

Ryacas

A computer algebra system in R

Mikkel Meyer Andersen and Søren Højsgaard

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Genesis of Rycas

[Rd] Computer algebra in R - would that be an idea??

From: Søren Højsgaard Date: Tue 12 Jul 2005 - 11:19:48 GMT

From time to time people request symbolic computations beyond what `D()` and `deriv()` etc can provide. A brief look at the internet shows that there are many more or less developed computer algebra packages freely available. Therefore, I wondered if it would be an idea to try to 'integrate' one of these packages in R, which I guess can be done in more or less elegant ways... I do not know any of the computer algebra people around the World, but perhaps some other people from the R-community do and would be able to/interested in establishing such a connection... Just an idea; comments appreciated :-)

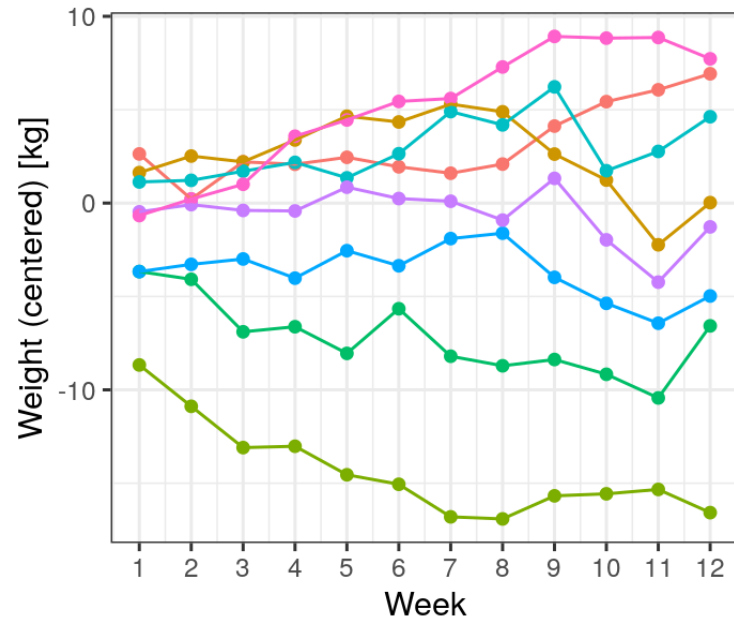
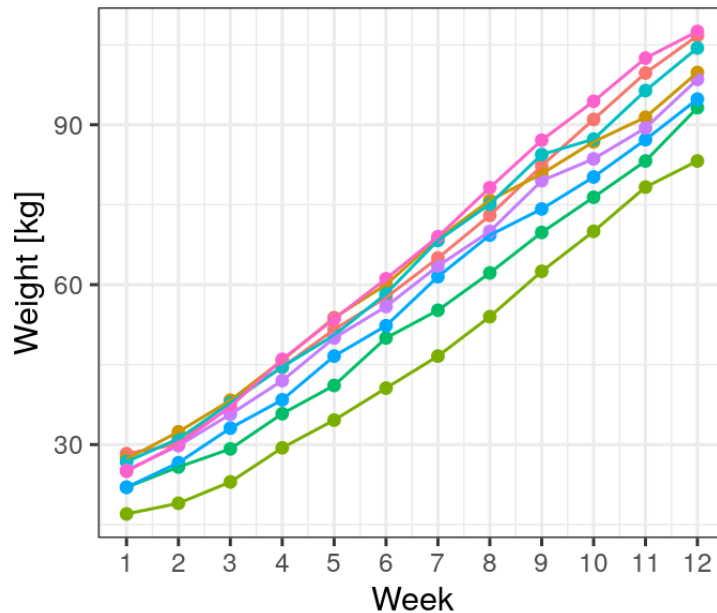
Original motivation

Modelling growth of slaughter pigs under different feed treatments.

One option is random regression model for i 'th individual:

$$y_{i,t} = b_0 + b_1 t + B_0 + B_1 t + e_{i,t},$$

where B_0 , B_1 , $e_{i,t}$ are normal random effects (and b_0 , b_1 are specific to treatment).



Motivation

Random regression model:

$$y_{i,t} = B_0 + B_1 t + e_{i,t}$$

where B_0 , B_1 , $e_{i,t}$ are normal random effects.

Question: What happens to the correlation between measurements on the same unit, i , as the distance between measurements increase. That is, what is the limit of

$$\text{cor}(y_{i,t}, y_{i,t+k}) \rightarrow ?? \quad \text{as} \quad k \rightarrow \infty$$

Background

- First version: yacasR; only on Windows; communication between R and yacas based client/server technology on local machine.
- Changed name to Ryacas; more contributors:
 - Rob Goedman
 - Gabor Grothendieck
 - **Søren Højsgaard**
 - Ayal Pinkus
 - Grzegorz Mazur
- Appeared on CRAN around 2009.

Background

- Has lived a quiet life until recently (2017) when **Mikkel Meyer Andersen** became maintainer
 - XML replaced by xml2, then skip XML communication with yacas's RForm()
- JOSS paper Andersen and Højsgaard (2019) **Ryacas: A computer algebra system in R**
- Synergy in open source projects
 - Bugs in yacas (Solve(), ())
 - New features in yacas (SumFunc(), Solve(), RForm(), Variables())
- Other resources: **Wolfram Alpha**

Getting started

Getting started

```
library(Ryacas)
```

- Stable version: <https://CRAN.R-project.org/package=Ryacas>
- Development version: <https://github.com/mikldk/ryacas/>
- Online documentation: <http://mikldk.github.io/ryacas/>

This talk was made using the development version available at <https://github.com/mikldk/ryacas/>:

```
devtools::install_github("mikldk/ryacas")
```

```
packageVersion("Ryacas")
```

```
## [1] '1.1.1.9005'
```

yacas symbols

```
x <- ysym("x")  
y <- ysym("y")  
eq <- x^2 + 3*x + 4*y + y^4  
eq
```

```
## y: x^2+3*x+4*y+y^4
```

...is just a class with a `yacas` command (for now)

```
str(eq)
```

```
## List of 3  
## $ yacas_cmd: chr "x^2+3*x+4*y+y^4"  
## $ is_mat : logi FALSE  
## $ is_vec : logi FALSE
```

```
class(eq)
```

```
## [1] "yac_symbol" "list"
```

```
as_r(eq)
```

```
## expression(x^2 + 3 * x + 4 * y + y^4)
```

```
as.character(eq)
```

```
## [1] "x^2+3*x+4*y+y^4"
```

Generic functions

```
methods(class = "yac_symbol")
```

```
## [1] [ [] [1] [<- %*% as_r
## [6] as_y as.character c cbind deriv
## [11] diag diag<- dim Hessian integrate
## [16] Jacobian length lim lower.tri Math
## [21] Ops print prod rbind simplify
## [26] solve str sum t tex
## [31] upper.tri with_value y_fn y_rmvars yac_assign
## [36] yac_expr yac_silent yac_str yac
## see '?methods' for accessing help and source code
```

Derivatives

```
deriv(eq, "x") # eq = x^2+3*x+4*y+y^4
```

```
## y: 2*x+3
```

```
H <- Hessian(eq, c("x", "y"))  
H
```

```
## {{      2,      0},  
## {      0, 12*y^2}}
```

```
eval(as_r(H), list(x = 1, y = 1))
```

```
##      [,1] [,2]  
## [1,]    2    0  
## [2,]    0   12
```

```
tex(H)
```

```
## [1] "\\left( \\begin{array}{cc} 2 & 0 \\\\ 0 & 12 y ^{2} \\end{array} \\right)"
```

Solving equations

Syntax:

```
solve(lhs, rhs, vars)
```

A brief example:

```
sol <- solve(x^2, -1, "x")  
sol
```

```
## {x==Complex(0, 1), x==Complex(0, -1)}
```

```
y_rmvars(sol)
```

```
## {Complex(0, 1), Complex(0, -1)}
```

```
as_r(y_rmvars(sol))
```

```
## [1] 0+1i 0-1i
```

Another example finding roots:

```
eq
```

```
## y: x^2+3*x+4*y+y^4
```

```
roots <- solve(eq, 0, "x") # shorthand rhs == 0: solve(eq, "x")  
roots
```

```
## {x==(Sqrt(9-4*(4*y+y^4))-3)/2, x==(-(Sqrt(9-4*(4*y+y^4))+3))/2}
```

```
tex(roots)
```

```
## [1] "\\left( x = \\frac{\\sqrt{9 - 4 \\left( 4 y + y ^{4} \\right) } - 3}{2}, x = \\frac{- \\left( \\sqrt{9 - 4 (4 y + y ^{4})} + 3 \\right) }{2} \\right)
```

```
### $$\\begin{align}`r tex(roots)`\\end{align}$$
```

$$\left(x = \frac{\sqrt{9 - 4(4y + y^4)} - 3}{2}, x = \frac{-\left(\sqrt{9 - 4(4y + y^4)} + 3\right)}{2} \right)$$

Solving a system of non-linear equations

```
x <- ysym("x")
y <- ysym("y")
lhs <- c(3*x*y - y, x)
rhs <- c(-5*x, y+4)
```

$$3xy - y = -5x$$
$$x = y + 4$$

```
sol <- solve(lhs, rhs, c("x", "y"))
sol
```

```
## {{      x==2,      y==(-2)},
## {      x==2/3, y==(-10)/3}}
```

```
as_r(y_rmvars(sol))
```

```
##           [,1]      [,2]
## [1,] 2.0000000 -2.0000000
## [2,] 0.6666667 -3.3333333
```


Integrals

Syntax:

```
integrate(expr, var)  
integrate(expr, var, from, to)
```

```
x <- ysym("x")  
res <- integrate(1/x, "x")  
res
```

```
## y: Ln(x)
```

```
res <- integrate(sin(x)^2, "x")  
res
```

```
## y: (x+Sin((-2)*x)/2)/2
```

```
as_r(res)
```

```
## expression((x + sin(-2 * x)/2)/2)
```

Sums

Syntax:

```
sum(expr, var, from, to)
```

```
x <- ysym("x")
k <- ysym("k")
res <- sum(x^k, "k", 0, "n")
res
```

```
## y: (1-x^(n+1))/(1-x)
```

Sums

```
k <- ysym("k")
res <- sum(1/k^2, "k", 1, Inf)
res
```

```
## y: Pi^2/6
```

```
as_r(res)
```

```
## [1] 1.644934
```

Limits

Syntax:

```
lim(expr, var, to)
lim(expr, var, to, from_left = TRUE)
lim(expr, var, to, from_right = TRUE)
```

```
x <- ysym("x")
lim(sin(x)/x, "x", 0)
```

```
## y: 1
```

```
lim(1/x, "x", 0)
```

```
## y: Undefined
```

```
lim(1/x, "x", 0, from_left = TRUE)
```

```
## y: -Infinity
```

```
lim(1/x, "x", 0, from_right = TRUE)
```

```
## y: Infinity
```

Linear algebra

```
A <- ysym(matrix(c(2, 1, 4, "x"), 2, 2))  
A
```

```
## {{2, 4},  
## {1, x}}
```

```
t(A)
```

```
## {{2, 1},  
## {4, x}}
```

```
A[1, ]
```

```
## {2, 4}
```

```
# solve(A)  
y_fn(A, "Determinant") # yacas function Determinant()
```

```
## y: 2*x-4
```

Linear algebra

```
b <- ysym(c("x", 3))  
y <- A %**% b  
y
```

```
## {2*x+12, 4*x}
```

```
solve(A, y)
```

```
## {((2*x+12)*x-16*x)/(2*x-4), (8*x-(2*x+12))/(2*x-4)}
```

```
solve(A, y) %>% simplify()
```

```
## {x, 3}
```

```
b
```

```
## {x, 3}
```

High-level interface (for everyday use)

- yacas symbols (`ysym()`)
- R syntax (`*`, `%*%`, `[`, `[<-`, `solve()`, etc.)

Low-level interface (for advanced stuff)

- `yac_str(x)`: Run yacas command `x` and return string

```
yac_str("Determinant({{2, 4}, {1, x}})")
```

```
## [1] "2*x-4"
```

- `yac_expr()`: Run yacas command `x` and return R expression

```
yac_expr("Determinant({{2, 4}, {1, x}})")
```

```
## expression(2 * x - 4)
```

See the documentation for yacas at <https://yacas.readthedocs.io/>.

Example: Multinomial likelihood

Multinomial likelihood

The multinomial likelihood for three categories is

$$\text{lik}(p \mid y) \propto p_1^{y_1} p_2^{y_2} p_3^{y_3}.$$

Taking log we get

$$\begin{aligned} l(p) &= y_1 \log(p_1) + y_2 \log(p_2) + y_3 \log(p_3) \\ g(p) &= p_1 + p_2 + p_3 - 1. \end{aligned}$$

Maximise $l(p)$ for $g(p) = 0$ using Lagrange multiplier to get the unconstrained optimisation problem

$$L = -l(p) + \lambda g(p)$$

```
p <- ysym(c("p1", "p2", "p3"))
y <- ysym(c("y1", "y2", "y3"))
lambda <- ysym("lambda")
l <- sum(y*log(p))
L <- -l + lambda*(sum(p) - 1)
L
```

```
## y: lambda*(p1+p2+p3-1)-(y1*Ln(p1)+y2*Ln(p2)+y3*Ln(p3))
```

Multinomial likelihood

```
gL <- deriv(L, c("p1", "p2", "p3"))  
gL
```

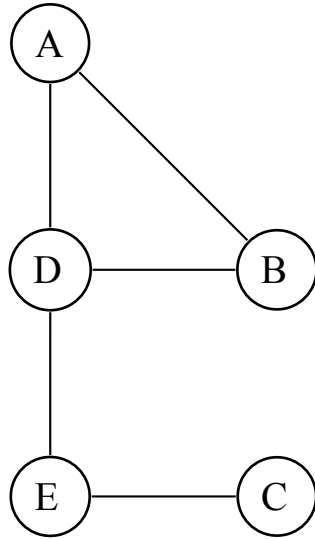
```
## {lambda-y1/p1, lambda-y2/p2, lambda-y3/p3}
```

- 3 equations by setting partial derivatives to 0
- 1 equation from the constraint

```
sol <- solve(c(gL, sum(p)),  
            c(rep(0, 3), 1),  
            c("p1", "p2", "p3", "lambda"))  
sol
```

```
## {{p1==y1/lambda, p2==y2/lambda, p3==y3/lambda, lambda==y1+y2+y3}}
```

Example: Graphical models



- Multivariate models with focus on conditional independence (CI) restrictions.
- Suppose $X = (X_A, X_B, \dots, X_E) \sim N_5(0, \Sigma)$.
- The key to interpretation is the concentration matrix $K = \Sigma^{-1}$
- $K_{ij} = 0$ iff X_i and X_j are independent given all other X s
- A missing edge reflects a CI-restriction.

- For example X_D and X_C are independent given all other X s
- A practical approach: X_C and X_D may be correlated. However
 - Regress X_D on X_A, X_B, X_E and extract residuals r_D .
 - Regress X_C on X_A, X_B, X_E and extract residuals r_C .
 - If the residuals r_D and r_C are uncorrelated then we have the CI.

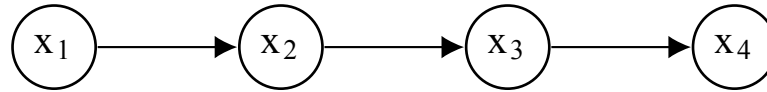
Many classical statistical models are built up on "modularization" based on CI-restrictions:

Examples:

- Autoregressive models
- State-space models / dynamic linear models
- Naive Bayesian models
- Probabilistic Principal Components

It is illustrative to see the connection between these model classes and CI-restrictions in the multivariate normal distribution.

Autoregression, AR(1)



Consider $AR(1)$ process: $x_i = ax_{i-1} + e_i$ where $i = 2, 3, 4$ and where $x_1 = e_1$.

$$x_1 = e_1$$

$$x_2 = ax_1 + e_2$$

$$x_3 = ax_2 + e_3$$

$$x_4 = ax_3 + e_4$$

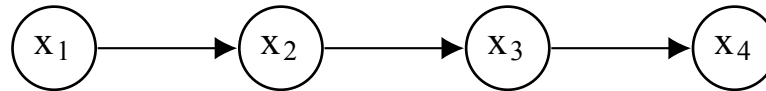
Let $e = (e_1, \dots, e_4)$ and $x = (x_1, \dots, x_4)$. Isolating error terms gives that

$$e = \begin{pmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -a & 1 & 0 & 0 \\ 0 & -a & 1 & 0 \\ 0 & 0 & -a & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = Lx$$

Define L :

```
# Or rbind(c(1, 0, 0, 0), ...)
L <- ysym("{ {1,0,0,0}, {-a,1,0,0}, {0,-a,1,0}, {0,0,-a,1} }")
L
```

```
## { { 1,  0,  0,  0},
##   {-a,  1,  0,  0},
##   { 0, -a,  1,  0},
##   { 0,  0, -a,  1}}
```



If error terms e_i are independent and $N(0, v^2)$ then $e = Lx$ gives

- $\mathbf{Var}(e) = v^2 I = L\mathbf{Var}(x)L'$
- Hence the covariance matrix of x is $V = \mathbf{Var}(x) = v^2 L^{-1}(L^{-1})'$
- The concentration matrix is $K = V^{-1} = LL'/v^2$

We skip v^2 in the following (set $v^2 = 1$)

```
Li <- solve(L)
Li
```

```
## {{ 1, 0, 0, 0},
## { a, 1, 0, 0},
## {a^2, a, 1, 0},
## {a^3, a^2, a, 1}}
```

```
V <- Li %*% t(Li)
K <- L %*% t(L)
```

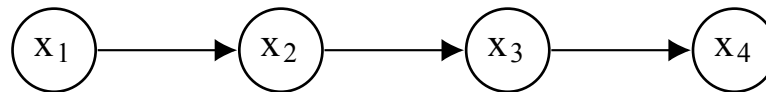
$$K = \begin{pmatrix} 1 & -a & 0 & 0 \\ -a & a^2 + 1 & -a & 0 \\ 0 & -a & a^2 + 1 & -a \\ 0 & 0 & -a & a^2 + 1 \end{pmatrix}$$
$$V = \begin{pmatrix} 1 & a & a^2 & a^3 \\ a & a^2 + 1 & a^3 + a & a^4 + a^2 \\ a^2 & a^3 + a & a^4 + a^2 + 1 & a^5 + a^3 + a \\ a^3 & a^4 + a^2 & a^5 + a^3 + a & a^6 + a^4 + a^2 + 1 \end{pmatrix}$$

The pattern of 0s in K is important:

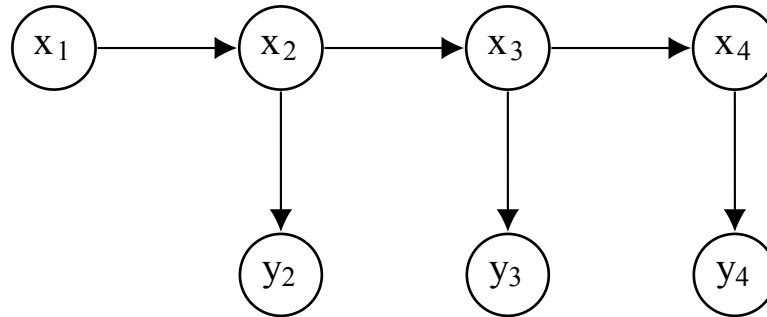
K

```
## {{ 1, -a, 0, 0},  
## { -a, a^2+1, -a, 0},  
## { 0, -a, a^2+1, -a},  
## { 0, 0, -a, a^2+1}}
```

$K_{ij} = 0$ iff x_i is independent of x_j given all other x 's



State space models



Same story, except that the setting is slightly more involved:

$$x_i = ax_{i-1} + e_i$$

$$y_i = bx_i + u_i$$

This gives a different L , but the method to find the concentration matrix is as before.

Further down the road

Further down the road

Symbolic math in R is limited to finding derivatives.

With Ryacas we have added a bit (still in R syntax thanks to S3)

- Integration
- Finding limits
- Simplifying expressions
- Solving (potentially systems of) non-linear equations
- Linear algebra
- Technical properties
 - No SystemRequirements
 - R expressions thanks to RForm() in yacas
 - LaTeX format thanks to TeXForm() in yacas

It may well be that in the future another engine than yacas should be invoked.

Original motivation - revisited

Random regression model:

$$y_t = B_0 + B_1 t + e_t$$

where $B = (B_0, B_1) \sim N(0, \Sigma)$, $e_t \sim N(0, w^2)$ are independent normal random effects.

What is:

$$\text{cor}(y_t, y_{t+k}) \rightarrow ?? \quad \text{as } k \rightarrow \infty$$

Solution

From:

$$y_t = B_0 + B_1 t + e_t = [1 \quad t] \begin{bmatrix} B_0 \\ B_1 \end{bmatrix} + e_t$$

We get:

$$\mathbf{Var}(y_t) = \mathbf{Var} \left([1 \quad t] \begin{bmatrix} B_0 \\ B_1 \end{bmatrix} \right) + \mathbf{Var}(e_t) = [1 \quad t] \Sigma [1 \quad t]^\top + w^2.$$

Similarly:

$$\mathbf{Var}(y_{t+k}) = [1 \quad t+k] \Sigma [1 \quad t+k]^\top + w^2.$$

Finally:

$$\mathbf{Cov}(y_t, y_{t+k}) = [1 \quad t] \Sigma [1 \quad t+k]^\top$$
$$\mathbf{Cor}(y_t, y_{t+k}) = \frac{\mathbf{Cov}(y_t, y_{t+k})}{\sqrt{\mathbf{Var}(y_t) \mathbf{Var}(y_{t+k})}}.$$

Formulation in Rycas

```
ysym_make(c("v1", "v2", "c12"))
```

```
## Warning in FUN(X[[i]], ...): v1 already exists, skipping
```

```
## Warning in FUN(X[[i]], ...): v2 already exists, skipping
```

```
## Warning in FUN(X[[i]], ...): c12 already exists, skipping
```

```
S <- rbind(c(v1, c12), c(c12, v2))
```

```
ysym_make(c("w" = "w", "xt" = "{{1, t}}", "xtk" = "{{1, t+k}}"))
```

```
## Warning in FUN(X[[i]], ...): w already exists, skipping
```

```
## Warning in FUN(X[[i]], ...): xt already exists, skipping
```

```
## Warning in FUN(X[[i]], ...): xtk already exists, skipping
```

```
v_t <- (xt %*% S %*% t(xt) + w^2)[1, 1]
```

```
v_t
```

```
## y: w^2+v1+t*c12+(c12+t*v2)*t
```

Finding the limit

Now the progress stops

```
# lim Cor(y_t, y_{t+k}) for k -> Inf  
lim(cv_t_tk / sqrt(v_t * v_tk), "k", Inf)
```

```
## Error in yac_core(x): Yacas returned this error: CommandLine(1) : Max eval  
## Please use MaxEvalDepth to increase the stack size as needed.
```

```
k <- ysym("k")  
lim((cv_t_tk / k) / sqrt((v_t * v_tk) / k^2), "k", Inf)
```

```
## Error in yac_core(x): Yacas returned this error: CommandLine(1) : Max eval  
## Please use MaxEvalDepth to increase the stack size as needed.
```

(<https://github.com/grzegorzmazur/yacas/issues/282>)

Another CAS

```
library(symr) # Based on SymPy; work in progress...
num <- paste0("(", as.character(cv_t_tk), ")/k")
den <- paste0("sqrt((((", as.character(v_t), ") * ((",
              as.character(v_tk), ")/ k^2)))")
num <- gsub("^", "**", num, fixed = TRUE) # Python's way
den <- gsub("^", "**", den, fixed = TRUE)
sympy <- symr::get_sympy()
res <- sympy$limit(paste0(num, "/", den), "k", "oo")
res
```

```
## (c12 + t*v2)/sqrt(v2*(c12*t + t*(c12 + t*v2) + v1 + w**2))
```

```
sympy$latex(res)
```

```
## [1] "\\frac{c_{12} + t v_{2}}{\\sqrt{v_{2} \\left(c_{12} t + t \\left(c_{12} + t v_{2}\\right) + v_{1} + w^2\\right)}}
```

$$\text{cor}(y_t, y_{t+k}) \rightarrow \frac{c_{12} + tv_2}{\sqrt{v_2 (c_{12}t + t (c_{12} + tv_2) + v_1 + w^2)}} \quad \text{as } k \rightarrow \infty$$

More in 2020...

References

- Yacas (yet another computer algebra system): <http://www.yacas.org/>
 - Online docs: <http://yacas.readthedocs.org/>
- Stable version: <https://CRAN.R-project.org/package=Ryacas>
- Development version: <https://github.com/mikldk/ryacas/>
 - Online docs: <http://mikldk.github.io/ryacas/>