

SymPy: Symbolic Computing in Python

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ABSTRACT

SymPy is an open source computer algebra system written in pure Python. It is built with a focus on extensibility and ease of use, through both interactive and programmatic applications. These characteristics have led SymPy to become a popular symbolic library for the scientific Python ecosystem. This paper presents the architecture of SymPy, a description of its features, and a discussion of select domain specific submodules. The supplementary materials provide additional examples and further outline details of the architecture and features of SymPy.

Keywords: symbolic, Python, computer algebra system

1 INTRODUCTION

SymPy is a full featured computer algebra system (CAS) written in the Python [27] programming language. It is free and open source software, licensed under the 3-clause BSD license [40]. The SymPy project was started by Ondřej Čertík in 2005, and it has since grown to over 500 contributors. Currently, SymPy is developed on GitHub using a bazaar community model [36]. The accessibility of the codebase and the open community model allow SymPy to rapidly respond to the needs of users and developers.

Python is a dynamically typed programming language that has a focus on ease of use and readability.¹ Due in part to this focus, it has become a popular language for scientific computing and data science, with a broad ecosystem of libraries [31]. SymPy is itself used by many libraries and tools to support research within a variety of domains, such as SageMath [46] (pure and applied mathematics), yt [49] (astronomy and astrophysics), PyDY [15] (multibody dynamics), and SfePy [9] (finite elements).

Unlike many CAS's, SymPy does not invent its own programming language. Python itself is used both for the internal implementation and end user interaction. By using the operator overloading functionality of Python, SymPy follows the embedded domain specific language paradigm proposed by Hudak [20]. The exclusive usage of a single programming language makes it easier for people already familiar with that language to use or develop SymPy. Simultaneously, it enables developers to focus on mathematics, rather than language design. SymPy officially supports Python 2.6, 2.7 and 3.2–3.5.

SymPy is designed with a strong focus on usability as a library. Extensibility is important in its application program interface (API) design. Thus, SymPy makes no attempt to extend the Python language itself. The goal is for users of SymPy to be able to include SymPy alongside other Python libraries in their workflow, whether that be in an interactive environment or as a programmatic part in a larger system.

As a library, SymPy does not have a built-in graphical user interface (GUI). However, SymPy exposes a rich interactive display system, and supports registering display formatters with Jupyter [24] frontends, including the Notebook and Qt Console, which will render SymPy expressions using MathJax [8] or L^AT_EX.

The remainder of this paper discusses key components of the SymPy library. Section 5 discusses the architecture of SymPy. Section 2 enumerates the features of SymPy and takes a closer look at some of the important ones. The section 3 looks at the numerical features of

¹This paper assumes a moderate familiarity with the Python programming language.

100 SymPy and its dependency library, mpmath. Section 4 looks at the domain specific physics
 101 submodules for performing symbolic and numerical calculations in classical mechanics and
 102 quantum mechanics. Conclusions and future directions for SymPy are given in section 6. All
 103 examples in this paper use SymPy version 1.0 and mpmath version 0.19.

104 The following statement imports all SymPy functions into the global Python namespace.²
 105 From here on, all examples in this paper assume that this statement has been executed:³

106 `>>> from sympy import *`

107 All examples could be tested on the SymPy Live instance, that is an online Python shell,
 108 which uses the Google App Engine to execute SymPy code.

109 2 OVERVIEW OF CAPABILITIES

110 Although SymPy’s extensive feature set cannot be covered in-depth in this paper, calculus and
 111 other bedrock areas are discussed in their own subsections. Additionally, Table 1 gives a compact
 112 listing of all major capabilities present in the SymPy codebase. This grants a sampling from the
 113 breadth of topics and application domains that SymPy services. Unless stated otherwise, all
 114 features noted in Table 1 are symbolic in nature. Numeric features are discussed in Section 3.

Table 1. SymPy Features and Descriptions

Feature (submodules)	Description
Calculus (<code>sympy.core</code> , <code>sympy.series</code> , <code>sympy.integrals</code>)	Algorithms for computing derivatives, integrals, and limits.
Category Theory (<code>sympy.categories</code>)	Representation of objects, morphisms, and diagrams. Tools for drawing diagrams with Xy-pic.
Code Generation (<code>sympy.printing</code> , <code>sympy.codegen</code>)	Generation of compilable and executable code in a variety of different programming languages from expressions directly. Target languages include C, Fortran, Julia, JavaScript, Mathematica, MATLAB and Octave, Python, and Theano.
Combinatorics & Group Theory (<code>sympy.combinatorics</code>)	Permutations, combinations, partitions, subsets, various permutation groups (such as polyhedral, Rubik, symmetric, and others), Gray codes [30], and Prufer sequences [4].
Concrete Math (<code>sympy.concrete</code>)	Summation, products, tools for determining whether summation and product expressions are convergent, absolutely convergent, hypergeometric, and for determining other properties; computation of Gosper’s normal form [35] for two univariate polynomials.
Cryptography (<code>sympy.crypto</code>)	Block and stream ciphers, including shift, Affine, substitution, Vigenère’s, Hill’s, bifid, RSA, Kid RSA, linear-feedback shift registers, and Elgamal encryption.
Differential Geometry (<code>sympy.diffgeom</code>)	Representations of manifolds, metrics, tensor products, and coordinate systems in Riemannian and pseudo-Riemannian geometries [43].
Geometry (<code>sympy.geometry</code>)	Representations of 2D geometrical entities, such as lines and circles. Enables queries on these entities, such as asking the area of an ellipse, checking for collinearity of a set of points, or finding the intersection between objects.

²`import *` has been used here to aid the readability of the paper, but is best to avoid such wildcard import statements in production code, as they make it unclear which names are present in the namespace. Furthermore, imported names could clash with already existing imports from another package. For example, SymPy, the standard Python `math` library, and NumPy all define the `exp` function, but only the SymPy one will work with SymPy symbolic expressions.

³The three greater-than signs denote the user input for the Python interactive session, with the result, if there is one, shown on the next line.

Lie Algebras (<code>sympy.liealgebras</code>) Logic (<code>sympy.logic</code>)	Representations of Lie algebras and root systems. Boolean expressions, equivalence testing, satisfiability, and normal forms.
Matrices (<code>sympy.matrices</code>)	Tools for creating matrices of symbols and expressions. Both sparse and dense representations, as well as symbolic linear algebraic operations (e.g., inversion and factorization), are supported.
Matrix Expressions (<code>sympy.matrices.expressions</code>)	Matrices with symbolic dimensions (unspecified entries). Block matrices.
Number Theory (<code>sympy.ntheory</code>)	Prime number generation, primality testing, integer factorization, continued fractions, Egyptian fractions, modular arithmetic, quadratic residues, partitions, binomial and multinomial coefficients, prime number tools, hexadecimal digits of π , and integer factorization.
Plotting (<code>sympy.plotting</code>)	Hooks for visualizing expressions via matplotlib [21] or as text drawings when lacking a graphical back-end. 2D function plotting, 3D function plotting, and 2D implicit function plotting are supported.
Polynomials (<code>sympy.polys</code>)	Polynomial algebras over various coefficient domains. Functionality ranges from simple operations (e.g., polynomial division) to advanced computations (e.g., Gröbner bases [1] and multivariate factorization over algebraic number domains).
Printing (<code>sympy.printing</code>)	Functions for printing SymPy expressions in the terminal with ASCII or Unicode characters and converting SymPy expressions to L ^A T _E X and MathML.
Quantum Mechanics (<code>sympy.physics.quantum</code>)	Quantum states, bra-ket notation, operators, basis sets, representations, tensor products, inner products, outer products, commutators, anticommutators, and specific quantum system implementations.
Series (<code>sympy.series</code>)	Series expansion, sequences, and limits of sequences. This includes Taylor, Laurent, and Puiseux series as well as special series, such as Fourier and formal power series.
Sets (<code>sympy.sets</code>)	Representations of empty, finite, and infinite sets (including special sets such as the natural, integer, and complex numbers). Operations on sets such as union, intersection, Cartesian product, and building sets from other sets are supported.
Simplification (<code>sympy.simplify</code>)	Functions for manipulating and simplifying expressions. Includes algorithms for simplifying hypergeometric functions, trigonometric expressions, rational functions, combinatorial functions, square root denesting, and common subexpression elimination.
Solvers (<code>sympy.solvers</code>)	Functions for symbolically solving equations, systems of equations, both linear and non-linear, inequalities, ordinary differential equations, partial differential equations, Diophantine equations, and recurrence relations.

Special Functions (<code>sympy.functions</code>)	Implementations of a number of well known special functions, including Dirac delta, Gamma, Beta, Gauss error functions, Fresnel integrals, Exponential integrals, Logarithmic integrals, Trigonometric integrals, Bessel, Hankel, Airy, B-spline, Riemann Zeta, Dirichlet eta, polylogarithm, Lerch transcendent, hypergeometric, elliptic integrals, Mathieu, Jacobi polynomials, Gegenbauer polynomial, Chebyshev polynomial, Legendre polynomial, Hermite polynomial, Laguerre polynomial, and spherical harmonic functions.
Statistics (<code>sympy.stats</code>)	Support for a random variable type as well as the ability to declare this variable from prebuilt distribution functions such as Normal, Exponential, Coin, Die, and other custom distributions [39].
Tensors (<code>sympy.tensor</code>) Vectors (<code>sympy.vector</code>)	Symbolic manipulation of indexed objects. Basic operations on vectors and differential calculus with respect to 3D Cartesian coordinate systems.

2.1 Basic Usage

Symbolic variables, called symbols, must be defined and assigned to Python variables before they can be used. This is typically done through the `symbols` function, which may create multiple symbols in a single function call. For instance,

```
>>> x, y, z = symbols('x y z')
```

creates three symbols representing variables named x , y , and z . In this particular instance, these symbols are all assigned to Python variables of the same name. However, the user is free to assign them to different Python variables, while representing the same symbol, such as `a`, `b`, `c = symbols('x y z')`. In order to minimize potential confusion, though, all examples in this paper will assume that the symbols x , y , and z have been assigned to Python variables identical to their symbolic names.

Expressions are created from symbols using Python's mathematical syntax. For instance, the following Python code creates the expression $(x^2 - 2x + 3)/y$. Note that the expression remains unevaluated: it is represented symbolically.

```
>>> (x**2 - 2*x + 3)/y
(x**2 - 2*x + 3)/y
```

Importantly, SymPy expressions are immutable. This simplifies the design of SymPy by allowing expression interning. It also enables expressions to be hashed, that is used to implement caching in SymPy.

2.2 Assumptions

SymPy performs logical inference through its assumptions system. The assumptions system allows users to specify that symbols have certain common mathematical properties, such as being positive, imaginary, or integral. SymPy is careful to never perform simplifications on an expression unless the assumptions allow them. For instance, the identity $\sqrt{t^2} = t$ holds if t is nonnegative ($t \geq 0$). However, for general complex t , no such identity holds.

By default, SymPy performs all calculations assuming that symbols are complex valued. This assumption makes it easier to treat mathematical problems in full generality.

```
>>> t = Symbol('t')
>>> sqrt(t**2)
sqrt(t**2)
```

By assuming the most general case, that `t` is complex by default, SymPy avoids performing mathematically invalid operations. However, in many cases users will wish to simplify expressions containing terms like $\sqrt{t^2}$.

Assumptions are set on `Symbol` objects when they are created. For instance `Symbol('t', positive=True)` will create a symbol named `t` that is assumed to be positive.

```

150 >>> t = Symbol('t', positive=True)
151 >>> sqrt(t**2)
152 t

```

Some of the common assumptions that SymPy allows are `positive`, `negative`, `real`, `nonpositive`, `integer`, `prime` and `commutative`.⁴ Assumptions on any object can be checked with the `is_assumption` attributes, like `t.is_positive`.

Assumptions are only needed to restrict a domain so that certain simplifications can be performed. They are not required to make the domain match the input of a function. For instance, one can create the object $\sum_{n=0}^m f(n)$ as `Sum(f(n), (n, 0, m))` without setting `integer=True` when creating the Symbol object `n`.

The assumptions system additionally has deductive capabilities. The assumptions use a three-valued logic using the Python built in objects `True`, `False`, and `None`. Note that `False` is returned if the SymPy object doesn't or can't have the assumption. For example, both `I.is_real` and `I.is_prime` return `False` for the imaginary unit `I`.

`None` represents the “unknown” case. This could mean that given assumptions do not unambiguously specify the truth of an attribute. For instance, `Symbol('x', real=True).is_positive` will give `None` because a real symbol might be positive or negative. The `None` could also mean that not enough is known or implemented to compute the given fact. For instance, `(pi + E).is_irrational` gives `None`, because determining whether $\pi + e$ is rational or irrational is an open problem in mathematics [26].

Basic implications between the facts are used to deduce assumptions. For instance, the assumptions system knows that being an integer implies being rational.

```

172 >>> i = Symbol('i', integer=True)
173 >>> i.is_rational
174 True

```

Furthermore, expressions compute the assumptions on themselves based on the assumptions of their arguments. For instance, if `x` and `y` are both created with `positive=True`, then `(x + y).is_positive` will be `True` whereas `(x - y).is_positive` will be `None`.

2.3 Simplification

The generic way to simplify an expression is by calling the `simplify` function. It must be emphasized that simplification is not a rigorously defined mathematical operation [28]. The `simplify` function applies several simplification routines along with heuristics to make the output expression “simple”.⁵

It is often preferable to apply more directed simplification functions. These apply very specific rules to the input expression and are typically able to make guarantees about the output. For instance, the `factor` function, given a polynomial with rational coefficients in several variables, is guaranteed to produce a factorization into irreducible factors. Table 2 lists common simplification functions.

Table 2. Some SymPy Simplification Functions

<code>expand</code>	expand the expression
<code>factor</code>	factor a polynomial into irreducibles
<code>collect</code>	collect polynomial coefficients
<code>cancel</code>	rewrite a rational function as p/q with common factors canceled
<code>apart</code>	compute the partial fraction decomposition of a rational function
<code>trigsimp</code>	simplify trigonometric expressions [14]
<code>hyperexpand</code>	expand hypergeometric functions [37, 38]

⁴SymPy assumes that two expressions A and B commute with each other multiplicatively, that is, $A \cdot B = B \cdot A$, unless they both have `commutative=False`. Many algorithms in SymPy require special consideration to work correctly with noncommutative products.

⁵The `measure` parameter of the `simplify` function lets the user specify the Python function used to determine how complex an expression is. The default measure function returns the total number of operations in the expression.

188 2.4 Calculus

189 SymPy provides all the basic operations of calculus, such as calculating limits, derivatives,
190 integrals, or summations.

191 Limits are computed with the `limit` function, using the Gruntz algorithm [18] for computing
192 symbolic limits and heuristics (a description of the Gruntz algorithm may be found in the
193 supplement). For example, the following computes $\lim_{x \rightarrow \infty} x \sin(\frac{1}{x}) = 1$. Note that SymPy denotes
194 ∞ as `oo`.

```
195 >>> limit(x*sin(1/x), x, oo)
196 1
```

As a more complex example, SymPy computes

$$\lim_{x \rightarrow 0} \left(2e^{\frac{1 - \cos(x)}{\sin(x)}} - 1 \right)^{\frac{\sinh(x)}{\operatorname{atan}^2(x)}} = e.$$

```
197 >>> limit((2*E**((1-cos(x))/sin(x))-1)**(sinh(x)/atan(x)**2), x, 0)
198 E
```

199 Derivatives are computed with the `diff` function, which recursively uses the various differen-
200 tiation rules.

```
201 >>> diff(sin(x)*exp(x), x)
202 exp(x)*sin(x) + exp(x)*cos(x)
```

Integrals are calculated with the `integrate` function. SymPy implements a combination of the Risch algorithm [6], table lookups, a reimplementaion of Manuel Bronstein’s “Poor Man’s Integrator” [5], and an algorithm for computing integrals based on Meijer G-functions [37, 38]. These allow SymPy to compute a wide variety of indefinite and definite integrals. The Meijer G-function algorithm and the Risch algorithm are respectively demonstrated below by the computation of

$$\int_0^\infty e^{-st} \log(t) dt = -\frac{\log(s) + \gamma}{s}$$

and

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

```
203 >>> s, t = symbols('s t', positive=True)
204 >>> integrate(exp(-s*t)*log(t), (t, 0, oo)).simplify()
205 -(log(s) + EulerGamma)/s
206 >>> integrate((-2*x**2*(log(x) + 1)*exp(x**2) +
207 ... (exp(x**2) + 1)**2)/(x*(exp(x**2) + 1)**2*(log(x) + 1)), x)
208 log(log(x) + 1) + 1/(exp(x**2) + 1)
```

209 Summations are computed with `summation` using a combination of Gosper’s algorithm [17],
210 an algorithm that uses Meijer G-functions [37, 38], and heuristics. Products are computed with
211 `product` function via a suite of heuristics.

```
212 >>> i, n = symbols('i n')
213 >>> summation(2**i, (i, 0, n - 1))
214 2**n - 1
215 >>> summation(i*factorial(i), (i, 1, n))
216 n*factorial(n) + factorial(n) - 1
```

217 Integrals, derivatives, summations, products, and limits that cannot be computed return
218 unevaluated objects. These can also be created directly if the user chooses.

```

219 >>> integrate(x**x, x)
220 Integral(x**x, x)
221 >>> Sum(2**i, (i, 0, n - 1))
222 Sum(2**i, (i, 0, n - 1))

```

2.5 Polynomials

SymPy implements a suite of algorithms for polynomial manipulation, which ranges from relatively simple algorithms for doing arithmetic of polynomials, to advanced methods for factoring multivariate polynomials into irreducibles, symbolically determining real and complex root isolation intervals, or computing Gröbner bases.

Polynomial manipulation is useful in its own right. Within SymPy, though, it is mostly used indirectly as a tool in other areas of the library. In fact, many mathematical problems in symbolic computing are first expressed using entities from the symbolic core, preprocessed, and then transformed into a problem in the polynomial algebra, where generic and efficient algorithms are used to solve the problem. The solutions to the original problem are subsequently recovered from the results. This is a common scheme in symbolic integration or summation algorithms.

SymPy implements dense and sparse polynomial representations.⁶ Both are used in the univariate and multivariate cases. The dense representation is the default for univariate polynomials. For multivariate polynomials, the choice of representation is based on the application. The most common case for the sparse representation is algorithms for computing Gröbner bases (Buchberger, F4, and F5) [7, 10, 11]. This is because different monomial orderings can be expressed easily in this representation. However, algorithms for computing multivariate GCDs or factorizations, at least those currently implemented in SymPy [32], are better expressed when the representation is dense. The dense multivariate representation is specifically a recursively-dense representation, where polynomials in $K[x_0, x_1, \dots, x_n]$ are viewed as a polynomials in $K[x_0][x_1] \dots [x_n]$. Note that despite this, the coefficient domain K , can be a multivariate polynomial domain as well. The dense recursive representation in Python gets inefficient as the number of variables increases.

Some examples for the `sympy.polys` submodule can be found in the supplement.

2.6 Printers

SymPy has a rich collection of expression printers. By default, an interactive Python session will render the `str` form of an expression, which has been used in all the examples in this paper so far. The `str` form of an expression is valid Python and roughly matches what a user would type to enter the expression.⁷

```

252 >>> phi0 = Symbol('phi0')
253 >>> str(Integral(sqrt(phi0), phi0))
254 'Integral(sqrt(phi0), phi0)'

```

A two-dimensional (2D) textual representation of the expression can be printed with monospace fonts via `pprint`. Unicode characters are used for rendering mathematical symbols such as integral signs, square roots, and parentheses. Greek letters and subscripts in symbol names that have Unicode code points associated are also rendered automatically.

```

255 >>> pprint(Integral(sqrt(phi0 + 1), phi0))
256
257
258

```

$$\int \sqrt{\varphi_0 + 1} \, d(\varphi_0)$$

Alternately, the `use_unicode=False` flag can be set, which causes the expression to be printed using only ASCII characters.

⁶In a dense representation, the coefficients for all terms up to the degree of each variable are stored in memory. In a sparse representation, only the nonzero coefficients are stored.

⁷Many Python libraries distinguish the `str` form of an object, which is meant to be human-readable, and the `repr` form, which is meant to be valid Python that recreates the object. In SymPy, `str(expr) == repr(expr)`. In other words, the string representation of an expression is designed to be compact, human-readable, and valid Python code that could be used to recreate the expression. As it was noted in section 5.1, the `srepr` function prints the exact, verbose form of an expression.


```

262 >>> pprint(Integral(sqrt(phi0 + 1), phi0), use_unicode=False)
263 /
264 |
265 | _____
266 | \sqrt{phi0 + 1} d(phi0)
267 |
268 /

```

269 The function `latex` returns a \LaTeX representation of an expression.

```

270 >>> print(latex(Integral(sqrt(phi0 + 1), phi0)))
271 \int \sqrt{\phi_{0} + 1}\, d\phi_{0}

```

272 Users are encouraged to run the `init_printing` function at the beginning of interactive
273 sessions, which automatically enables the best pretty printing supported by their environment.
274 In the Jupyter Notebook or Qt Console [33], the \LaTeX printer is used to render expressions
275 using MathJax or \LaTeX , if it is installed on the system. The 2D text representation is used
276 otherwise.

277 Other printers such as MathML are also available. SymPy uses an extensible printer subsystem
278 for customizing any given printer, and allows custom objects to define their printing behavior for
279 any printer. The code generation functionality of SymPy relies on this subsystem to convert
280 expressions into code in various target programming languages.

281 2.7 Solvers

282 SymPy has equation solvers that can handle ordinary differential equations, recurrence relation-
283 ships, Diophantine equations, and algebraic equations. There is also rudimentary support for
284 simple partial differential equations.

285 There are two functions for solving algebraic equations in SymPy: `solve` and `solveset`.
286 `solveset` has several design changes with respect to the older `solve` function. This distinction
287 is present in order to resolve the usability issues with the previous `solve` function API while
288 maintaining backward compatibility with earlier versions of SymPy. `solveset` only requires
289 essential input information from the user. The function signatures of `solve` and `solveset` are

```

290 solve(f, *symbols, **flags)
291 solveset(f, symbol, domain=S.Complexes)

```

292 The `domain` parameter is typically either `S.Complexes` (the default) or `S.Reals`; the latter causes
293 `solveset` to only return real solutions.

294 An important difference between the two functions is that the output API of `solve` varies
295 with input (sometimes returning a Python list and sometimes a Python dictionary) whereas
296 `solveset` always returns a SymPy set object.

297 Both functions implicitly assume that expressions are equal to 0. For instance, `solveset(x -`
298 `1, x)` solves $x - 1 = 0$ for x .

299 `solveset` is under active development as a planned replacement for `solve`. There are certain
300 features which are implemented in `solve` that are not yet implemented in `solveset`, including
301 multivariate systems, and some transcendental equations.

302 More examples of `solveset` and `solve` can be found in the supplement.

303 2.8 Matrices

304 Besides being an important feature in its own right, computations on matrices with symbolic
305 entries are important for many algorithms within SymPy. The following code shows some basic
306 usage of the `Matrix` class.

```

307 >>> A = Matrix([[x, x + y], [y, x]])
308 >>> A
309 Matrix([
310 [x, x + y],
311 [y, x]])

```


good performance, singularities in the middle of the interval must be specified by the user. To evaluate slowly converging limits and infinite series, mpmath automatically tries Richardson extrapolation and the Shanks transformation (Euler-Maclaurin summation can also be used) [3]. A function to evaluate oscillatory integrals by means of convergence acceleration is also available.

A wide array of higher mathematical functions is implemented with full support for complex values of all parameters and arguments, including complete and incomplete gamma functions, Bessel functions, orthogonal polynomials, elliptic functions and integrals, zeta and polylogarithm functions, the generalized hypergeometric function, and the Meijer G-function. The Meijer G-function instance $G_{1,3}^{3,0}(0; \frac{1}{2}, -1, -\frac{3}{2}|x)$ is a good test case [48]; past versions of both Maple and Mathematica produced incorrect numerical values for large $x > 0$. Here, mpmath automatically removes an internal singularity and compensates for cancellations (amounting to 656 bits of precision when $x = 10000$), giving correct values:

```
>>> mpmath.mp.dps = 15
>>> mpmath.meijerg([], [0], [[-0.5, -1, -1.5], []], 10000)
mpf('2.4392576907199564e-94')
```

Equivalently, with SymPy's interface this function can be evaluated as:

```
>>> meijerg([], [0], [[-S(1)/2, -1, -S(3)/2], []], 10000).evalf()
2.43925769071996e-94
```

Symbolic integration and summation often produce hypergeometric and Meijer G-function closed forms (see Subsection 2.4); numerical evaluation of such special functions is a useful complement to direct numerical integration and summation.

4 PHYSICS SUBMODULE

SymPy includes several submodules that allow users to solve domain specific problems. For example, a comprehensive physics submodule is included that is useful for solving problems in mechanics, optics, and quantum mechanics along with support for manipulating physical quantities with units.

4.1 Classical Mechanics

One of the core domains that SymPy supports is the physics of classical mechanics. This is in turn separated into two distinct components: vector algebra and mechanics.

4.1.1 Vector Algebra

The `sympy.physics.vector` submodule provides reference frame-, time-, and space-aware vector and dyadic objects that allow for three-dimensional operations such as addition, subtraction, scalar multiplication, inner and outer products, and cross products. The vector and dyadic objects can both be written in very compact notation that make it easy to express the vectors and dyadics in terms of multiple reference frames with arbitrarily defined relative orientations. The vectors are used to specify the positions, velocities, and accelerations of points; orientations, angular velocities, and angular accelerations of reference frames; and forces and torques. The dyadics are essentially reference frame-aware 3×3 tensors [44]. The vector and dyadic objects can be used for any one-, two-, or three-dimensional vector algebra, and they provide a strong framework for building physics and engineering tools.

The following Python code demonstrates how a vector is created using the orthogonal unit vectors of three reference frames that are oriented with respect to each other, and the result of expressing the vector in the A frame. The B frame is oriented with respect to the A frame using Z-X-Z Euler Angles of magnitude π , $\frac{\pi}{2}$, and $\frac{\pi}{3}$, respectively, whereas the C frame is oriented with respect to the B frame through a simple rotation about the B frame's X unit vector through $\frac{\pi}{2}$.

```
>>> from sympy.physics.vector import ReferenceFrame
>>> A = ReferenceFrame('A')
>>> B = ReferenceFrame('B')
>>> C = ReferenceFrame('C')
```

```

458 >>> B.orient(A, 'body', (pi, pi/3, pi/4), 'zxz')
459 >>> C.orient(B, 'axis', (pi/2, B.x))
460 >>> v = 1*A.x + 2*B.z + 3*C.y
461 >>> v
462 A.x + 2*B.z + 3*C.y
463 >>> v.express(A)
464 A.x + 5*sqrt(3)/2*A.y + 5/2*A.z

```

4.1.2 Mechanics

The `sympy.physics.mechanics` submodule utilizes the `sympy.physics.vector` submodule to populate time-aware particle and rigid-body objects to fully describe the kinematics and kinetics of a rigid multi-body system. These objects store all of the information needed to derive the ordinary differential or differential algebraic equations that govern the motion of the system, i.e., the equations of motion. These equations of motion abide by Newton's laws of motion and can handle arbitrary kinematic constraints or complex loads. The submodule offers two automated methods for formulating the equations of motion based on Lagrangian Dynamics [25] and Kane's Method [23]. Lastly, there are automated linearization routines for constrained dynamical systems [34].

4.2 Quantum Mechanics

The `sympy.physics.quantum` submodule has extensive capabilities to solve problems in quantum mechanics, using Python objects to represent the different mathematical objects relevant in quantum theory [41]: states (bras and kets), operators (unitary, Hermitian, etc.), and basis sets, as well as operations on these objects such as representations, tensor products, inner products, outer products, commutators, and anticommutators. The base objects are designed in the most general way possible to enable any particular quantum system to be implemented by subclassing the base operators and defining the relevant class methods to provide system-specific logic.

Symbolic quantum operators and states may be defined, and one can perform a full range of operations with them.

```

485 >>> from sympy.physics.quantum import Commutator, Dagger, Operator
486 >>> from sympy.physics.quantum import Ket, qapply
487 >>> A = Operator('A')
488 >>> B = Operator('B')
489 >>> C = Operator('C')
490 >>> D = Operator('D')
491 >>> a = Ket('a')
492 >>> comm = Commutator(A, B)
493 >>> comm
494 [A,B]
495 >>> qapply(Dagger(comm*a)).doit()
496 -<a|*(Dagger(A)*Dagger(B) - Dagger(B)*Dagger(A))

```

Commutators can be expanded using common commutator identities:

```

498 >>> Commutator(C+B, A*D).expand(commutator=True)
499 -[A,B]*D - [A,C]*D + A*[B,D] + A*[C,D]

```

On top of this set of base objects, a number of specific quantum systems have been implemented in a fully symbolic framework. These include:

- Many of the exactly solvable quantum systems, including simple harmonic oscillator states and raising/lowering operators, infinite square well states, and 3D position and momentum operators and states.
- Second quantized formalism of non-relativistic many-body quantum mechanics [12].

- Quantum angular momentum [50]. Spin operators and their eigenstates can be represented in any basis and for any quantum numbers. A rotation operator representing the Wigner-D matrix, which may be defined symbolically or numerically, is also implemented to rotate spin eigenstates. Functionality for coupling and uncoupling of arbitrary spin eigenstates is provided, including symbolic representations of Clebsch-Gordon coefficients and Wigner symbols.
- Quantum information and computing [29]. Multidimensional qubit states, and a full set of one- and two-qubit gates are provided and can be represented symbolically or as matrices/vectors. With these building blocks, it is possible to implement a number of basic quantum algorithms including the quantum Fourier transform, quantum error correction, quantum teleportation, Grover's algorithm, dense coding, etc. In addition, any quantum circuit may be plotted using the `circuit_plot` function (Figure 1).

Here are a few short examples of the quantum information and computing capabilities in `sympy.physics.quantum`. Start with a simple four-qubit state and flip the second qubit from the right using a Pauli-X gate:

```
>>> from sympy.physics.quantum.qubit import Qubit
>>> from sympy.physics.quantum.gate import XGate
>>> q = Qubit('0101')
>>> q
|0101>
>>> X = XGate(1)
>>> qapply(X*q)
|0111>
```

Qubit states can also be used in adjoint operations, tensor products, inner/outer products:

```
>>> Dagger(q)
<0101|
>>> ip = Dagger(q)*q
>>> ip
<0101|0101>
>>> ip.doit()
1
```

Quantum gates (unitary operators) can be applied to transform these states and then classical measurements can be performed on the results:

```
>>> from sympy.physics.quantum.qubit import measure_all
>>> from sympy.physics.quantum.gate import H, X, Y, Z
>>> c = H(0)*H(1)*Qubit('00')
>>> c
H(0)*H(1)*|00>
>>> q = qapply(c)
>>> measure_all(q)
[ (|00>, 1/4), (|01>, 1/4), (|10>, 1/4), (|11>, 1/4) ]
```

Lastly, the following example demonstrates creating a three-qubit quantum Fourier transform, decomposing it into one- and two-qubit gates, and then generating a circuit plot for the sequence of gates (see Figure 1).

```
>>> from sympy.physics.quantum.qft import QFT
>>> from sympy.physics.quantum.circuitplot import circuit_plot
>>> fourier = QFT(0,3).decompose()
>>> fourier
SWAP(0,2)*H(0)*C((0),S(1))*H(1)*C((0),T(2))*C((1),S(2))*H(2)
>>> c = circuit_plot(fourier, nqubits=3)
```



Figure 1. The circuit diagram for a three-qubit quantum Fourier transform generated by SymPy.

5 ARCHITECTURE

Software architecture is of central importance in any large software project because it establishes predictable patterns of usage and development [42]. This section describes the essential structural components of SymPy, provides justifications for the design decisions that have been made, and gives example user-facing code as appropriate.

5.1 The Core

A computer algebra system stores mathematical expressions as data structures. For example, the mathematical expression $x + y$ is represented as a tree with three nodes, $+$, x , and y , where x and y are ordered children of $+$. As users manipulate mathematical expressions with traditional mathematical syntax, the CAS manipulates the underlying data structures. Automated optimizations and computations such as integration, simplification, etc. are all functions that consume and produce expression trees.

In SymPy every symbolic expression is an instance of a Python `Basic` class,⁹ a superclass of all SymPy types providing common methods to all SymPy tree-elements, such as traversals. The children of a node in the tree are held in the `args` attribute. A terminal or leaf node in the expression tree has empty `args`.

For example, consider the expression $xy + 2$:

```
>>> expr = x*y + 2
```

By order of operations, the parent of the expression tree for `expr` is an addition, so it is of type `Add`. The child nodes of `expr` are 2 and `x*y`.

```
>>> type(expr)
<class 'sympy.core.add.Add'>
>>> expr.args
(2, x*y)
```

Descending further down into the expression tree yields the full expression. For example, the next child node (given by `expr.args[0]`) is 2. Its class is `Integer`, and it has an empty `args` tuple, indicating that it is a leaf node.

```
>>> expr.args[0]
2
>>> type(expr.args[0])
<class 'sympy.core.numbers.Integer'>
>>> expr.args[0].args
()
```

⁹Some internal classes, such as those used in the polynomial submodule, do not follow this rule for efficiency reasons.

589 Symbols or symbolic constants, like e or π , are examples of leaf nodes.

```
590 >>> exp(1)
591 E
592 >>> exp(1).args
593 ()
594 >>> x.args
595 ()
```

596 A useful way to view an expression tree is using the `srepr` function, which returns a string
597 representation of an expression as valid Python code¹⁰ with all the nested class constructor calls
598 to create the given expression.

```
599 >>> srepr(expr)
600 "Add(Mul(Symbol('x'), Symbol('y')), Integer(2))"
```

601 Every SymPy expression satisfies a key identity invariant:

```
602 expr.func(*expr.args) == expr
```

603 This means that expressions are rebuildable from their `args`.¹¹ Note that in SymPy the `==`
604 operator represents exact structural equality, not mathematical equality. This allows testing if
605 any two expressions are equal to one another as expression trees. For example, even though
606 $(x+1)^2$ and x^2+2x+1 are equal mathematically, SymPy gives

```
607 >>> (x + 1)**2 == x**2 + 2*x + 1
608 False
```

609 because they are different as expression trees (the former is a `Pow` object and the latter is an `Add`
610 object).

611 Python allows classes to override mathematical operators. The Python interpreter translates
612 the above `x*y + 2` to, roughly, `(x.__mul__(y)).__add__(2)`. Both `x` and `y`, returned from the
613 `symbols` function, are `Symbol` instances. The `2` in the expression is processed by Python as a
614 literal, and is stored as Python's built in `int` type. When `2` is passed to the `__add__` method
615 of `Symbol`, it is converted to the SymPy type `Integer(2)` before being stored in the resulting
616 expression tree. In this way, SymPy expressions can be built in the natural way using Python
617 operators and numeric literals.

618 5.2 Extensibility

619 While the core of SymPy is relatively small, it has been extended to a wide variety of domains
620 by a broad range of contributors. This is due, in part, to the fact that the same language,
621 Python, is used both for the internal implementation and the external usage by users. All of
622 the extensibility capabilities available to users are also utilized by SymPy itself. This eases the
623 transition pathway from SymPy user to SymPy developer.

624 The typical way to create a custom SymPy object is to subclass an existing SymPy class,
625 usually `Basic`, `Expr`, or `Function`. As it was stated before, all SymPy classes used for expression
626 trees should be subclasses of the base class `Basic`. `Expr` is the `Basic` subclass for mathematical
627 that can be added and multiplied together. The most commonly seen classes in SymPy are
628 subclasses of `Expr`, including `Add`, `Mul`, and `Symbol`. Instances of `Expr` typically represent complex
629 numbers, but may also include other “rings”, like matrix expressions. Not all SymPy classes are
630 subclasses of `Expr`. For instance, logic expressions, such as `And(x, y)`, are subclasses of `Basic`
631 but not of `Expr`.

632 The `Function` class is a subclass of `Expr` which makes it easier to define mathematical functions
633 called with arguments. This includes named functions like $\sin(x)$ and $\log(x)$ as well as undefined
634 functions like $f(x)$. Subclasses of `Function` should define a class method `eval`, which returns a

¹⁰ The `dotprint` function from the `sympy.printing.dot` submodule prints output to dot format, which can be rendered with `Graphviz` to visualize expression trees graphically.

¹¹ `expr.func` is used instead of `type(expr)` to allow the function of an expression to be distinct from its actual Python class. In most cases the two are the same.

635 canonical form of the function application (usually an instance of some other class, i.e., a `Number`)
636 or `None`, if for given arguments that function should not be automatically evaluated.

637 Many SymPy functions perform various evaluations down the expression tree. Classes
638 define their behavior in such functions by defining a relevant `_eval_*` method. For instance,
639 an object can indicate to the `diff` function how to take the derivative of itself by defining the
640 `_eval_derivative(self, x)` method, which may in turn call `diff` on its `args`. (Subclasses of
641 `Function` should implement `fdiff` method instead, it returns the derivative of the function without
642 considering the chain rule.) The most common `_eval_*` methods relate to the assumptions:
643 `_eval_is_assumption` is used to deduce *assumption* on the object.

644 As an example of the notions presented in this section, Listing 1 presents a minimal version
645 of the gamma function $\Gamma(x)$ from SymPy, which evaluates itself on positive integer arguments,
646 has the positive and real assumptions defined, can be rewritten in terms of factorial with
647 `gamma(x).rewrite(factorial)`, and can be differentiated. `self.func` is used throughout instead
648 of referencing `gamma` explicitly so that potential subclasses of `gamma` can reuse the methods.

Listing 1. A minimal implementation of `sympy.gamma`.

```
649 from sympy import Integer, Function, floor, factorial, polygamma
650
651 class gamma(Function)
652     @classmethod
653     def eval(cls, arg):
654         if isinstance(arg, Integer) and arg.is_positive:
655             return factorial(arg - 1)
656
657     def _eval_is_positive(self):
658         x = self.args[0]
659         if x.is_positive:
660             return True
661         elif x.is_noninteger:
662             return floor(x).is_even
663
664     def _eval_is_real(self):
665         x = self.args[0]
666         # noninteger means real and not integer
667         if x.is_positive or x.is_noninteger:
668             return True
669
670     def _eval_rewrite_as_factorial(self, z):
671         return factorial(z - 1)
672
673     def fdiff(self, argindex=1):
674         from sympy.core.function import ArgumentIndexError
675         if argindex == 1:
676             return self.func(self.args[0])*polygamma(0, self.args[0])
677         else:
678             raise ArgumentIndexError(self, argindex)
```

679 The gamma function implemented in SymPy has many more capabilities than the above listing,
680 such as evaluation at rational points and series expansion.

681 5.3 Speed

682 Due to being written in pure Python, SymPy's speed is generally slower compared with its
683 commercial competitors. For many applications and uses of SymPy, that is not a problem, as
684 SymPy is able to return the answer quickly enough, but for some applications that require
685 handling of very long expressions and/or lots of small expressions, the speed becomes a problem.

686 For this reason, a new library called SymEngine [47] was started. It is a pure C++ library

687 with thin wrappers to other languages (Python, Ruby, Julia, ...) whose aim is to be the fastest
688 manipulation library. Preliminary benchmarks suggest that SymEngine is as fast or faster than
689 the commercial or open source competitors.

690 The development branch of SymPy recently started to use SymEngine as an optional backend,
691 initially in `sympy.physics.mechanics` only. The plan is to allow more algorithms in SymPy to
692 take advantage of the speed of SymEngine.

693 6 CONCLUSION AND FUTURE WORK

694 SymPy is a robust computer algebra system that provides a wide spectrum of features both in
695 traditional computer algebra and in a plethora of scientific disciplines. This allows SymPy to be
696 used in a first-class way with other Python projects, including the scientific Python stack. Unlike
697 many other CAS's, SymPy is designed to be used in an extensible way: both as an end-user
698 application and as a library.

699 SymPy expressions are immutable trees of Python objects. SymPy uses Python both as the
700 internal language and the user language. This permits users to access to the same methods that
701 the library implements in order to extend it for their needs. Additionally, SymPy has a powerful
702 assumptions system for declaring and deducing mathematical properties of expressions.

703 SymPy supports a wide array of mathematical facilities. This includes functions for simplify-
704 ing expressions, performing common calculus operations, pretty printing expressions, solving
705 equations, and representing symbolic matrices. Other supported facilities include discrete math,
706 concrete math, plotting, geometry, statistics, polynomials, sets, series, vectors, combinatorics,
707 group theory, code generation, tensors, Lie algebras, cryptography, and special functions. Ad-
708 ditionally, SymPy contains submodules targeting certain specific domains, such as classical
709 mechanics and quantum mechanics. This breadth of domains has been engendered by a strong
710 and vibrant user community. Anecdotally, these users likely chose SymPy because of its ease of
711 access.

712 Some of the planned future work for SymPy includes work on improving code generation,
713 improvements to the speed of SymPy using SymEngine, improving the assumptions system, and
714 improving the solvers submodule.

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