frac{t}{2}\right) e^t$$

Limits and series:

Out [18]:
$$\frac{\sin(2x)}{x}$$

In [19]: sp.limit(f,x,0) # limit of
$$f(x)$$
 as x goes to 0

Out [20]:
$$2 - \frac{4x^2}{3} + \frac{4x^4}{15} - \frac{8x^6}{315} + \mathcal{O}(x^8)$$

Out [21]:
$$\frac{8x^6}{315} + \frac{4x^4}{15} - \frac{4x^2}{3} + 2$$

Exercise 10.2a

Consider the function

$$f(x,y) = \sin(x+y)\cos(2x-y) .$$

Using SymPy,

- Differentiate f(x,y) with respect to x and simplify the result.
- Integrate f(x,y) with respect to x and simplify the result.

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• Integrate f(x,y) with respect to x from x=-1 to x=1, substitute the value y=2, and evaluate the answer numerically to 8 significant figures.

Exercise 10.2b

Solve the differential equation

$$x^{2} \frac{d^{2}}{dx^{2}} F(x) - x \frac{d}{dx} F(x) - 3F(x) = 4x^{3}$$

using SymPy.

Exercise 10.2c

With SymPy, compute the Taylor series for

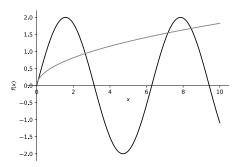
$$f(x) = \ln(x + \cos(x)) ,$$

about x=0. Include terms up to x^7 . Remove the $\mathcal{O}(x^8)$ symbol and evaluate the expression at x=1/2. Compare the series approximation to f(1/2).

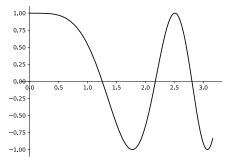
10.3 Plotting graphs with SymPy

In [1]: import sympy as sp # import sympy x,y,u = sp.symbols('x y u') # define symbols

In [2]: # plot $2*\sin(x)$ and sqrt(x/3) for x from 0 to 10 $sp.plot(2*\sin(x), sqrt(x/3), (x,0,10))$



In [3]: # parametric plot of x = sqrt(u), y = cos(u)
for u from 0 to 10
sp.plot_parametric((sqrt(u),cos(u)), (u,0,10))



Exercise 10.3a

Use SymPy to plot (on the same graph) the functions $\sin(x)$ and $\sin((\pi/2)\sin(x))$ over the domain $-2\pi \le x \le 2\pi$.

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Exercise 10.3b

A cycloid is the path made by a point on a circle as the circle rolls along the x-axis. For a circle of radius R, a cycloid is defined parametrically by the equations

$$x = R(t - \sin t) ,$$

$$y = R(1 - \cos t) .$$

Use SymPy to plot the cycloid with R = 1.

10.4 Linear algebra with SymPy

In [1]: import sympy as sp # import sympy x,y = sp.symbols('x y') # define symbols

${\bf Matrices:}$

In [2]: A = sp.Matrix([[1,3],[2,5]]) # Define a 2x2 matrix A

 $[1\ 3]$ Out [2]: 2 5

In [3]: A[1,0] # second row, first column

Out [3]: 2

> In [4]: A[0,1] # first row, second column

Out [4]: 3

> In [5]: det(A) # determinant of A

Out [5]: -1

> In [6]: A.inv() # inverse of A

Out [6]:

In [7]: sp.eye(3) # 3x3 identity matrix

 $[1 \ 0 \ 0]$ Out [7]: 0 1 0 0 0 1

Out [8]:
$$\begin{bmatrix} 3x & 1 \\ 2 & -y \end{bmatrix}$$

Out [9]:
$$\begin{bmatrix} 3x + 6 & 1 - 3y \\ 6x + 10 & 2 - 5y \end{bmatrix}$$

Out [10]:
$$\begin{bmatrix} 1 - 3x & 2 \\ 0 & y + 5 \end{bmatrix}$$

Matrix equations:

Out [11]:
$$\begin{bmatrix} 2 \\ 3 \end{bmatrix}$$

Out [12]:
$$\begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Vectors:

Out [13]:
$$\begin{bmatrix} 4 \\ 5 \\ 6 \end{bmatrix}$$

Out [14]:

In [15]: v1.cross(v2) # cross product v1 x v2

Out [15]: $\begin{bmatrix} -3 \\ 6 \\ -3 \end{bmatrix}$

Exercise 10.4a

Use SymPy to define the matrices

$$M = \begin{pmatrix} 3 & -5 & 2 \\ -1 & 4 & 4 \\ 2 & 3 & -2 \end{pmatrix} ,$$

$$N = \begin{pmatrix} 1 & 3 & -2 \\ 2 & 5 & -3 \\ 4 & -3 & -2 \end{pmatrix} .$$

Compute the product MN. Find the determinant of MN and the inverse of MN.

Exercise 10.4b

Let

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

$$b = \begin{pmatrix} 3 \\ 5 \\ 1 \end{pmatrix}$$

With SymPy, solve the matrix equation Av = b for the vector v.

Exercise 10.4c

Use SymPy to define the vector

$$v_1 = \begin{pmatrix} a_1 \\ b_1 \\ c_1 \end{pmatrix} ,$$

along with two more vectors v_2 and v_3 . Verify the triple product identity $v_1 \times (v_2 \times v_3) = (v_1 \cdot v_3)v_2 - (v_1 \cdot v_2)v_3$.

10.5 From SymPy to NumPy

```
In [1]:
           import sympy as sp
                                          # import sympy
           import numpy as np
                                          # import numpy
           x = sp.symbols('x')
                                          # define variables
  In [2]:
           f = sp.sin(sp.log(x))
                                          # define a sympy function
                                           # print
Out [2]:
           \sin(\log(x))
 In [3]:
           f = sp.lambdify(x,f,"numpy") # convert to numpy function
           f(2)
                                          # evaluate f at 2
Out [3]:
           0.6389612763136348
 In [4]:
           x = np.linspace(2,5,4)
                                          # create array of x values
           f(x)
                                          # evaluate f at x
Out [4]:
           array([0.63896128, 0.89057704, 0.98302774, 0.99925351])
```

Exercise 10.5

Use SymPy to compute

$$f(x) = \int x \sin^2(x) \, dx \; .$$

Convert f(x) to a NumPy function, then use Matplotlib to plot the function.

10.6 Printing with SymPy

A final word on printing with SymPy. When we type a variable name such as f (or a command such as factor(f)) into the last line of a jupyter notebook cell, Python responds by printing the result to the screen. You can always use the print() function to tell Python to print. However, the output might be less readable when you use print() explicitly. For example, consider the function $f = x^2 - y^2$. The output from f is

$$x^2 - y^2$$
,

whereas the output from print(f) is

$$x**2 - y**2$$
.

 SymPy also has a "pretty print" feature. The command $\operatorname{\mathsf{pprint}}(\mathtt{f})$ produces

$$x^2 - y^2$$
.

These results may differ on different platforms.