

Mr.CAS— A Minimalistic (pure) *Ruby* CAS for Fast Prototyping and Code Generation

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Abstract

There are Computer Algebra System (CAS) systems on the market with complete solutions for manipulation of analytical models. But exporting a model that implements specific algorithms on specific platforms, for target languages or for particular numerical library, is often a rigid procedure that requires manual post-processing. This work presents a *Ruby* library that exposes core CAS capabilities, i.e. simplification, substitution, evaluation, etc. The library aims at programmers that need to rapidly prototype and generate numerical code for different target languages, while keeping separated mathematical expression from the code generation rules, where best practices for numerical conditioning are implemented. The library is written in pure *Ruby* language and is compatible with most *Ruby* interpreters.

Keywords: CAS, code-generation, Ruby

1. Motivation and significance

Ruby [1] is a purely object-oriented scripting language designed in the mid-1990s by Yukihiro Matsumoto, internationally standardized since 2012 as ISO/IEC 30170.

With the advent of the *Internet of Things*, a compact version of the *Ruby* interpreter called *mRuby* (*eMbedded Ruby*) [2] was published on *GitHub* by Matsumoto, in 2014. The new interpreter is a lightweight implementation, aimed at both low power devices and personal computers, and complies with the standard [3]. *mRuby* has a completely new API, and it is designed to be embedded in complex projects as a front-end interface—for example, a numerical optimization suite may use *mRuby* for problem definition.

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12 The *Ruby* code-base exposes a large set of utilities in core and standard
 13 libraries, that can be furthermore expanded through third party libraries,
 14 or *gems*. Among the large number of available gems, *Ruby* still lacks an
 15 Automatic and Symbolic Differentiation (ASD) [4] engine that handles basic
 16 computer algebra routines, compatible with all different *Ruby* interpreters.

17 Nowadays *Ruby* is mainly known thanks to the web-oriented *Rails* frame-
 18 work. Its expressiveness and elegance make it interesting for use in the sci-
 19 entific and technical field. An ASD-capable gem would prove a fundamental
 20 step in this direction, including the support for flexible code generation for
 21 high-level software—for example, IPOPT [5, 6].

22 *Mr.CAS*¹ is a gem implemented in pure *Ruby* that supports symbolic
 23 differentiation (SD) and fundamentals computer algebra operations [7]. The
 24 library aims at supporting programmers in rapid prototyping of numerical
 25 algorithms and in code generation, for different target languages. It permits
 26 to implement mathematical models with a clean separation between actual
 27 mathematical formulations and conditioning rules for numerical instabilities,
 28 in order to support generation of code that is more robust with respect to
 29 issues that can be introduced by specific applications. As a long-term effort,
 30 it will become a complete open-source CAS system for the standard *Ruby*
 31 language.

32 Other CAS libraries for *Ruby* are available:

33 ***Rucas*** [8], ***Symbolic*** [9] : milestone gems, yet at an early stage and with
 34 discontinued development status. Both offer basic simplification rou-
 35 tines, although they lack differentiation.

36 ***Symengine*** [10] : is a wrapper of the *symengine* C++ library. The back-
 37 end library is very complete, but it is compatible only with the *vanilla*
 38 *C Ruby* interpreter and has several dependencies. At best of Author
 39 knowledge, the gem does not work with *Ruby* 2.x interpreter.

40 In Section 2, *Mr.CAS* containers and tree structure are explained in de-
 41 tail and applied to basic CAS tasks. In Section 3, examples on how to use
 42 the library as code generator or as interface are described. Finally, the rea-
 43 sons behind the implementation and the long term desired impact are de-
 44 picted in Section 4. All code listings are available at [http://bit.ly/Mr_](http://bit.ly/Mr_CAS_examples)
 45 [CAS_examples](http://bit.ly/Mr_CAS_examples).

¹Minimalistic Ruby Computer Algebra System

2. Software description

2.1. Software Architecture

Mr.CAS is an object oriented ASD gem that supports computer algebra routines such as simplifications and substitutions. When gem is required, it overloads methods of `Fixnum` and `Float` classes, making them compatible with fundamental symbolic classes.

Each symbolic expression (or operation) is the instance of an object, that inherits from a common virtual ancestor: `CAS::Op`. An operation encapsulates sub-operations recursively, building a tree, that is the mathematical equivalent of function composition:

$$(f \circ g) \tag{1}$$

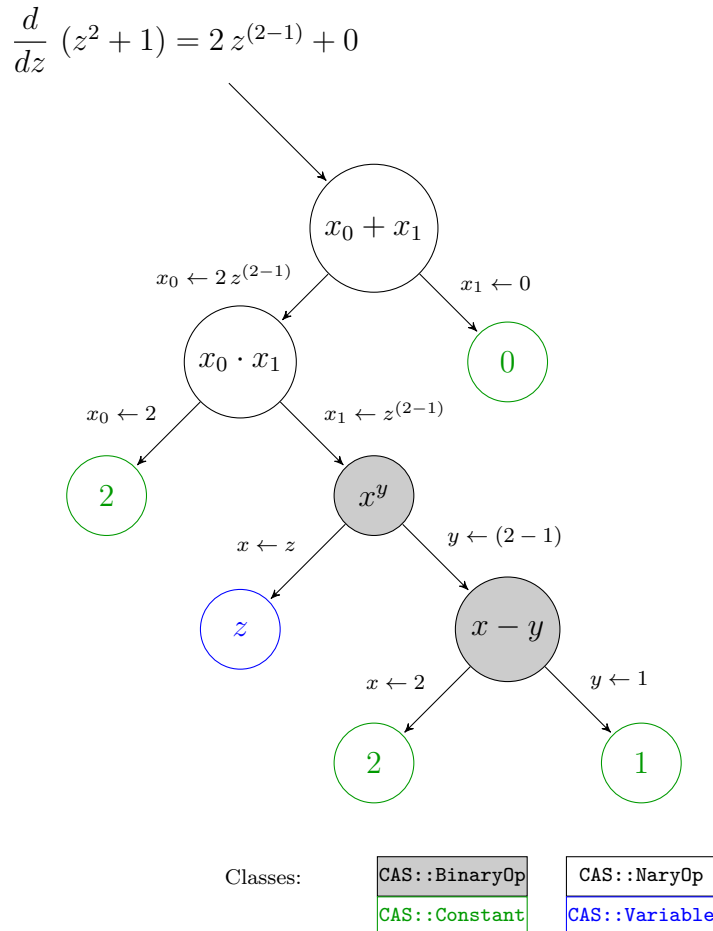


Figure 1: Tree of the expression derived in Listing 1

56 When a new operation is created, it is appended to the tree. The num-
 57 ber of branches are determined by the parent container class of the current
 58 symbolic function. There are three possible containers:

59 **CAS::Op** single sub-tree operation—e.g. $\sin(\cdot)$.

60 **CAS::BinaryOp** dual sub-tree operation—e.g. exponent x^y —that inherits
 61 from **CAS::Op**.

62 **CAS::NaryOp** operation with arbitrary number of sub-tree—e.g. sum $x_1 +$
 63 $\dots + x_N$ —that inherits from **CAS::Op**.

64 Fig. 1 contains a graphical representation of a expression tree. The different
 65 kind of containers allows to introduce some properties—i.e. *associativity* and
 66 *commutativity* for sums and multiplications [11]. Each container exposes the
 67 sub-tree as instance properties. Basic containers interfaces and inheritances
 68 are shown in Fig. 2. For a complete overview of all classes and inheritance,
 69 please refer to software documentation.

70 The terminal leaves of the graph are the classes **CAS::Constant**, **CAS::Va-**
 71 **riable** and **CAS::Function**. The first models a simple numerical value,
 72 while the second represents an independent variable, that can be used to
 73 perform derivatives and evaluations, and the latter is a prototype of im-
 74 plicit functions. Those leaves exemplify only real scalar expressions, with
 75 definition of complex, vectorial, and matricial extensions as milestones for
 76 the next major release.

77 The symbolic differentiation (**CAS::Op#diff**) explores the graph until it
 78 reaches ending nodes. A terminal node is the starting point for derivatives
 79 accumulation, the mathematical equivalent of the chain rule:

$$(f \circ g)' = (f' \circ g) g' \quad (2)$$

80 The recursiveness is used also for simplifications (**CAS::Op#simplify**), sub-
 81 stitutions (**CAS::Op#subs**), evaluations (**CAS::Op#call**) and code genera-
 82 tion.

83 2.2. Software Functionalities

84 2.2.1. Basic Functionalities

85 *No additional dependencies are required.* The gem can be installed through
 86 the *rubygems.org* provider². Gem functionalities are required using the Ker-
 87 nel method: `require 'Mr.CAS'`. All methods and classes are encapsulated
 88 in the module **CAS**.

²gem install Mr.CAS

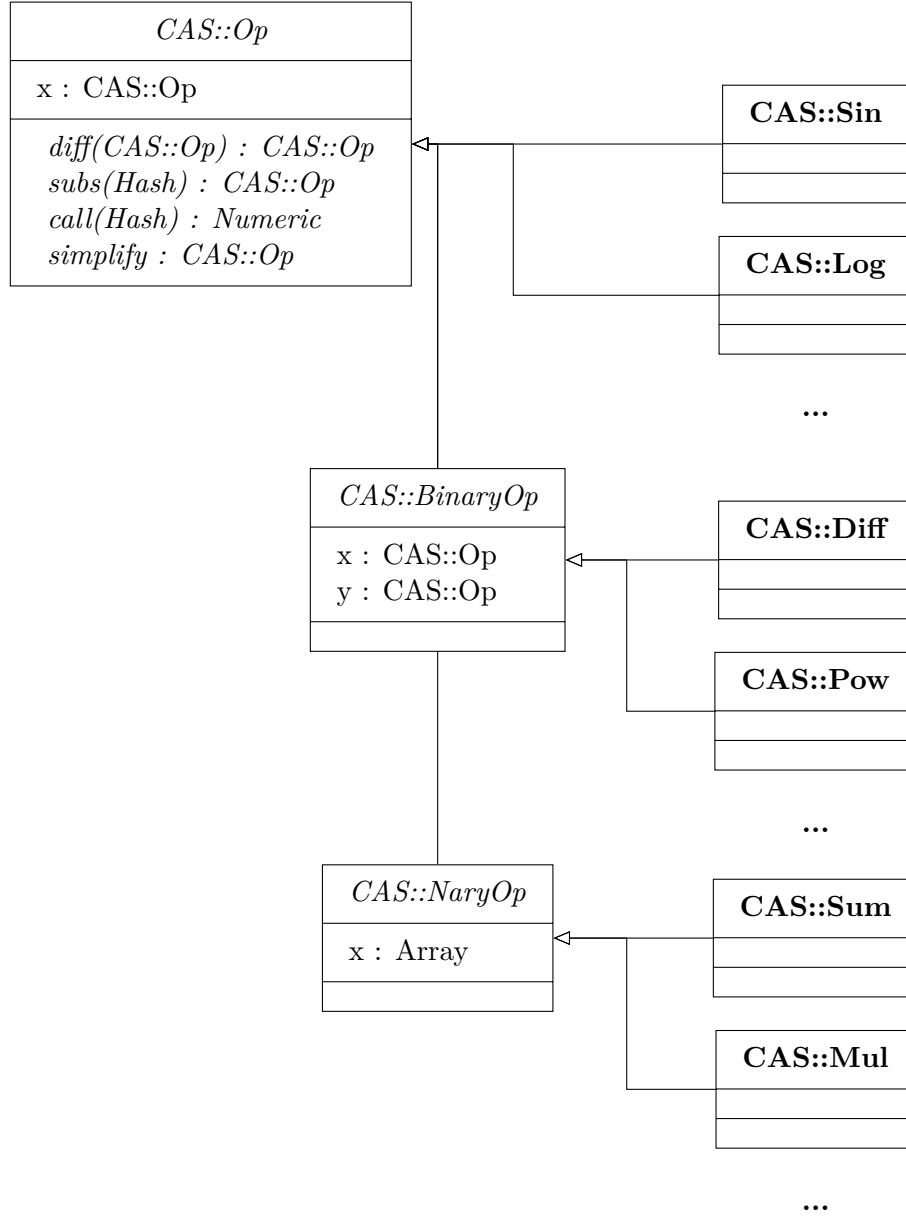


Figure 2: Reduced version of classes interface and inheritance. The figure depicts the basic abstract class `CAS::Op`, from which the *single argument* operations inherit. `CAS::Op` is also the ancestor for other kind of containers, namely the `CAS::BinaryOp` and `CAS::NaryOp`, the models of container with *two* and *more arguments*

89 Symbolic Differentiation (SD) is performed with respect to independent
 90 variables (`CAS::Variable`) through forward accumulation, even for implicit
 91 functions. The differentiation is done by the method `CAS::Op#diff`, having

92 a `CAS::Variable` as argument, as shown in Listing 1.

Listing 1: Differentiation example

```

93
94 z = CAS.vars 'z'           # creates a variable
95 f = z ** 2 + 1             # define a symbolic expression
96 f.diff(z)                  # derivative w.r.t. z
97 # => (((z)^(2-1)) * 2 * 1) + 0
98 g = CAS.declare :g, f      # creates implicit expression
99 g.diff(z)                  # derivative w.r.t. z
100 # => (((z)^(2-1)) * 2 * 1) + 0 * Dg[0](((z)^(2) + 1)))
101

```

102 Automatic differentiation (AD) is included as a plugin and exploits the
103 properties of dual numbers to efficiently perform differentiation, see [12] for
104 further details. The AD strategy is useful in case of complex expressions,
105 where explicit derivative's tree may exceed the call stack depth.

106 Simplifications are not executed automatically, after differentiation. Each
107 node of the tree knows rules for simplify itself, and rules are called recursively,
108 exactly like ASD. Simplifications that require a *heuristic expansion* of the
109 sub-graph—i.e. some trigonometric identities—are not defined for now, but
110 can be easily achieved through substitutions, as shown in Listing 2.

Listing 2: Simplification example

```

111
112 x, y = CAS::vars 'x', 'y'   # creates two variables
113 f = CAS.log( CAS.sin( y ) ) # symbolic expression
114 f.subs y => CAS.asin(CAS.exp(x)) # performs substitution
115 f.simplify                  # simplifies expression
116 # => x
117

```

118 The tree is numerically evaluated when the independent variables values
119 are provided in a feed dictionary. The graph is reduced recursively to a single
120 numeric value, as shown in Listing 3.

Listing 3: Tree evaluation example

```

121
122 x = CAS.vars 'x'           # creates a variable
123 f = x ** 2 + 1             # defines a symbolic expression
124 f.call x => 2              # evaluates for x = 2
125 # => 5.0
126

```

127 Symbolic expressions can be used to create comparative expressions, that
128 are stored in special container classes, modeled by the ancestor `CAS::Con-`
129 `dition`—for example, $f(\cdot) \geq g(\cdot)$. This allow the definition of piecewise
130 functions, in `CAS::Piecewise`. Internally, `max(\cdot)` and `min(\cdot)` functions are
131 declared as operations that inherits from `CAS::Piecewise`—for example,
132 $\max(f(\cdot), g(\cdot))$. Usage is shown in Listing 4.

Listing 4: Expressions and Piecewise functions

```

133
134 x, y = CAS.vars 'x', 'y'
135 f = CAS.declare :f, x
136 g = CAS.declare :g, x, y
137 h = CAS.declare :h, y
138
139 f.greater_equal g
140 # => (f(x) >= g(x, y))
141 pw = CAS::Piecewise.new(f,
142     CAS::Piecewise.new(g, h, y.equal(0)),
143     x.greater(0))
144 # => ((x > 0) ? f(x) : ((y == 0) ? g(x, y) : h(y)))
145 CAS::max f, g
146 # => ((f(x) >= g(x, y)) ? f(x) : g(x, y))
147

```

2.2.2. Meta-programming and Code-Generation

Mr.CAS is developed explicitly for metaprogramming and code generation. Expressions can be exported as source code or used as prototypes for callable *closures* (the **Proc** object in Listing 5):

Listing 5: Graph evaluation example

```

152
153 x = CAS::vars 'x'           # creates a variable
154 f = CAS::log(CAS::sin(x))   # define a symbolic function
155
156 proc = f.as_proc           # exports callable lambda
157 proc.call 'x' => Math::PI/2
158 # => 0.0
159

```

Compiling a closure of a tree is like making its snapshot, thus any further manipulation of the expression does not update the callable object. This drawback is balanced by the faster execution time of a **Proc**: when a graph needs *only to be evaluated*, transforming it in a *closure* reduces the execution time—for example, in an iterative algorithm, where a closure is called at each iteration.

Code generation should be flexible enough to export expression trees in a user's target language. Generation methods for common languages are included in specific *plugins*. Users can furthermore expand exporting capabilities by writing specific exportation rules, overriding method for existing plugin, or designing their own exporter, like the one shown in Listing 6:

Listing 6: Example of Ruby code generation plugin

```

171
172 # Rules definition for Fortran Language
173 module CAS
174 {
175     # . . .
176     CAS::Variable => Proc.new { "#{name}" }

```

```

177     CAS::Sin      => Proc.new { "sin(#{x.to_fortran})" },
178     # . . .
179   }.each do |cls, prc|
180     cls.send(:define_method, :to_fortran, &prc)
181   end
182 end
183
184 # Usage
185 x = CAS.vars 'x'
186 code = (CAS.sin(x)).to_fortran
187 # => sin(x)
188

```

189 3. Illustrative Examples

190 3.1. Code Generation as C Library

191 This example shows how a *user of* Mr.CAS can export a mathematical
192 model as a C library. The `c-opt` plugin implements advanced features such
193 as code optimization and generation of libraries.

194 The library `example` implements the model:

$$f(x, y) = x^y + g(x) \log(\sin(x^y)) \quad (3)$$

195 where the expression $g(x)$ belongs to a external object, declared as `g_impl`,
196 which interface is described in `g_impl.h` header. What should be noted is
197 the corpus of the exported code: the intermediate operation x^y is evaluated
198 once, even if appears twice in eq. 3. The C function that implements $f(x, y)$
199 is declared with the token `f_impl`. The exporter uses as default type `double`
200 for variables and function returned values. Library created by `CLib` contains
201 the code shown in Listing 9.

Listing 7: Calling optimized-C exporter for library generation

```

202 # Model
203 x, y = CAS.vars :x, :y
204 g = CAS.declare :g, x
205
206 f = x ** y + g * CAS.log(CAS.sin(x ** y))
207
208 # Code Generation
209 g.c_name = 'g_impl'          # g token
210
211 CAS::CLib.create "example" do
212   include_local "g_impl"      # g header
213   implements_as "f_impl", f    # token for f
214 end
215
216

```

Listing 8: C Header

```

// Header file for library: example.c

#ifndef example_H
#define example_H

// Standard Libraries
#include <math.h>

217 // Local Libraries
#include "g_impl"

// Definitions

// Functions
double f_impl(double x, double y);

#endif // example_H

```

Listing 9: C Source

```

// Source file for library: example.c

#include "example.h"

double f_impl(double x, double y) {
    double __t_0 = pow(x, y);
    double __t_1 = g_impl(x);
    double __t_2 = sin(__t_0);
    double __t_3 = log(__t_2);
    double __t_4 = (__t_1 + __t_3);
    double __t_5 = (__t_0 + __t_4);

    return __t_5;
}

// end of example.c

```

218 The function $g(x)$ models the following operation:

$$g(x) = (\sqrt{x+a} - \sqrt{x}) + \sqrt{\pi+x} \quad (4)$$

219 and may suffer from *catastrophic numerical cancellation* [13] when the x
 220 value is considerably greater than a . The user may decide to specialize code
 221 generation rules for this particular expression, stabilizing it through ratio-
 222 nalization. Without modifying the actual model, $g(x)$ the rationalization for
 223 differences of square roots³ is inserted into the exportation rules, as in List-
 224 ing 10. The rules are valid only for the current user script. For more insight
 225 about `__to_c` and `__to_c_impl`, refer to the software manual.

Listing 10: Conditioning in exporting function

```

226 # Model
227 a = CAS.declare "PARAM_A"
228
229
230 g = (CAS.sqrt(x + a) - CAS.sqrt(x)) + CAS.sqrt(CAS::Pi + x)
231
232 # Particular Code Generation for difference between square roots.
233 module CAS
234   class Diff
235     alias :__to_c_impl_old :__to_c_impl
236
237     def __to_c_impl(v)

```

³i.e.: $\sqrt{\phi(\cdot)} - \sqrt{\psi(\cdot)} = \frac{\phi(\cdot) - \psi(\cdot)}{\sqrt{\phi(\cdot)} + \sqrt{\psi(\cdot)}}$

```

238         if @x.is_a? CAS::Sqrt and @y.is_a? CAS::Sqrt
239             "{@x.x.__to_c(v)} + {@y.x.__to_c(v)} / " +
240             "( {@x.__to_c(v)} + {@y.__to_c(v)} )"
241         else
242             self.__to_c_impl_old(v)
243         end
244     end
245 end
246 end
247
248 CAS::Clib.create "g_impl" do
249     define "PARAM_A()", 1.0 # Arbitrary value for PARAM_A
250     define "M_PI", Math::Pi
251     implements_as "g_impl", g
252 end
253
254 puts g
255 # => ((sqrt((x + PARAM_A())) - sqrt(x)) + sqrtπ(( + x)))
256

```

It should be noted the separation between the *model*, which does not contain stabilization, and the *code generation rule*. For this particular case, the code generation rule in Listing 10 overloads the predefined one, in order to obtain the conditioned code. Obviously, the user can decide to apply directly the conditioning on the model itself, but this may change the calculus behavior in further manipulation.

Listing 11: `g_impl` Header

```

// Header file for library: g_impl.c

#ifndef g_impl_H
#define g_impl_H

// Standard Libraries
#include <math.h>

// Local Libraries

// Definitions
#define PARAM_A() 1.0
#define M_PI 3.141592653589793

// Functions
double g_impl(double x);

#endif // g_impl_H

```

Listing 12: `g_impl` Source

```

// Source file for library: g_impl.c

#include "g_impl.h"

double g_impl(double x) {
    double __t_0 = PARAM_A();
    double __t_1 = (x + __t_0);
    double __t_2 = sqrt(__t_1);
    double __t_3 = sqrt(x);
    double __t_4 = (__t_1 + x) / ( __t_2 +
    __t_3 );
    double __t_5 = (M_PI + x);
    double __t_6 = sqrt(__t_5);
    double __t_7 = (__t_4 + __t_6);

    return __t_7;
}

// end of g_impl.c

```

264 3.2. Using the module as interface

265 As example, an implementation of an algorithm that estimates the *order*
 266 *of convergence* for trapezoidal integration scheme [14] is provided, using the
 267 symbolic differentiation as interface.

268 Given a function $f(x)$, the trapezoidal rule for primitive estimation for
 269 the interval $[a, b]$ is:

$$I_n(a, b) = h \left(\frac{f(a) + f(b)}{2} + \sum_{k=1}^{n-1} f(a + k h) \right) \quad (5)$$

270 with $h = (b - a)/n$, where n mediates the step size of the integration. When
 271 exact primitive $F(x)$ is known, approximation error is:

$$E[n] = F(b) - F(a) - I_n(a, b) \quad (6)$$

272 The error has an asymptotic expansion of the form:

$$E[n] \propto C n^{-p} \quad (7)$$

273 where p is the convergence order. Using a different value for n , for example
 274 $2n$, the ratio 8 takes the approximate vale:

$$\frac{E[n]}{E[2n]} \approx 2^p \quad \rightarrow \quad p \approx \log_2 \left(\frac{E[n]}{E[2n]} \right) \quad (8)$$

275 The Listings 13 and 14 contain the implementation of the described procedure
 276 using the proposed gem and the well known *Python* [15] library *SymPy* [16].

Listing 13: Ruby version

```

require 'Mr.CAS'

def integrate(f, a, b, n)
  h = (b - a) / n

  func = f.as_proc

  sum = ((func.call 'x' => a) +
        (func.call 'x' => b)) / 2.0

  for i in (1...n)
    sum += (func.call 'x' => (a + i*h))
  end
  return sum * h
end

277 def order(f, a, b, n)
  x = CAS.vars 'x'

  f_ab = (f.call x => b) -
        (f.call x => a)
  df = f.diff(x).simplify
  f_1n = integrate(df, a, b, n)
  f_2n = integrate(df, a, b, 2 * n)

  return Math.log(
    (f_ab - f_1n) /
    (f_ab - f_2n),
    2)
end

x = CAS.vars 'x'
f = CAS.arctan x

puts(order f, -1.0, 1.0, 100)
# => 1.9999999974244451

```

Listing 14: Python version

```

import sympy
import math

def integrate(f, a, b, n):
  h = (b - a)/n
  x = sympy.symbols('x')
  func = sympy.lambdify((x), f)

  sums = (func(a) +
        func(b)) / 2.0

  for i in range(1, n):
    sums += func(a + i*h)

  return sums * h

def order(f, a, b, n):
  x = sympy.symbols('x')

  f_ab = sympy.Subs(f, (x), (b)).n() - \
        sympy.Subs(f, (x), (a)).n()
  df = f.diff(x)
  f_1n = integrate(df, a, b, n)
  f_2n = integrate(df, a, b, 2 * n)

  return math.log(
    (f_ab - f_1n) /
    (f_ab - f_2n),
    2)

x = sympy.symbols('x')
f = sympy.atan(x)

print(order(f, -1.0, 1.0, 100))
# => 1.9999999974244451

```

278 3.3. ODE Solver with Taylor's series

279 In this example, a solving step for a specific ordinary differential equation
 280 (ODE) using Taylor's series method [17] is derived. Given an ODE in the
 281 form:

$$y'(x) = f(x, y(x)) \quad (9)$$

282 the integration step with order n has the form:

$$y(x+h) = y(x) + h y'(x) + \cdots + \frac{h^n}{n!} y^{(n)}(x) + E_n(x) \quad (10)$$

283 where it is possible to substitute equation 9:

$$y^{(i)}(x) = \frac{\partial y^{(i-1)}(x)}{\partial x} + \frac{\partial y^{(i-1)}(x)}{\partial y} y'(x) \quad (11)$$

284 For this algorithm, three methods are defined. The first evaluates the facto-
 285 rial, the second evaluates the list of required derivatives, and the third returns
 286 the integration step in a symbolic form. The result of the third method is
 287 transformed in a C function. In this particular case, the ODE is $y' = xy$. For
 288 the resulting C code of Listing 15, refer to the online version of the examples.

Listing 15: Generator for ODE integration step

```

289 $x, $y, $h = CAS::vars :x, :y, :h
290 # Evaluates n!
291 def fact(n); (n < 2 ? 1 : n * fact(n-1)); end
292 # Evaluates all derivatives required by the order
293 def coeff(f, n)
294   df = [f]
295   for _ in 2..n
296     df << df[-1].diff($x).simplify + (df[-1].diff($y).simplify * df[0])
297   end
298   return df
299 end
300 # Generates the symbolic form for a Taylor step
301 def taylor(f, n)
302   df = coeff(f, n)
303   y = $y
304   for i in 0...df.size
305     y = y + (($h ** (i + 1))/(fact(i + 1)) * df[i])
306   end
307   return y.simplify
308 end
309
310
311 # Example function for the integrator
312 f = $x * $y
313 # Exporting a C function
314 clib = CAS::CLib.create "taylor" do
315   implements_as "taylor_step", taylor(f, 4)
316 end

```

318 Other examples are available online⁴: (a) adding a user defined `CAS::Op-`
 319 that implements the `sign(·)` function with the appropriate optimized C gener-

⁴http://bit.ly/Mr_CAS_examples

320 ation rule; (b) exporting the operation as a continuous function through over-
321 loading or substitutions; (c) performing a symbolic Taylor’s series; (d) writing
322 an exporter for the L^AT_EX language; (e) a Newton-Raphson algorithm using
323 automatic differentiation plugin.

324 4. Impact

325 *Mr.CAS* is a midpoint between a CAS and an ASD library. It allows
326 to manipulate expressions while maintaining the complete control on how
327 the code is exported. Each rule is overloaded and applied run-time, without
328 the need of compilation. Each user’s model may include the mathematical
329 description, code generation rules and high level logic that should be intrinsic
330 to such a rule—for example, exporting a Hessian as pattern instead of matrix.

331 Our research group is including *Mr.CAS* in a solver for optimal control
332 problem with indirect methods, as interface for problems description [18].

333 As a long term ambitious impact, this library will become a complete
334 CAS for *Ruby* language, filling the empty space reported by *SciRuby* for
335 symbolic math engines.

336 5. Conclusions

337 This work presents a pure *Ruby* library that implements a minimalis-
338 tics CAS with automatic and symbolic differentiation that is aimed at code
339 generation and meta-programming. Although at an early developing stage,
340 *Mr.CAS* has promising feature, some of them shown in Section 3. Also, this
341 is the only gem that implements symbolic manipulation for this language.

342 Language features and lack of dependencies simplify the use of the module
343 as interface, extending model definition capabilities for numerical algorithms.
344 All core functionalities and basic mathematics are defined, with the plan to
345 include more features in next releases. Reopening a class guarantees a *liquid*
346 behaviour, in which users are free to modify core methods at their needs.

347 Library is published in *rubygems.org* repository and versioned on *github.com*,
348 under MIT license. It can be included easily in projects and in inline inter-
349 preter, or installed as a standalone gem.

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394 **Current code version**

Nr.	Code metadata description	Please fill in this column
C1	Current code version	0.2.7
C2	Permanent link to code/repository used for this code version	github.com/MatteoRagni/cas-rb & rubygems.org/gems/Mr.CAS
C3	Legal Code License	MIT
C4	Code versioning system used	<i>git</i> (GitHub)
C5	Software code languages, tools, and services used	<i>Ruby</i> language
C6	Compilation requirements, operating environments	<i>Ruby</i> $\geq 2.x$
C7	If available Link to developer documentation/manual	rubydoc.info/gems/Mr.CAS
C8	Support email for questions	info@ragni.me

Table 1: Code metadata (mandatory)