SymPy: Symbolic Computing in Python

Supplementary material

As in the paper, all examples in the supplement assume that the following has been run:

```
4 >>> from sympy import *
5 >>> x, y, z = symbols('x y z')
```

6 1 LIMITS: THE GRUNTZ ALGORITHM

SymPy calculates limits using the Gruntz algorithm, as described in [7]. The basic idea is as follows: any limit can be converted to a limit $\lim_{x\to\infty} f(x)$ by substitutions like $x\to \frac{1}{x}$. Then the subexpression ω (that converges to zero as $x\to\infty$ faster than all other subexpressions) is identified in f(x), and f(x) is expanded into a series with respect to ω . Any positive powers of ω converge to zero (while negative powers indicate an infinite limit) and any constant term independent of ω determines the limit. When a constant term still dependends on x the Gruntz algorithm is applied again until a final numerical value is obtained as the limit.

To determine the most rapidly varying subexpression, the comparability classes must first be defined, by calculating L:

$$L \equiv \lim_{x \to \infty} \frac{\log |f(x)|}{\log |g(x)|} \tag{1}$$

The relations <, >, and \sim are defined as follows: f>g when $L=\pm\infty$ (it is said that f is more rapidly varying than g, i.e., f goes to ∞ or 0 faster than g), f< g when L=0 (f is less rapidly varying than g) and $f\sim g$ when $L\neq 0,\pm\infty$ (both f and g are bounded from above and below by suitable integral powers of the other). Note that if f>g, then $f>g^n$ for any n. Here are some examples of comparability classes:

$$2 < x < e^x < e^{x^2} < e^{e^x}$$

$$2 \sim 3 \sim -5$$

$$x \sim x^2 \sim x^3 \sim \frac{1}{x} \sim x^m \sim -x$$

$$e^x \sim e^{-x} \sim e^{2x} \sim e^{x+e^{-x}}$$

$$f(x) \sim \frac{1}{f(x)}$$

The Gruntz algorithm is now illustrated with the following example:

$$f(x) = e^{x+2e^{-x}} - e^x + \frac{1}{x}. (2)$$

First, the set of most rapidly varying subexpressions is determined — the so-called mrv set. For (2), the mrv set $\{e^x, e^{-x}, e^{x+2}e^{-x}\}$ is obtained. These are all subexpressions of (2) and they all belong to the same comparability class. This calculation can be done using SymPy as follows:

```
17 >>> from sympy.series.gruntz import mrv
18 >>> mrv(exp(x+2*exp(-x))-exp(x) + 1/x, x)[0].keys()
19 dict keys([exp(x + 2*exp(-x)), exp(x), exp(-x)])
```

Next, an arbitrary item ω is taken from mrv set that converges to zero for $x \to \infty$ and doesn't have subexpressions in the given mrv set. If such a term is not present in the mrv set (i.e., all terms converge to infinity instead of zero), the relation $f(x) \sim \frac{1}{f(x)}$ can be used. In the considered case, only item $\omega = e^{-x}$ can be accepted.

The next step is to rewrite the mrv set in terms of $\omega = g(x)$. Every element f(x) of the mrv set is rewritten as $A\omega^c$, where

$$c = \lim_{x \to \infty} \frac{\log f(x)}{\log g(x)}, \qquad A = e^{\log f - c \log g}$$
(3)

Note that this step includes calculation of more simple limits, for instance

$$\lim_{x \to \infty} \frac{\log e^{x + 2e^{-x}}}{\log e^{-x}} = \lim_{x \to \infty} \frac{x + 2e^{-x}}{-x} = -1 \tag{4}$$

In this example we obtain the rewritten mrv set: $\{\frac{1}{\omega}, \omega, \frac{1}{\omega}e^{2\omega}\}$. This can be done in SymPy with

```
25 >>> from sympy.series.gruntz import mrv, rewrite
26 >>> m = mrv(exp(x+2*exp(-x))-exp(x) + 1/x, x)
```

27 >>> w = Symbol('w')

28 >>> rewrite(m[1], m[0], x, w)[0]

 $\frac{1}{x} + \exp(2^*w)/w - \frac{1}{w}$

Then the rewritten subexpressions are substituted back into f(x) in (2) and the result is expanded with respect to ω :

$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega} e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2)$$
 (5)

Since ω is from the mrv set, then in the limit as $x \to \infty$, $\omega \to 0$, and so $2\omega + O(\omega^2) \to 0$ in (5):

$$f(x) = \frac{1}{x} - \frac{1}{\omega} + \frac{1}{\omega}e^{2\omega} = 2 + \frac{1}{x} + 2\omega + O(\omega^2) \to 2 + \frac{1}{x}$$
 (6)

In this example the result $(2+\frac{1}{x})$ still depends on x, so the above procedure is repeated until just a value independent of x is obtained. This is the final limit. In the above case the limit is 2, as can be verified by SymPy:

```
33 >>> limit(exp(x+2*exp(-x))-exp(x) + 1/x, x, oo)
34 2
```

In general, when f(x) is expanded in terms of ω , the following is obtained:

$$f(x) = \underbrace{O\left(\frac{1}{\omega^3}\right)}_{\infty} + \underbrace{\frac{C_{-2}(x)}{\omega^2}}_{\infty} + \underbrace{\frac{C_{-1}(x)}{\omega}}_{\infty} + C_0(x) + \underbrace{C_1(x)\omega}_{0} + \underbrace{O(\omega^2)}_{0}$$
 (7)

The positive powers of ω are zero. If there are any negative powers of ω , then the result of the limit is infinity, otherwise the limit is equal to $\lim_{x\to\infty} C_0(x)$. The expression $C_0(x)$ is always simpler than original f(x), same is true for limits, arising in the rewrite stage (3), so the algorithm converges. A proof of this and further details on the algorithm are given in Gruntz's PhD thesis [7].

2 SERIES

2.1 Series Expansion

SymPy is able to calculate the symbolic series expansion of an arbitrary series or expression involving elementary and special functions and multiple variables. For this it has two different implementations: the series method and Ring Series.

The first approach stores a series as an instance of the Expr class. Each function has its specific implementation of its expansion, which is able to evaluate the Puiseux series expansion about a specified point. For example, consider a Taylor expansion about 0:

```
48 >>> series(\sin(x+y) + \cos(x*y), x, 0, 2)
49 1 + \sin(y) + x*\cos(y) + 0(x**2)
```

The newer and much faster approach called Ring Series makes use of the fact that a truncated Taylor series is simply a polynomial. Correspondingly, they may be represented by sparse polynomials which perform well in a under a wide range of cases. Ring Series also gives the user the freedom to choose the type of coefficients to use, resulting in faster operations on certain types.

For this, several low-level methods for expansion of trigonometric, hyperbolic and other elementary operations (like series inversion, calculating the *n*th root, etc.) are implemented using variants of the Newton Method [Brent and Zimmermann]. All these support Puiseux series expansion. The following example demonstrates the use of an elementary function that calculates the Taylor expansion of the sine of a series.

```
60 >>> from sympy.polys.ring_series import rs_sin
61 >>> R, t = ring('t', QQ)
62 >>> rs_sin(t**2 + t, t, 5)
63 -1/2*t**4 - 1/6*t**3 + t**2 + t
```

The function sympy.polys.rs_series makes use of these elementary functions to expand an arbitrary SymPy expression. It does so by following a recursive strategy of expanding the lowermost functions first and then composing them recursively to calculate the desired expansion. Currently, it only supports expansion about 0 and is under active development. Ring Series is several times faster than the default implementation with the speed difference increasing with the size of the series. The sympy.polys.rs_series takes as input any SymPy expression and hence there is no need to explicitly create a polynomial ring. An example demonstrating its use:

```
71 >>> from sympy.polys.ring_series import rs_series
72 >>> from sympy.abc import a, b
73 >>> rs_series(sin(a + b), a, 4)
74 -1/2*(sin(b))*a**2 + (sin(b)) - 1/6*a**3*(cos(b)) + a*(cos(b))
```

5 2.2 Formal Power Series

SymPy can be used for computing the formal power series of a function. The implementation
 is based on the algorithm described in the paper on formal power series [8]. The advantage of
 this approach is that an explicit formula for the coefficients of the series expansion is generated
 rather than just computing a few terms.

The following example shows how to use fps:

```
81 >>> f = fps(sin(x), x, x0=0)

82 >>> f.truncate(6)

83 x - x**3/6 + x**5/120 + 0(x**6)

84 >>> f[15]

85 -x**15/1307674368000
```

2.3 Fourier Series

87 SymPy provides functionality to compute Fourier series of a function using the fourier_series
88 function:

```
89 >>> L = symbols('L')
90 >>> expr = 2 * (Heaviside(x/L) - Heaviside(x/L - 1)) - 1
91 >>> f = fourier_series(expr, (x, 0, 2*L))
92 >>> f.truncate(3)
93 4*sin(pi*x/L)/pi + 4*sin(3*pi*x/L)/(3*pi) + 4*sin(5*pi*x/L)/(5*pi)
```

3 LOGIC

SymPy supports construction and manipulation of boolean expressions through the sympy.logic
 module. SymPy symbols can be used as propositional variables and subsequently be replaced
 with True or False values. Many functions for manipulating boolean expressions have been
 implemented in the logic module.

9 3.1 Constructing boolean expressions

A boolean variable can be declared as a SymPy Symbol. Python operators &, | and ~ are overridden when using SymPy objects to use the SymPy functionality for logical And, Or, and Not. Other logic functions are also integrated into SymPy, including Xor and Implies, which are constructed with ^ and >>, respectively. Expressions can therefore be constructed either by using the shortcut operator notation or by directly creating the relevant objects: And(), Or(), Not(), Xor(), Implies(), Nand(), Nor(), etc.:

```
106 >>> e = (x & y) | z
107 >>> e.subs({x: True, y: True, z: False})
108 True
```

3.2 CNF and DNF

109

Any boolean expression can be converted to conjunctive normal form, disjunctive normal form, or negation normal form. The API also exposes methods to check if a boolean expression is in any of the aforementioned forms.

```
>>> from sympy.logic.boolalg import is_dnf, is_cnf
113
    >>> to_cnf((x & y) | z)
114
   And(0r(x, z), 0r(y, z))
115
   >> to dnf(x & (y | z))
116
   Or(And(x, y), And(x, z))
   >> is cnf((x | y) \& z)
118
    True
119
   >> is_dnf((x \& y) | z)
120
121
    True
```

3.3 Simplification and Equivalence

The sympy.logic module supports simplification of given boolean expression by making deductions from the expression. Equivalence of two logical expressions can also be checked. In the case of equivalence, the function bool_map can be used to show which variables of the first expression correspond to which variables of the second one.

3.4 SAT solving

135

The module also supports satisfiability (SAT) checking of a given boolean expression. If an expression is satisfiable, it is possible to return a variable assignment which satisfies it. The API also supports listing all possible assignments. The SAT solver has a clause learning DPLL algorithm implemented with a watch literal scheme and VSIDS heuristic [11].

```
140 >>> satisfiable(a & (~a | b) & (~b | c) & ~c)
141 False
142 >>> satisfiable(a & (~a | b) & (~b | c) & c)
143 {a: True, b: True, c: True}
```

4 DIOPHANTINE EQUATIONS

144

151

152

153

154

155

Diophantine equations play a central role in number theory. A Diophantine equation has the form, $f(x_1, x_2, ..., x_n) = 0$ where $n \ge 2$ and $x_1, x_2, ..., x_n$ are integer variables. If there are n integers $a_1, a_2, ..., a_n$ such that $x_1 = a_1, x_2 = a_2, ..., x_n = a_n$ satisfies the above equation, the equation is said to be solvable.

Currently, the following five types of Diophantine equations can be solved using SymPy's Diophantine module $(a_1, ..., a_{n+1}, a, b, c, d, e, f, and k$ are explicitly given rational constants):

- Linear Diophantine equations: $a_1x_1 + a_2x_2 + \cdots + a_nx_n = b$
- General binary quadratic equation: $ax^2 + bxy + cy^2 + dx + ey + f = 0$
- Homogeneous ternary quadratic equation: $ax^2 + by^2 + cz^2 + dxy + eyz + fzx = 0$
 - Extended Pythagorean equation: $a_1x_1^2 + a_2x_2^2 + \cdots + a_nx_n^2 = a_{n+1}x_{n+1}^2$
- General sum of squares: $x_1^2 + x_2^2 + \dots + x_n^2 = k$

The diophantine function factors the equation it is given (if possible), solves each factor separately, and combines the results to give a final solution set. The following examples illustrate some of the basic functionalities of the Diophantine module.

```
>>> from sympy.solvers.diophantine import *
159
    >>> diophantine(2*x + 3*y - 5)
160
    set([(3*t_0 - 5, -2*t_0 + 5)])
161
162
    >>> diophantine(2*x + 4*y - 3)
163
    set()
164
165
    >>> diophantine(x**2 - 4*x*y + 8*y**2 - 3*x + 7*y - 5)
166
    set([(2, 1), (5, 1)])
167
168
    >>> diophantine(x**2 - 4*x*y + 4*y**2 - 3*x + 7*y - 5)
    set([(-2*t**2 - 7*t + 10, -t**2 - 3*t + 5)])
170
171
    \Rightarrow diophantine(3*x**2 + 4*y**2 - 5*z**2 + 4*x*y - 7*y*z + 7*z*x)
172
    set([(-16*p**2 + 28*p*q + 20*q**2,
    3*p**2 + 38*p*q - 25*q**2,
174
    4*p**2 - 24*p*q + 68*q**2)])
176
    >>> x1, x2, x3, x4, x5, x6 = symbols('x1, x2, x3, x4, x5, x6')
177
    >>> diophantine(9*x1**2 + 16*x2**2 + x3**2 + 49*x4**2 + 4*x5**2 - 25*x6**2)
178
    set([(70*t1**2 + 70*t2**2 + 70*t3**2 + 70*t4**2 - 70*t5**2, 105*t1*t5,
179
    420*t2*t5. 60*t3*t5. 210*t4*t5.
180
    42*t1**2 + 42*t2**2 + 42*t3**2 + 42*t4**2 + 42*t5**2)])
181
182
    >>> a, b, c, d = symbols('a b c d')
183
    >>> diophantine(a^{**2} + b^{**2} + c^{**2} + d^{**2} - 23)
    set([(2, 3, 3, 1)])
185
```

5 SETS

186

188

189

190

191

192

193

SymPy supports representation of a wide variety of mathematical sets. This is achieved by first defining abstract representations of atomic set classes and then combining and transforming them using various set operations.

Each of the set classes inherits from the base class Set and defines methods to check membership and calculate unions, intersections, and set differences. When these methods are not able to evaluate to atomic set classes, they are represented as abstract unevaluated objects.

SymPy has the following atomic set classes:

• EmptySet represents the empty set \emptyset .

- UniversalSet is an abstract "universal set" of which everything is a member. The union of the universal set with any set gives the universal set and the intersection gives the other set itself.
- FiniteSet is functionally equivalent to Python's built in set object. Its members can be any SymPy object including other sets.
 - Integers represents the set of integers \mathbb{Z} .
 - Naturals represents the set of natural numbers \mathbb{N} , i.e., the set of positive integers.
 - Naturals0 represents the set of whole numbers \mathbb{N}_0 , which are all the non-negative integers.
 - Range represents a range of integers. A range is defined by specifying a start value, an end value, and a step size. The enumeration of a Range object is functionally equivalent to Python's range except it supports infinite endpoints, allowing the representation of infinite ranges.
- Interval represents an interval of real numbers. It is defined by giving the start and the end points and by specifying if the interval is open or closed on the respective ends.

Other than unevaluated classes of Union, Intersection, and Complement operations, SymPy has the following set classes.

- ProductSet defines the Cartesian product of two or more sets. The product set is useful when representing higher dimensional spaces. For example, to represent a three-dimensional space, SymPy uses the Cartesian product of three real sets.
- ImageSet represents the image of a function when applied to a particular set. The image set of a function F with respect to a set S is $\{F(x) \mid x \in S\}$. SymPy uses image sets to represent sets of infinite solutions of equations such as $\sin(x) = 0$.
- ConditionSet represents a subset of a set whose members satisfy a particular condition. The subset of set S given by the condition H is $\{x \mid H(x), x \in S\}$. SymPy uses condition sets to represent the set of solutions of equations and inequalities, where the equation or the inequality is the condition and the set is the domain over which it is being solved.

A few other classes are implemented as special cases of the classes described above. The set of real numbers, Reals, is implemented as a special case of Interval. ComplexRegion is implemented as a special case of ImageSet. ComplexRegion supports both polar and rectangular representation of regions on the complex plane.

6 STATISTICS

The sympy.stats module provides random variable types and methods for computing of statistical properties of expressions involving random variables, which can be either continuous or discrete, the latter ones being further divided into finite and infinite. The variables are associated with probability densities on corresponding domains and internally defined in terms of probability spaces. Apart from the possibility of defining the random variables from user supplied density distribution, SymPy provides definitions of most common distributions, including Uniform, Poisson, Normal, Binomial, Bernoulli, and many others.

Properties of random expressions can be calculated using, e.g., expectation (abbreviated E) and variance to calculate expectation and variance. Internally, these functions generate integrals and summations, which are automatically evaluated. The evaluation can be suppressed using evaluate=False keyword argument.

Conditions on random variables can be defined with inequalities, equalities, and logical operators and their overall probabilities are obtained using P. The features can be illustrated on a model of two dice throws:

```
>>> from sympy.stats import Die, P, E
    >>> X, Y = Die("X"), Die("Y")
    >>> P(Eq(X, 6) \& Eq(Y, 6))
242
    1/36
243
    >>> P(X>Y)
244
    5/12
    The conditions can also be supplied as a second parameter to E, P, and other methods to calculate
    the property given the condition:
    >>> E(X, X+Y<5)
    5/3
249
       Using the facilities of the sympy.stats module, one can, for example, calculate the well known
250
    properties of maxwellian velocity distribution
251
    >>> from sympy.stats import Maxwell, density
252
    >>> kT, m, x = symbols("kT m x", positive=True)
253
    >>> v = Maxwell("v", sqrt(kT/m))
254
    >>> E(v)
                                               # mean velocity
    2*sqrt(2)*sqrt(kT)/(sqrt(pi)*sqrt(m))
                                               # unevaluated mean velocity
    >>> E(v, evaluate=False)
    Integral(sqrt(2)*m**(3/2)*v**3*exp(-m*v**2/(2*kT))/(sqrt(pi)*kT**(3/2)),
    (v, 0, oo))
    >>> E(m*v**2/2)
                                               # mean energy
260
    3*kT/2
    >>> solve(density(v)(x).diff(x), x)[0] # most probable velocity
    sqrt(2)*sqrt(kT)/sqrt(m)
263
```

More information on the sympy.stats module can be found in [13].

7 CATEGORY THEORY

264

269

270

271

272

273

274

275

276

278

280

281

282

284

SymPy includes a module for dealing with categories—abstract mathematical objects representing classes of structures as classes of objects (points) and morphisms (arrows) between the objects.

The module was designed with the following two goals in mind:

- 1. automatic typesetting of diagrams given by a collection of objects and of morphisms between them, and
 - 2. specification and semi-automatic derivation of properties using commutative diagrams.

As of version 1.0, SymPy only implements the first goal, while a partially working draft of implementation of the second goal is available at https://github.com/scolobb/sympy/tree/ct4-commutativity.

In order to achieve the two goals, the module <code>sympy.categories</code> defines several classes representing some of the essential concepts: objects, morphisms, categories, and diagrams. In category theory, the inner structure of objects is often discarded in the favor of studying the properties of morphisms, so the class <code>Object</code> is essentially a synonym of the class <code>Symbol</code>. There are several morphism classes which do not have a particular internal structure either, though an exception is <code>CompositeMorphism</code>, which essentially stores a list of morphisms.

The class Diagram captures the properties of morphisms. This class stores a family of morphisms, the corresponding source and target objects, and, possibly, some properties of the morphisms. Generally, no restrictions are imposed on what the properties may be—for example, one might use strings of the form "forall", "exists", "unique", etc. Furthermore, the morphisms of a diagram are grouped into *premises* and *conclusions* in order to be able to represent logical implications of the form "for a collection of morphisms P with properties $p: P \to \Omega$ (the premises), there exists a collection of morphisms C with properties $c: C \to \Omega$ (the conclusions)", where Ω is

the universal collection of properties. Finally, the class Category includes a collection of diagrams which are deemed commutative and which therefore define the properties of this category.

Automatic typesetting of diagrams takes a Diagram and produces LATEX code using the Xy-pic package. Typesetting is done in two stages: layout and generation of Xy-pic code. The layout stage is taken care of by the class DiagramGrid, which takes a Diagram and lays out the objects in a grid, trying to reduce the average length of the arrows in the final picture. By default, DiagramGrid uses a series of triangle-based heuristics to produce a rectangular grid. A linear layout can also be imposed. Furthermore, groups of objects can be given; in this case, the groups will be treated as atomic cells, and the member objects will be typeset independently of the other objects.

The second phase of diagram typesetting consists in actually drawing the picture and is carried out by the class <code>XypicDiagramDrawer</code>. An example of a diagram automatically typeset by <code>DiagramgGrid</code> and <code>XypicDiagramDrawer</code> in given in Figure 1.

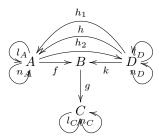


Figure 1. An automatically typeset commutative diagram

As far as the second main goal of the module is concerned, the principal idea consists in automatically deciding whether a diagram is commutative or not, given a collection of "axioms": diagrams known to be commutative. The implementation is based on graph embeddings (injective maps): whenever an embedding of a commutative diagram into a given diagram is found, one concludes that the subdiagram is commutative. Deciding commutativity of the whole diagram is therefore based (theoretically) on finding a "cover" of the target diagram by embeddings of the axioms. The naïve implementation proved to be prohibitively slow; a better optimized version is therefore in order, as well as application of heuristics.

8 SYMPY GAMMA

SymPy Gamma is a simple web application that runs on Google App Engine. It executes and displays the results of SymPy expressions as well as additional related computations, in a fashion similar to that of Wolfram|Alpha. For instance, entering an integer will display its prime factors, digits in the base-10 expansion, and a factorization diagram. Entering a function will display its docstring; in general, entering an arbitrary expression will display its derivative, integral, series expansion, plot, and roots.

SymPy Gamma also has several features beyond just computing the results using SymPy.

• SymPy Gamma displays integration and differentiation steps in detail, which can be viewed in Figure 2:

Integral Steps: integrate(tan(x), x) Fullscreen 1. Rewrite the integrand: $\tan(x) = \frac{\sin(x)}{\cos(x)}$ 2. Let $u = \cos(x)$ Then let $du = -\sin(x)dx$ and substitute du: $\int -\frac{1}{u} du$ The integral of a constant times a function is the constant times the integral of the function: $\int -\frac{1}{u} du = -\int \frac{1}{u} du$ The integral of $\frac{1}{u}$ is $\log(u)$. So, the result is: $-\log(u)$ Now substitute u back in: $-\log(\cos(x))$ Add the constant of integration: $-\log(\cos(x)) + \text{constant}$ The answer is: $-\log(\cos(x)) + \text{constant}$

Figure 2. Integral steps of tan(x)

- SymPy Gamma displays the factor tree diagrams for different numbers.
- SymPy Gamma saves user search queries, and offers many such similar features for free, which Wolfram Alpha only offers to its paid users.

Every input query from the user on SymPy Gamma is first parsed by its own parser capable of handling several different forms of function names which SymPy as a library does not support. For instance, SymPy Gamma supports queries like sin x, whereas SymPy will only recognise sin(x).

This parser converts the input query to the equivalent SymPy readable code, which is then processed by SymPy, and the result is finally printed with the built-in IATEX output and rendered by the SymPy Gamma web application.

9 SYMPY LIVE

319

320

321

322

323

324

325

326

328

329

330

331

332

333

335

SymPy Live is an online Python shell, which uses the Google App Engine to executes SymPy code. It is integrated in the SymPy documentation examples at http://docs.sympy.org.

This is accomplished by providing a HTML/JavaScript GUI for entering source code and visualization of output, and a server that evaluates the requested source code. It is an interactive AJAX shell that runs SymPy code using Python on the server.

10 COMPARISON WITH MATHEMATICA

Wolfram Mathematica is a popular proprietary CAS that features highly advanced algorithms, has a core written in C++[16], and interprets its own programming language, Wolfram Language.

Analogous to Lisp S-expressions, Mathematica uses its own style of M-expressions, which are arrays of either atoms or other M-expressions. The first element of the expression identifies the type of the expression and is indexed by zero, and the first argument is indexed starting with one. In SymPy, expression arguments are stored in a Python tuple (that is, an immutable array), while the expression type is identified by the type of the object storing the expression.

Mathematica can associate attributes to its atoms. Attributes may define mathematical properties and behavior of the nodes associated to the atom. In SymPy, the usage of static class fields is roughly similar to Mathematica's attributes, though other programming patterns may also be used to achieve an equivalent behavior such as class inheritance.

Unlike SymPy, Mathematica's expressions are mutable: one can change parts of the expression tree without the need of creating a new object. The mutability of Mathematica expressions allows for a lazy updating of any references to a given data structure.

Products in Mathematica are determined by some built in node types, such as Times, Dot, and others. Times is a representation of the * operator, and is always meant to represent a commutative product operator. The other notable product is Dot, which represents the . operator. This product represents matrix multiplication. It is not commutative. Unlike Mathematica, SymPy determines commutativity with respect to multiplication from the expression type of the factors. Mathematica puts the Orderless attribute on the expression type.

Regarding associative expressions, SymPy handles associativity of sums and products by automatically flattening them, Mathematica specifies the Flat attribute on the expression type.

Mathematica relies heavily on pattern matching—even the so-called equivalent of function declaration is in reality the definition of a pattern generating an expression tree transformation on input expressions. Mathematica's pattern matching is sensitive to associative, commutative, and one-identity properties of its expression tree nodes. SymPy has various ways to perform pattern matching. All of them play a lesser role in the CAS than in Mathematica and are basically available as a tool to rewrite expressions. The differential equation solver in SymPy somewhat relies on pattern matching to identify differential equation types, but it is envisaged to replace that strategy with analysis of Lie symmetries in the future. Mathematica's real advantage is the ability to add (at runtime) new overloading to the expression builder or specific subnodes. Consider for example:

```
370  In[1]:= Unprotect[Plus]
371  Out[1]= {Plus}
372
373  In[2]:= Sin[x_]^2 + Cos[y_]^2 := 1
374
375  In[3]:= x + Sin[t]^2 + y + Cos[t]^2
376  Out[3]= 1 + x + y
```

This expression in Mathematica defines a substitution rule that overloads the functionality of the Plus node (the node for additions in Mathematica). A symbol with a trailing underscore is treated as a wildcard. Although one may wish to keep this identity unevaluated, this example clearly illustrates the potential to define one's own immediate transformation rules. In SymPy, the operations constructing the addition node in the expression tree are Python class constructors and cannot be modified at runtime.¹ The way SymPy deals with extending the missing runtime overloadability functionality is by subclassing the node types: subclasses may redefine the class constructor to yield the proper extended functionality.

Unlike SymPy, Mathematica does not support type inheritance or polymorphism [4]. SymPy relies heavily on class inheritance, but for the most part, class inheritance is used to make sure that SymPy objects inherit the proper methods and implement the basic hashing system.

¹Nonetheless, Python supports monkey patching but it is a discouraged programming pattern.

While Mathematica interprets nested lists as matrices whenever the sublists have the same length, matrices in SymPy are a type in their own right, allowing ordinary operators and functions (like multiplication and exponentiation) to be used as they traditionally are in mathematics.

```
391 >>> exp(Matrix([[1, 1],[0, 2]])) * Matrix([a, b])
392 Matrix([
393 [E*a + b*(-E + exp(2))],
394 [ b*exp(2)]])
```

Using the standard multiplication in Mathematica performs an element-wise product and calling the exponential function Exp on a matrix returns an element-wise exponentiation of its elements.

Unevaluated expressions in Mathematica can be achieved in various ways, most commonly with the HoldForm or Hold nodes, that block the evaluation of subnodes by the parser. Such a node cannot be expressed in Python because of greedy evaluation. Whenever needed in SymPy, it is necessary to add the parameter evaluate=False to all subnodes.

In Mathematica, the operator == returns a boolean whenever it is able to immediately evaluate the truth of the equality, otherwise it returns an Equal expression. In SymPy, == means structural equality and is always guaranteed to return a boolean expression. To express a mathematical equality in SymPy it is necessary to explicitly construct an instance of the Equality class.

SymPy, in accordance with Python (and unlike the usual programming convention), uses ** to express the power operator, while Mathematica uses the more common ^.

SymPy's use of floating-point numbers is similar to that of most other CASs, including Maple and Maxima. By contrast, Mathematica uses a form of significance arithmetic [14] for approximate numbers. This offers further protection against numerical errors, although it comes with its own set of problems (for a critique of significance arithmetic, see Fateman [4]). Internally, SymPy's evalf method works similarly to Mathematica's significance arithmetic, but the semantics are isolated from the rest of the system.

11 OTHER PROJECTS THAT USE SYMPY

There are several projects that use SymPy as a library for implementing a part of their functionality. Some of them are listed below:

- Cadabra: Cadabra is a CAS designed specifically for the resolution of problems encountered in field theory.
- Octave Symbolic: The Octave-Forge Symbolic package adds symbolic calculation features to GNU Octave. These include common CAS tools such as algebraic operations, calculus, equation solving, Fourier and Laplace transforms, variable precision arithmetic, and other features.
- SymPy.jl: Provides a Julia interface to SymPy using PyCall.
- Mathics: Mathics is a free, general-purpose online CAS featuring Mathematica compatible syntax and functions. It is backed by highly extensible Python code, relying on SymPy for most mathematical tasks.
- Mathpix: An iOS App, that detects handwritten math as input, and uses SymPy Gamma to evaluate the math input and generate the relevant steps to solve the problem.
- **IKFast**: IKFast is a robot kinematics compiler provided by OpenRAVE. It analytically solves robot inverse kinematics equations and generates optimized C++ files. It uses SymPy for its internal symbolic mathematics.
- Sage: A CAS, visioned to be a viable free open source alternative to Magma, Maple, Mathematica and MATLAB. Sage includes many open source mathematical libraries, including SymPy.

- SageMathCloud: SageMathCloud is a web-based cloud computing and course management platform for computational mathematics.
- PyDy: Multibody Dynamics with Python.
- galgebra: Geometric algebra (previously sympy.galgebra).
- yt: Python package for analyzing and visualizing volumetric data (yt.units uses SymPy).
- **SfePy**: Simple finite elements in Python, see section 11.1.
- Quameon: Quantum Monte Carlo in Python.
- Lcapy: Experimental Python package for teaching linear circuit analysis.
- Quantum Programming in Python: Quantum 1D Simple Harmonic Oscillator and Quantum Mapping Gate.
 - LaTeX Expression project: Easy LATeX typesetting of algebraic expressions in symbolic form with automatic substitution and result computation.
- Symbolic statistical modeling: Adding statistical operations to complex physical models.

49 11.1 SfePy

445

453

454

455

456

457

458

459

460

461

463

465

466

467

SfePy (Simple finite elements in Python), cf. [3], is a Python package for solving partial differential equations (PDEs) in 1D, 2D and 3D by the finite element (FE) method [17]. SymPy is used within this package mostly for code generation and testing, namely:

- generation of the hierarchical FE basis module, involving generation and symbolic differentiation of 1D Legendre and Lobatto polynomials, constructing the FE basis polynomials [15] and generating the C code;
- generation of symbolic conversion formulas for various groups of elastic constants [6]: provide any two of the Young's modulus, Poisson's ratio, bulk modulus, Lamé's first parameter, shear modulus (Lamé's second parameter) or longitudinal wave modulus and get the other ones;
 - simple physical unit conversions, generation of consistent unit sets;
 - testing FE solutions using method of manufactured (analytical) solutions: the differential operator of a PDE is symbolically applied and a symbolic right-hand side is created, evaluated in quadrature points, and subsequently used to obtain a numerical solution that is then compared to the analytical one;
- testing accuracy of 1D, 2D and 3D numerical quadrature formulas (cf. [1]) by generating polynomials of suitable orders, integrating them, and comparing the results with those obtained by the numerical quadrature.

12 TENSORS

Ongoing work to provide the capabilities of tensor computer algebra has so far produced the tensor module. It comprises three submodules whose purposes are quite different: sympy. tensor.indexed and sympy.tensor.indexed_methods support indexed symbols, sympy.tensor. array contains facilities to operate on symbolic N-dimensional arrays, and finally sympy.tensor. tensor is used to define abstract tensors. The abstract tensors submodule is inspired by xAct [10] and Cadabra [12]. Canonicalization based on the Butler-Portugal [9] algorithm is supported in SymPy. Tensor support in SymPy is currently limited to polynomial tensor expressions.

13 NUMERICAL SIMPLIFICATION

The nsimplify function in SymPy (a wrapper of identify in mpmath) attempts to find a simple symbolic expression that evaluates to the same numerical value as the given input. It works by applying a few simple transformations (including square roots, reciprocals, logarithms and exponentials) to the input and, for each transformed value, using the PSLQ algorithm [5] to search for a matching algebraic number or optionally a linear combination of user-provided base constants (such as π).

```
483 >>> t = 1 / (sin(pi/5)+sin(2*pi/5)+sin(3*pi/5)+sin(4*pi/5))**2
484 >>> nsimplify(t)
485 -2*sqrt(5)/5 + 1
486 >>> nsimplify(pi, tolerance=0.01)
487 22/7
488 >>> nsimplify(1.783919626661888, [pi], tolerance=1e-12)
489 pi/(-1/3 + 2*pi/3)
```

490 14 EXAMPLES

```
14.1 Simplification
491
        · expand:
492
          >> expand((x + y)**3)
493
          x^{**3} + 3^*x^{**2}y + 3^*x^*y^{**2} + y^{**3}
494
        factor:
495
          \Rightarrow factor(x**3 + 3*x**2*y + 3*x*y**2 + y**3)
496
          (x + y)**3
497
        • collect:
498
          >> collect(y*x**2 + 3*x**2 - x*y + x - 1, x)
499
          x^{**}2^{*}(y + 3) + x^{*}(-y + 1) - 1
500
        • cancel:
501
          >>> cancel((x**2 + 2*x + 1)/(x**2 - 1))
502
          (x + 1)/(x - 1)
503
        • apart:
504
          >> apart((x**3 + 4*x - 1)/(x**2 - 1))
          x + 3/(x + 1) + 2/(x - 1)
506
```

• trigsimp:

507

510

511

14.2 Polynomials

• Factorization:

```
y^{**}2^{*}t^{**}2 + 3^{*}z^{**}6^{*}t^{**}2 + 2^{*}z^{**}4^{*}t^{**}3 - 3^{*}z^{**}3^{*}t^{**}2 -
516
                   2*z*t**3)
         >>> factor(f)
518
          (t**2*z**3 - t**2 + 47*x*y)*(2*t*z + 45*x**3 - 9*y**3 - y**2 +
519
           3*z**3)
520
       • Gröbner bases:
521
         >>> x0, x1, x2 = symbols('x:3')
522
         >>> I = [x0 + 2*x1 + 2*x2 - 1,
523
                   x0**2 + 2*x1**2 + 2*x2**2 - x0
524
                    2*x0*x1 + 2*x1*x2 - x1
525
         >>> groebner(I, order='lex')
         GroebnerBasis([7*x0 - 420*x2**3 + 158*x2**2 + 8*x2 - 7,
527
         7*x1 + 210*x2**3 - 79*x2**2 + 3*x2
         84*x2**4 - 40*x2**3 + x2**2 + x2, x0, x1, x2, domain='ZZ',
         order='lex')
       • Root isolation:
531
          \Rightarrow f = 7*z**4 - 19*z**3 + 20*z**2 + 17*z + 20
532
         >>> intervals(f, all=True, eps=0.001)
533
          ([],
           [((-425/1024 - 625*I/1024, -1485/3584 - 2185*I/3584), 1),
            ((-425/1024 + 2185*I/3584, -1485/3584 + 625*I/1024), 1),
536
            ((3175/1792 - 2605*I/1792, 1815/1024 - 10415*I/7168), 1),
537
            ((3175/1792 + 10415*I/7168, 1815/1024 + 2605*I/1792), 1)])
    14.3 Solvers
       • Single solution:
540
         >>> solveset(x - 1, x)
541
         {1}
542
       • Finite solution set, quadratic equation:
543
         >>> solveset(x**2 - pi**2, x)
         {-pi, pi}
545
       • No solution:
         >>> solveset(1, x)
          EmptySet()
548
       • Interval solution:
549
         >>> solveset(x**2 - 3 > 0, x, domain=S.Reals)
          (-oo, -sqrt(3)) U (sqrt(3), oo)
551
       • Infinitely many solutions:
552
         >>> solveset(x - x, x, domain=S.Reals)
553
          (-00, 00)
554
         >>> solveset(x - x, x, domain=S.Complexes)
          S.Complexes
556
```

```
• Linear systems (linsolve)
557
         >>> A = Matrix([[1, 2, 3], [4, 5, 6], [7, 8, 10]])
         >>> b = Matrix([3, 6, 9])
559
         >>> linsolve((A, b), x, y, z)
560
         \{(-1, 2, 0)\}
561
         >>> linsolve(Matrix(([1, 1, 1, 1], [1, 1, 2, 3])), (x, y, z))
562
         \{(-y - 1, y, 2)\}
       Below are examples of solve applied to problems not yet handled by solveset.
564
       • Nonlinear (multivariate) system of equations (the intersection of a circle and a parabola):
565
         >>> solve([x**2 + y**2 - 16, 4*x - y**2 + 6], x, y)
566
567
         [(-2 + sqrt(14), -sqrt(-2 + 4*sqrt(14))),
          (-2 + sqrt(14), sqrt(-2 + 4*sqrt(14))),
          (-sqrt(14) - 2, -I*sqrt(2 + 4*sqrt(14))),
          (-sqrt(14) - 2, I*sqrt(2 + 4*sqrt(14)))]
570
       • Transcendental equations:
571
         >>> solve((x + log(x))**2 - 5*(x + log(x)) + 6, x)
572
         [LambertW(exp(2)), LambertW(exp(3))]
         >> solve(x**3 + exp(x))
574
         [-3*LambertW((-1)**(2/3)/3)]
    14.4 Matrices
576
       • Matrix expressions
577
         >>> m, n, p = symbols('m n p', integer=True)
578
         >>> R = MatrixSymbol('R', m, n)
579
         >>> S = MatrixSymbol('S', n, p)
580
         >>> T = MatrixSymbol('T', m, p)
         >>> U = R*S + 2*T
582
         >>> U.shape
583
         (m, p)
         >>> U[0, 1]
         2*T[0, 1] + Sum(R[0, k]*S[k, 1], (k, 0, n - 1))
586
       • Block Matrices
587
         >>> n, m, l = symbols('n m l')
588
         >>> X = MatrixSymbol('X', n, n)
589
         >>> Y = MatrixSymbol('Y', m ,m)
590
         >>> Z = MatrixSymbol('Z', n, m)
         >>> B = BlockMatrix([[X, Z], [ZeroMatrix(m, n), Y]])
592
         >>> B
         Matrix([
594
         [X, Z],
         [0, Y]])
596
597
         >>> B[0, 0]
         X[0, 0]
         >>> B.shape
599
         (m + n, m + n)
```

600

15 REFERENCES

REFERENCES

602

- [1] Abramowitz, M. and Stegun, I. A. (1964). Handbook of Mathematical Functions with
 Formulas, Graphs, and Mathematical Tables. Dover Publications, New York, NY, USA, ninth
 printing edition.
- [Brent and Zimmermann] Brent, R. P. and Zimmermann, P. Modern Computer Arithmetic.

 Cambridge University Press, version 0.5.1 edition.
- Cimrman, R. (2014). SfePy write your own FE application. In de Buyl, P. and Varoquaux, N., editors, *Proceedings of the 6th European Conference on Python in Science (EuroSciPy 2013)*, pages 65–70. http://arxiv.org/abs/1404.6391.
- ⁶¹¹ [4] Fateman, R. J. (1992). A review of Mathematica. Journal of Symbolic Computation, 13(5):545–579.
- Ferguson, H. R. P., Bailey, D. H., and Arno, S. (1999). Analysis of PSLQ, an integer relation finding algorithm. *Mathematics of Computation*, 68(225):351–369.
- ⁶¹⁵ Fung, Y. C. (1993). A first course in continuum mechanics. Pearson, third edition edition.
- Gruntz, D. (1996). On Computing Limits in a Symbolic Manipulation System. PhD thesis,
 Swiss Federal Institute of Technology, Zürich, Switzerland.
- [8] Gruntz, D. and Koepf, W. (1993). Formal power series.
- Manssur, L. R. U., Portugal, R., and Svaiter, B. F. (2002). Group-theoretic approach for symbolic tensor manipulation. *International Journal of Modern Physics C*, 13.
- [10] Martín-García, J. (2002-2016). xAct, efficient tensor computer algebra.
- [11] Moskewicz, M., Madigan, C., and Malik, S. (2008). Method and system for efficient
 implementation of boolean satisfiability. US Patent 7,418,369.
- Peeters, K. (2007). Cadabra: a field-theory motivated symbolic computer algebra system.

 Computer Physics Communications.
- [13] Rocklin, M. and Terrel, A. R. (2012). Symbolic statistics with SymPy. Computing in Science
 and Engineering, 14.
- ⁶²⁸ [14] Sofroniou, M. and Spaletta, G. (2005). Precise numerical computation. *Journal of Logic* ⁶²⁹ and Algebraic Programming, 64(1):113–134.
- [15] Solin, P., Segeth, K., and Dolezel, I. (2003). Higher-Order Finite Element Methods. Chapman
 & Hall / CRC Press.
- [16] Wolfram, S. (2003). The Mathematica Book. Wolfram Media, Champaign, IL, USA, fifth
 edition.
- ⁶³⁴ [17] Zienkiewicz, O., Taylor, R., and Zhu, J. (2013). *The Finite Element Method: Its Basis and*⁶³⁵ Fundamentals. Butterworth-Heinemann, seventh edition.