Computing with polynomials in SymPy

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Presentation plan

- Short introduction to SymPy
- Polynomials manipulation module
- Tour of module's functionality
- Use cases of the module
  - Mathematics: Graph coloring
  - Embedding: Code generation
- Notes on the internal implementation
  - Multi–level structure
  - Ground types
  - Pure mode Cython
- Future plans

What is SymPy?

- A pure Python library for symbolic mathematics

```
>>> from sympy import *
>>> x = Symbol('x')

>>> limit(sin(pi*x)/x, x, 0)
pi

>>> integrate(x + sinh(x), x)
(1/2)*x**2 + cosh(x)

>>> diff(_, x)
x + sinh(x)
```

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```

How to get involved?

- Visit our main web site:
  - `www.sympy.org`
- and additional web sites:
  - `docs.sympy.org`
  - `wiki.sympy.org`
  - `live.sympy.org`
- Contact us on our mailing list:
  - `sympy@googlegroups.com`
- or/and IRC channel:
  - `#sympy` on FreeNode
- Clone source repository:

```
git clone git://git.sympy.org/sympy.git
```

My role in the project

A short historical background

- cooperation started in March 2007
  - a few simple bugfixes and improvements
- next came Google Summer of Code 2007
  - algorithms for solving recurrence relations
  - algorithms for definite and indefinite summations
- and this is how it works:
  - algorithms for symbolic integration
  - algebraic structures, polynomials
  - expression simplification, ...
- else:
  - Google Summer of Code 2009, 2010 mentor (PSU, PSF)
  - EuroSciPy 2009 and 2010, py4science (UC Berkeley)
  - master's thesis

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Why we need polynomials in SymPy?

- polynomials are useful on their own
  - many problems can be stated in terms of polynomials
- polynomials are ubiquitous in symbolic algorithms
  - symbolic integration, summation
    - resultant, GCDs, factorization, ...
  - simplification of expressions
    - GCDs, factorization, ...
  - truncated power series
    - fast arithmetics, compositions, ...
  - solvers
    - roots, Gröbner bases, ...
  - ...

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Why polynomials not expressions?

- take advantage of
  - additional knowledge
    - monomial orderings, ...
  - dedicated data structures
  - polynomials manipulation algorithms
- efficiency concerns

```
In [1]: var('x')

In [2]: f = Add(*[ k*x**k for k in xrange(1, 1000) ])

In [3]: %timeit f + 3*f;
1 loops, best of 3: 773 ms per loop

In [4]: F = Poly(f, expand=False)

In [5]: %timeit F + 3*F;
100 loops, best of 3: 12.8 ms per loop
```

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Module's functionality

- classical arithmetics
- GCD, LCM, cofactors
- functional decomposition
- square–free decomposition
- factorization into irreducibles
- root counting, isolation, finding
- Gröbner bases, monomial orderings
- polynomial remainder sequences
- subresultants, resultant, discriminant
- special polynomials
- polynomial forms
- ...

Module's functionality

Factorization of polynomials

- finite fields

```
In [1]: factor(x**2 + 1, modulus=2)
Out[1]: (1 + x)**2
```

- rational numbers

```
In [2]: factor(x**6 + 1)
Out[2]: (1 + x**2)*(1 - x**2 + x**4)

In [3]: factor(expand((x + 101*y + 703*z)**20))
Out[3]: (x + 101*y + 703*z)**20
```

- algebraic numbers

```
In [4]: factor(x**4 + 1, extension=I)
Out[4]: (I + x**2)*(-I + x**2)

In [5]: factor(x**2 - 2*y**2, extension=sqrt(2))
Out[5]: (x + y*2**(1/2))*(x - y*2**(1/2))
```

Module's functionality

Solving inequalities

- inequalities

```
In [1]: a = Symbol('a', real=True)

In [2]: solve(a**2 - 2 > 0, a)
Out[2]: [(-oo, -2**(1/2)), (2**(1/2), oo)]
```

- systems of inequalities

```
In [3]: solve([a**2 - 2 < 0, a**2 - 1 > 0], a)
Out[3]: [(-2**(1/2), -1), (1, 2**(1/2))]
```

- relational syntax

```
In [4]: solve([a**2 - 2 < 0, a**2 - 1 > 0], a, relational=True)
Out[4]: Or(And(-2**(1/2) < a, a < -1), And(1 < a, a < 2**(1/2)))
```

- symbolic roots

```
In [5]: solve(a**5 + 2*a**3 + 3*a + 4 > 0, a)
Out[5]: [(RootOf(a**5 + 2*a**3 + 3*a + 4, 0), oo)]
```

Module's functionality

Gröbner bases and monomial orderings

- monomial orderings

```
In [1]: LT(x*y**7 + 2*x**2*y**3, order='lex')
Out[1]: 2*x**2*y**3

In [2]: LT(x*y**7 + 2*x**2*y**3, order='grlex')
Out[2]: x*y**7
```

- Gröbner bases

```
In [3]: var('x1,x2,i1,i2,i3')
Out[3]: (x1, x2, i1, i2, i3)

In [4]: f1, f2, f3 = x1**2 + x2**2, x1**2*x2**2, x1**3*x2 - x1*x2**3

In [5]: G = groebner([f1 - i1, f2 - i2, f3 - i3], wrt='x1,x2')

In [6]: reduced(x1**7*x2 - x1*x2**7, G, wrt=[x1, x2])[1]
Out[6]: -i2*i3 + i3*i1**2

In [7]: _.subs({i1: f1, i2: f2, i3: f3}).expand()
Out[7]: x2*x1**7 - x1*x2**7
```

Module's functionality

Generating special polynomials

- symmetric polynomials

```
In [1]: symmetric_poly(2, x, y, z)
Out[1]: x*y + x*z + y*z
```

- cyclotomic polynomials

```
In [2]: cyclotomic_poly(10, x)
Out[2]: 1 - x + x**2 - x**3 + x**4
```

- orthogonal polynomials

```
In [3]: hermite_poly(6, x)
Out[3]: -120 + 720*x**2 - 480*x**4 + 64*x**6
```

- Swinnerton–Dyer polynomials

```
In [4]: swinnerton_dyer_poly(3, x)
Out[4]: 576 - 960*x**2 + 352*x**4 - 40*x**6 + x**8
```

Module's functionality

Polynomial forms: Horner

- univariate polynomials

```
In [1]: horner(x**6 + 2*x**3 + 3*x**2 + 4*x + 5)
Out[1]: 5 + x*(4 + x*(3 + x*(2 + x**3)))

In [2]: horner(a*x**6 + b*x**3 + c*x**2 + d*x + e, x)
Out[2]: e + x*(d + x*(c + x*(b + a*x**3)))
```

- multivariate polynomials

```
In [3]: sum(i*j*x**i*y**j, (i, 1, 2), (j, 1, 2))
Out[3]: x*y + 2*x*y**2 + 2*y*x**2 + 4*x**2*y**2

In [4]: horner(_3)
Out[4]: x*(y*(1 + 2*y) + x*y*(2 + 4*y))

In [5]: horner(_3, wrt=y)
Out[5]: y*(x*(1 + 2*x) + x*y*(2 + 4*x))
```

Module's functionality

Computing symmetric reduction

- symmetric polynomials

```
In [1]: symmetrize(x**2 + y**2)
Out[1]: (-2*x*y + (x + y)**2, 0)

In [2]: symmetrize(x**2 + y**2, formal=True)
Out[2]: (-2*s2 + s1**2, 0, {s1: x + y, s2: x*y})
```

- non–symmetric polynomials

```
In [3]: symmetrize(x**2 - y**2)
Out[3]: (-2*x*y + (x + y)**2, -2*y**2)

In [4]: symmetrize(x**2 - y**2, formal=True)
Out[4]: (-2*s2 + s1**2, -2*y**2, {s1: x + y, s2: x*y})
```

Implemented algorithms

Only most remarkable cases here

- square–free decomposition
  - Yun
- factorization into irreducibles
  - finite fields
    - Berlekamp, Zassenhaus, Shoup
  - rational numbers
    - Cantor–Zassenhaus, Wang
- functional decomposition
  - Landau–Zippel
- Gröbner bases
  - Buchberger
- root isolation
  - continued fractions, Collins–Krandick

Use cases of the module

And SymPy in general

- solving mathematical problems
  - e.g. in teaching mathematics
  - Why?
    - uses single, easy to learn programming language
    - core algorithms exposed to the user
  - Example: graph k–coloring
- embedding in other software
  - e.g. code generation, preprocessing
  - Why?
    - small library with no dependencies
  - Example: C code generation

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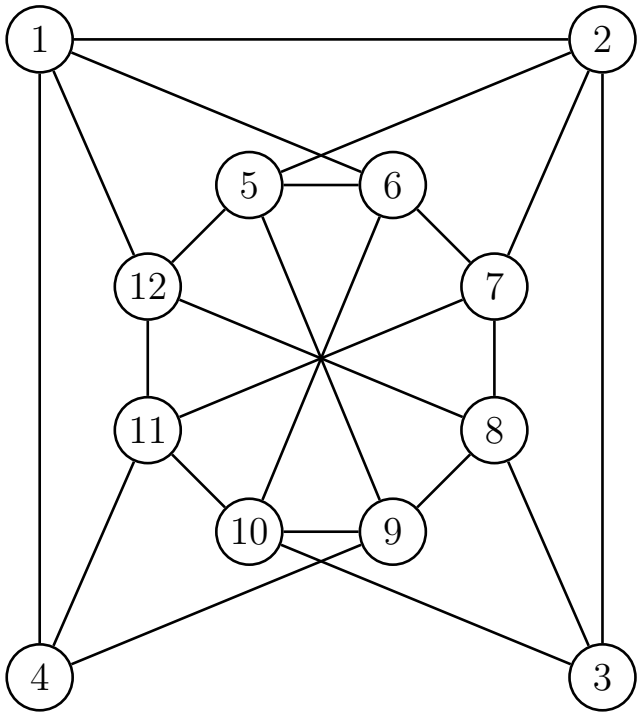
Use cases of the module

Graph k–coloring with Gröbner bases (1)



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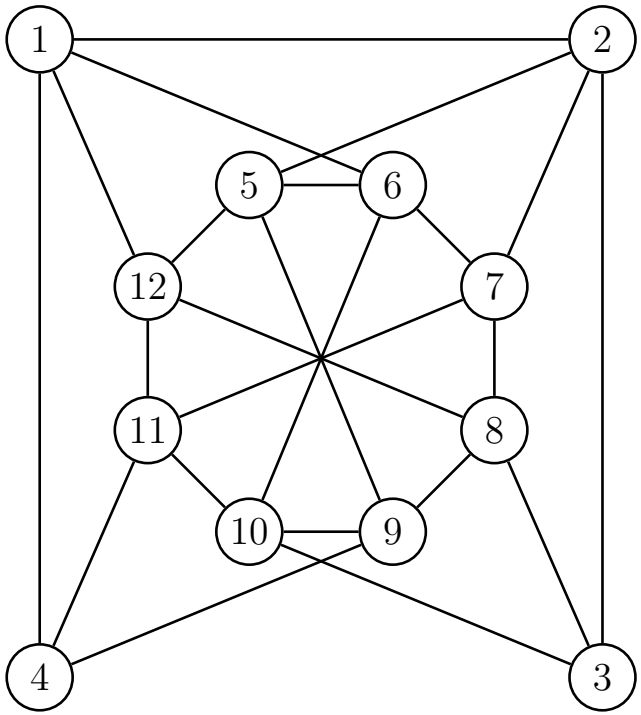

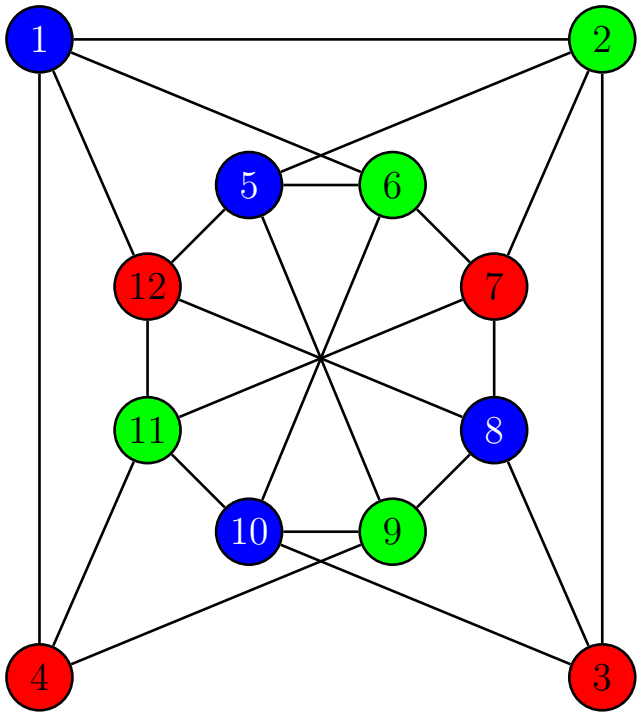

Use cases of the module

Graph k–coloring with Gröbner bases (2)

Given a graph $\mathcal{G}(V, E)$ we write two sets of equations:

- I_k — allow one of k colors per vertex

$$I_k = \{x_i^k - 1 : i \in V\}$$

- $I_{\mathcal{G}}$ — adjacent vertices have different colors assigned

$$I_{\mathcal{G}} = \{x_i^{k-1} + x_i^{k-2}x_j + \ldots + x_i x_j^{k-2} + x_j^{k-1} : (i,j) \in E\}$$

Next we solve $I_k \cup I_{\mathcal{G}}$ using the Gröbner bases method.

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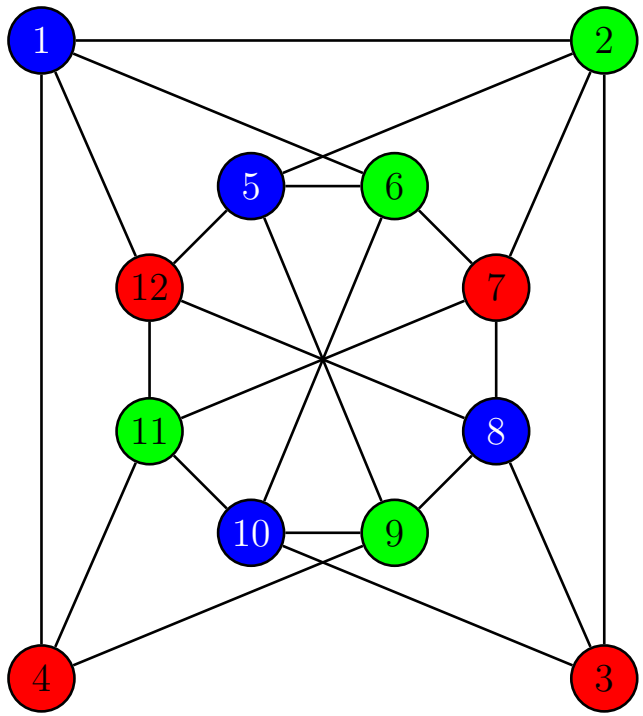
Use cases of the module

Graph k–coloring with Gröbner bases (3)

$$\{x_1 + x_{11} + x_{12},$$
$$x_2 - x_{11},$$
$$x_3 - x_{12},$$
$$x_4 - x_{12},$$
$$x_5 + x_{11} + x_{12},$$
$$x_6 - x_{11},$$
$$x_7 - x_{12},$$
$$x_8 + x_{11} + x_{12},$$
$$x_9 - x_{11},$$
$$x_{10} + x_{11} + x_{12},$$
$${x_{11}}^2 + x_{11}x_{12} + x_{12}^2,$$
$${x_{12}}^3 - 1\}$$



Use cases of the module

Graph k–coloring with Gröbner bases (4)

Here is how to solve 3–coloring problem in SymPy:

```
In [1]: V = range(1, 12+1)
In [2]: E = [(1,2),(2,3),(1,4),(1,6),(1,12),(2,5),(2,7),
(3,8),(3,10),(4,11),(4,9),(5,6),(6,7),(7,8),(8,9),(9,10),
(10,11),(11,12),(5,12),(5,9),(6,10),(7,11),(8,12)]

In [3]: X = [ Symbol('x' + str(i)) for i in V ]
In [4]: E = [ (X[i-1], X[j-1]) for i, j in E ]

In [5]: I3 = [ x**3 - 1 for x in X ]
In [6]: Ig = [ x**2 + x*y + y**2 for x, y in E ]

In [7]: G = groebner(I3 + Ig, X, order='lex')

In [8]: G != [1]
Out[8]: True
```

Use cases of the module

Graph k–coloring with Gröbner bases (4)

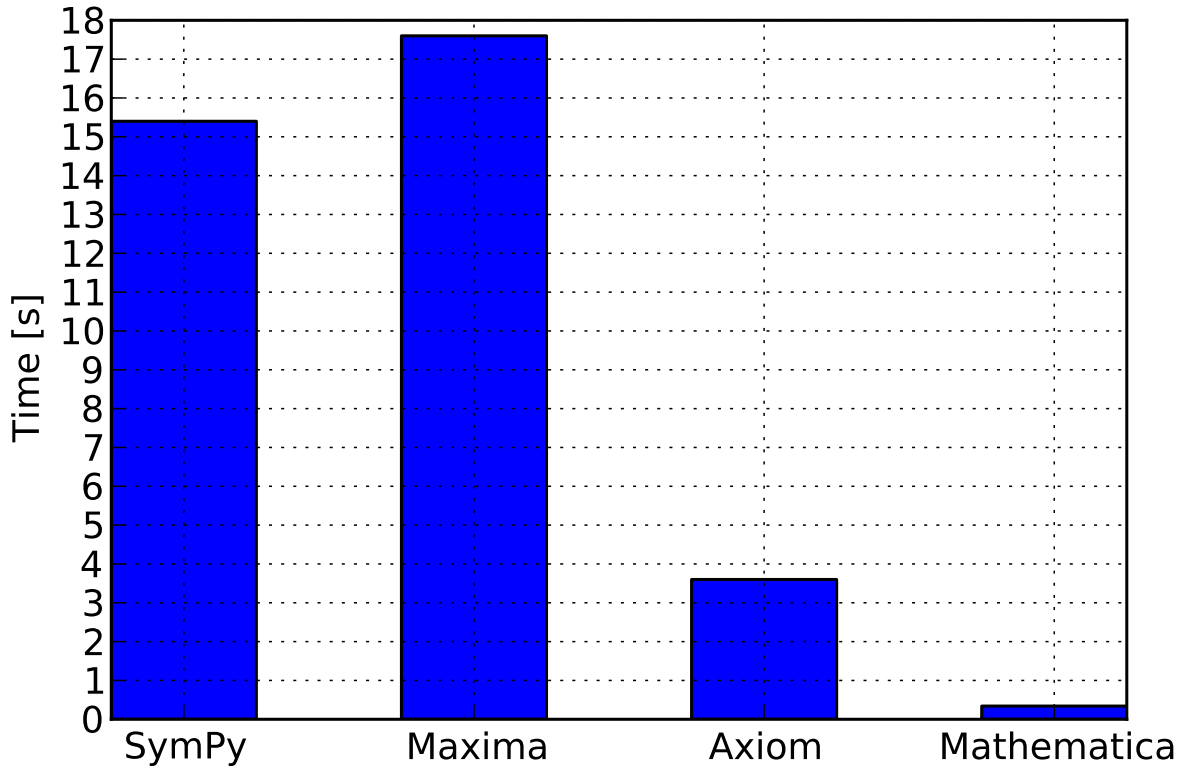


Figure: Average timing of Gröbner basis computation

Use cases of the module

C code generation (1)

The problem:

- transform expressions into Horner form
- generate equivalent C code
  - e.g. for fast evaluation
- assume we can't use `pow()` function

How we will approach the problem?

- define a new printer to generate code
- use `horner()` to transform expressions

Use cases of the module

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- define a new printer to generate code
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Use cases of the module

C code generation (2)

Lets define a dedicated printer for the task:

```
from sympy.printing import StrPrinter

class CPrinter(StrPrinter):
    """Print Lambda as C function and unroll Pow. """

    counter = 0

    def _print_Lambda(self, expr):
        self.counter += 1

        return """long _L%i(long %s) {\n  return (%s);\n}""" % \
            (self.counter, expr.args[0], self.doprint(expr.args[1]))

    def _print_Pow(self, expr):
        if expr.exp.is_Integer:
            return '*'.join([str(expr.base)]*int(expr.exp))
        else:
            return StrPrinter._print_Pow(self, expr)
```

Use cases of the module

C code generation (3)

Lets generate some code using the new `CPrinter`:

```
In [1]: from sympy import horner, Lambda

In [2]: from sympy.abc import x

In [3]: f = horner(x**6 + 2*x**3 + 3*x**2 + 4*x + 5)

In [4]: print CPrinter().doprint(Lambda(x, f))
Out[4]:
double _L1(double _x) {
  return (5 + (4 + (3 + (2 + _x*_x*_x)*_x)*_x)*_x);
}
```

Multi–level structure

- user level: L3

```
>>> f3 = x**10 - 1
>>> %timeit factor_list(f3)
100 loops, best of 3: 5.57 ms per loop
```

- user level: L2

```
>>> f2 = Poly(x**10 - 1, x, domain='ZZ')
>>> %timeit f2.factor_list()
100 loops, best of 3: 2.15 ms per loop
```

- internal level: L1

```
>>> f1 = DMP([1, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1], ZZ)
>>> %timeit f1.factor_list()
100 loops, best of 3: 1.90 ms per loop
```

- internal level: L0

```
>>> f0 = [1, 0, 0, 0, 0, 0, 0, 0, 0, 0, -1]
>>> %timeit dup_factor_list(f0, ZZ)
100 loops, best of 3: 1.88 ms per loop
```

Ground types

```
In [1]: from sympy.polys.algebratools import ZZ_python, ZZ_gmpy

In [2]: f = Poly(x**3 - 5, domain=ZZ_python())

In [3]: map(type, f.rep.all_coeffs())
Out[3]: [<type 'int'>, <type 'int'>, <type 'int'>, <type 'int'>]

In [4]: g = Poly(x**3 - 5, domain=ZZ_gmpy())

In [5]: map(type, g.rep.all_coeffs())
Out[5]: [<type 'mpz'>, <type 'mpz'>, <type 'mpz'>, <type 'mpz'>]

In [6]: f + g
Out[6]: Poly(2*x**3 - 10, x, domain='ZZ')

In [7]: map(type, _.rep.all_coeffs())
Out[7]: [<type 'mpz'>, <type 'mpz'>, <type 'mpz'>, <type 'mpz'>]
```

Ground types

Benchmark: Small coefficients

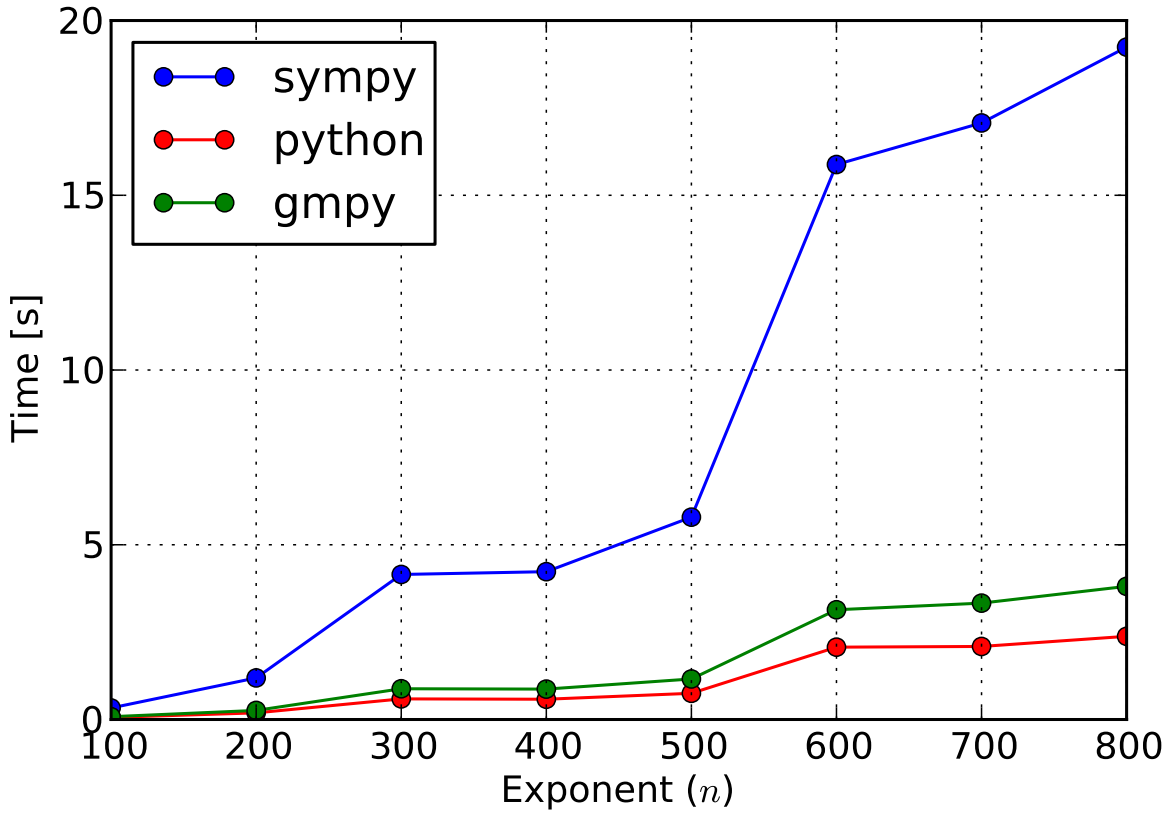

Figure: Factoring time of $x^n - 1$ polynomial

Ground types

Benchmark: Large coefficients

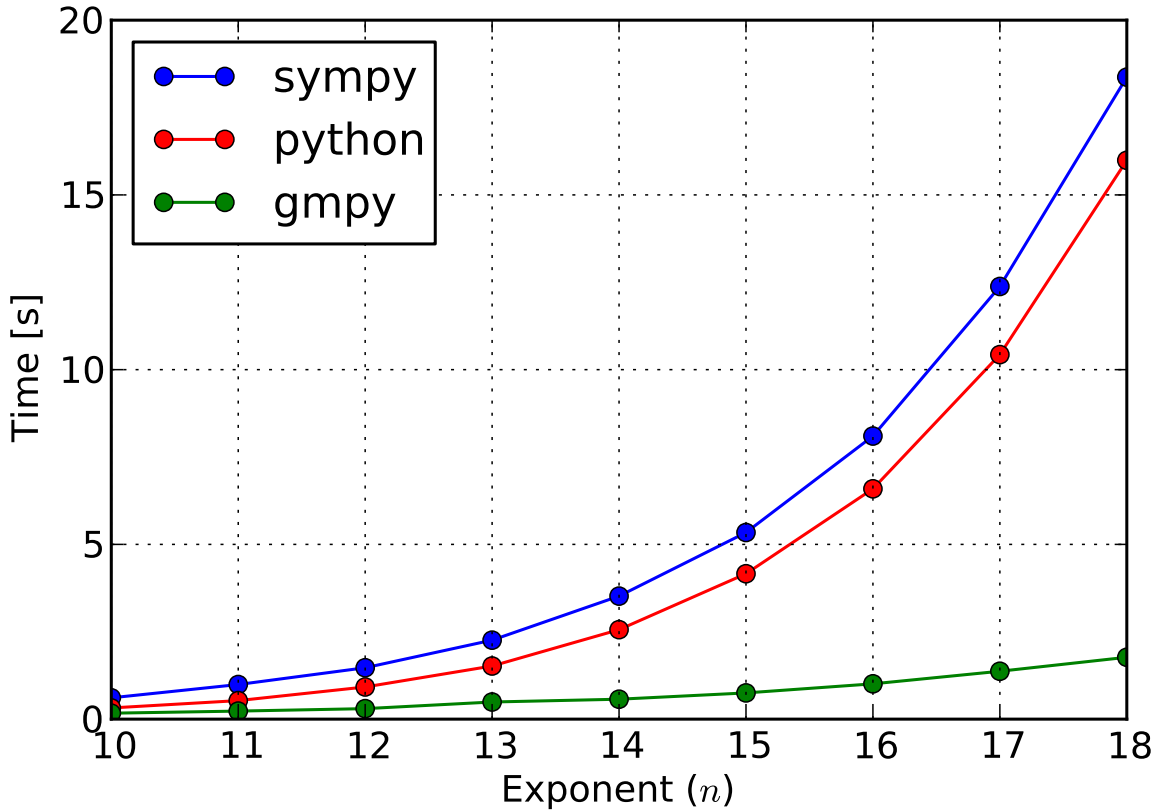

Figure: Factoring time of $(1234x + 123y + 12z + 1)^n$ polynomial

Pure mode Cython

Why want to use Cython?

- we want speed improvements
- we don't want to write C/C++ by hand

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Using pure mode Cython

How to use pure mode Cython in SymPy?

- install Cython (`www.cython.org`) on your system
- annotate selected functions with `cythonized` decorator
- choose which variables should be considered as native
- type `make` in your shell and rerun SymPy

Example:

```
@cythonized('i,n')
def dup_scale(f, a, K):
    """Compute ``f(a*x)`` in ``K[x]``. """
    f, n, b = list(f), dup_degree(f), a

    for i in xrange(n-1, -1, -1):
        f[i], b = b*f[i], b*a

    return f
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```

Using pure mode Cython

How cythonized decorator works?

- with Cython

```
def cythonized(specs):
    arg_types = {}

    for spec in specs.split(','):
        arg_types[spec] = cython.int

    return cython.locals(**arg_types)
```

- without Cython

```
def cythonized(specs):
    return lambda f: f
```

Using pure mode Cython

How cythonized decorator works?

- with Cython

```
def cythonized(specs):
    arg_types = {}

    for spec in specs.split(','):
        arg_types[spec] = cython.int

    return cython.locals(**arg_types)
```

- without Cython

```
def cythonized(specs):
    return lambda f: f
```

Using pure mode Cython

Benchmark: Polynomial exponentiation

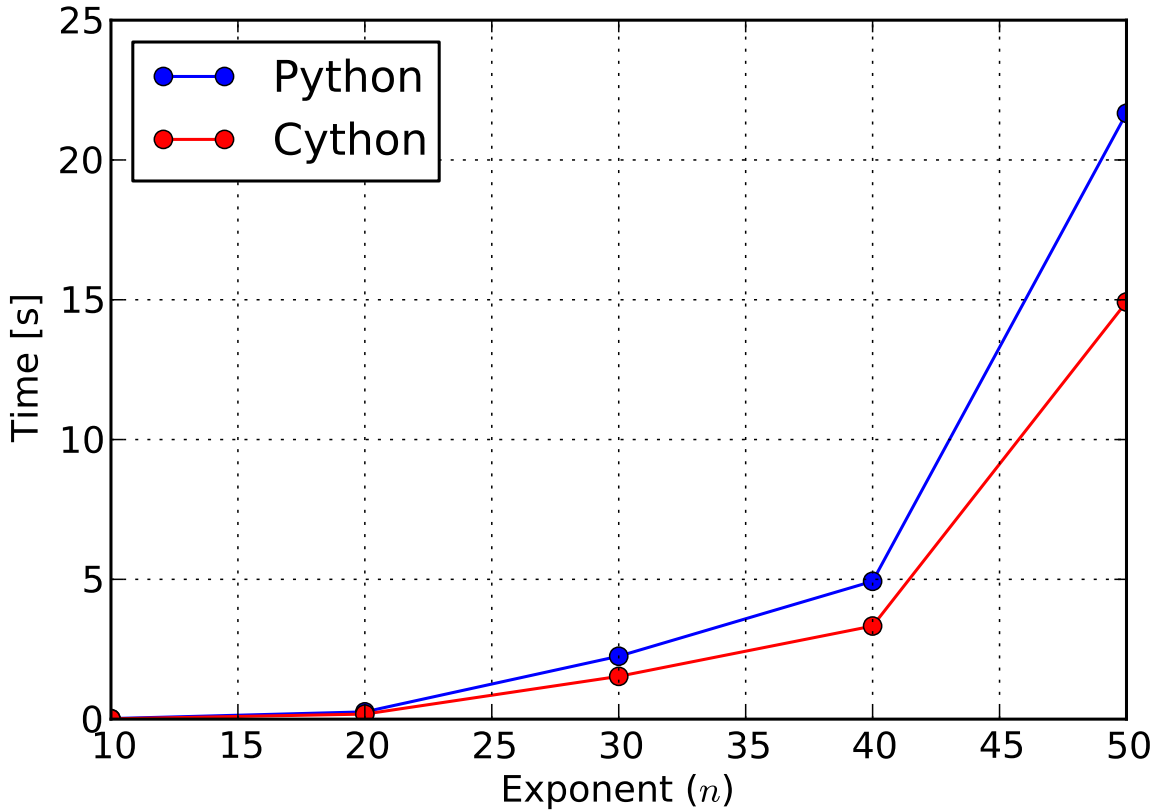

Figure: Computation time of $(27x + y^2 - 15z)^n$

Using pure mode Cython

Benchmark: Polynomial factorization

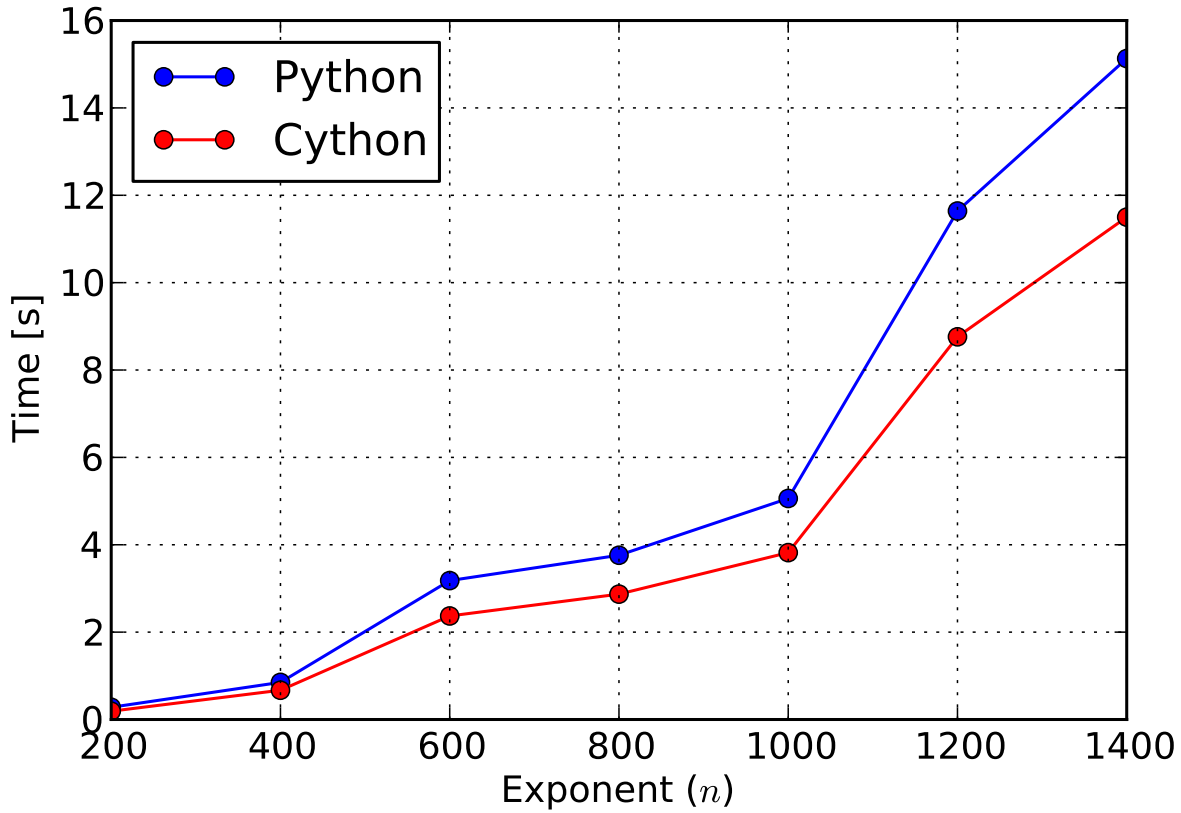

Figure: Factoring time of $x^n - 1$ polynomial

Future plans

- implement better algorithms
  - factorization, Gröbner bases, ...
- write more extensive documentation
- use the module for practical things
  - GSoC project: Algorithms for Symbolic Integration

Thank you for your attention!

Questions, remarks, discussion . . .