

# Computer Algebra Systems in R with *caracas*

by Mikkel Meyer Andersen and Søren Højsgaard

**Abstract** The capability of R to do symbolic mathematics is enhanced by the *caracas* package. This package uses the Python computer algebra library SymPy as a back-end but *caracas* is tightly integrated in the R environment, thereby enabling the R user with symbolic mathematics within R. Key components of the *caracas* package are illustrated in this paper. Examples are taken from statistics and mathematics. The *caracas* package integrates well with e.g. *Rmarkdown*, and as such creation of scientific reports and teaching is supported.

## Keywords

Differentiation, Factor analysis, Hessian matrix, Integration, Lagrange multiplier, Limit, Linear algebra, Principal component analysis, Score function, Symbolic mathematics, Taylor expansion, Teaching.

## Introduction

The capability of R (R Core Team, 2021) to handle symbolic mathematics is greatly enhanced by two packages: The *caracas* package, which is the main topic of this paper, and the *Ryacas* package described in Andersen and Højsgaard (2019). The *caracas* package is based on interfacing the Python library SymPy (Meurer et al., 2017), using the *reticulate* package, (Ushey et al., 2020). Similarly, *Ryacas* is based on interfacing the computer algebra system (CAS) yacas (Pinkus et al., 2016; Pinkus and Winitzki, 2002). The *caracas* package is open-source and the source code is available at <https://github.com/r-cas/caracas>. Several vignettes illustrating *caracas* are provided and these are also available online, see <https://r-cas.github.io/caracas/>.

One particular instance where we have found the packages useful is in connection with teaching where symbolic mathematics is helpful strongly aided by the packages ability to enter in a reproducible framework (provided e.g. by *Rmarkdown*). In this paper we provide a few examples of this, and we address the issue more generally towards the end of the paper.

**The *caracas* package versus other computer algebra systems** Neither *caracas* nor *Ryacas* are as powerful as some of the large commercial computer algebra systems. The virtue of the *caracas* and *Ryacas* packages lie elsewhere:

1. Tools like solving equations, summation, limits, symbolic linear algebra, outputting in tex format etc. are directly available from within R.
2. The packages enable working with the same language and in the same environment as the user does for statistical analyses.
3. Symbolic mathematics can easily be combined with data which is helpful in e.g. numerical optimization.
4. Lastly, the packages are part of the R project (since the packages are on CRAN). As such the packages are freely available, and therefore support e.g. education - also of people with limited economical means and thus contributing to United Nations sustainable development goals, cfr. United Nations General Assembly (2015).

With respect to freely available resources in a CAS context, we would like to draw attention to WolframAlpha, see <https://www.wolframalpha.com/>, which is an online for answering (mathematical) queries.

## Introductory examples

There are no other system requirements than Python for using *caracas*. This paper is based on the following version of *caracas*:

```
R> library(caracas)
R> packageVersion("caracas")
#> [1] '1.1.0'
```

## The interplay between R and SymPy

As mentioned above, `caracas` provides an interface from R to the Python package SymPy. This means that SymPy is “running under the hood” of R via the `reticulate` package. In `caracas` we have symbols, which is an R list with a `pyobj` slot and the class `caracas_symbol`. The `pyobj` refers to an object in Python (often a SymPy object). As such, a symbol (in R) provides a handle to a Python object. In the design of `caracas` we have tried to make this distinction something the user should not be concerned with, but it is worthwhile being aware of the distinction. There are several ways of creating symbols; one is with `def_sym()` that both declares the symbol in R and in Python:

```
R> ## Define symbols and assign in global environment
R> def_sym(s1, s2); s1 # Declares 's1'/'s2' in both R and Python
#> [caracas]: s1
R> str(s1)
#> List of 1
#> $ pyobj:s1
#> - attr(*, "class")= chr "caracas_symbol"
R> ## Create new symbol from existing ones
R> s3 <- s1 * s2; s3 # 's3' is a symbol in R; no corresponding object in Python
#> [caracas]: s1*s2
R> str(s3)
#> List of 1
#> $ pyobj:s1*s2
#> - attr(*, "class")= chr "caracas_symbol"
```

Note that above `def_sym(s1, s2)` is a short-hand for the following:

```
R> s1 <- symbol("s1")
R> s2 <- symbol("s2")
```

We can further exemplify that objects in R and Python are not necessarily identical. We look into a symbol, and to make the distinction clear we use different names. Symbols can be created with the `symbol()` function.

```
R> ## Create a symbol 'b1' corresponding to an entity called 'a' in SymPy:
R> b1 <- symbol("a"); str(b1)
#> List of 1
#> $ pyobj:a
#> - attr(*, "class")= chr "caracas_symbol"
R> ## A new symbol can be created as:
R> b2 <- b1 + 1; str(b2)
#> List of 1
#> $ pyobj:a + 1
#> - attr(*, "class")= chr "caracas_symbol"
R> ## The Python entity 'a' in the symbol can be modified with:
R> b3 <- subs(b2, "a", "k"); str(b3)
#> List of 1
#> $ pyobj:k + 1
#> - attr(*, "class")= chr "caracas_symbol"
```

Going back to the first example, we can substitute one symbol with another and simplify the result as (where we use the pipe operator `%>%` from `magrittr` by [Bache and Wickham \(2020\)](#)):

```
R> s4 <- s3 %>% subs("s1", "u + v") %>% subs("s2", "u - v"); s4
#> [caracas]: (u - v)*(u + v)
R> s5 <- expand(s4); s5
#> [caracas]: 2 2
#> u - v
```

It is also possible to convert to and from symbols and standard R expressions:

```
R> ## Coerce from symbol to expression:
R> e5 <- as_expr(s5); e5
#> expression(u^2 - v^2)
R> ## Coerce from expression to symbol:
R> as_sym(e5) # identical to s5
```

```
#> [caracas]:  2    2
#>             u  - v
```

### Finding a limit - the Euler constant

Define symbols  $n$  and  $f$ :

```
R> def_sym(n)
R> f <- (1 + 1/n)^n
```

We can calculate the limit of  $f$  for  $n \rightarrow \infty$ :

```
R> lim_f <- lim(f, n, Inf)
R> lim_f
#> [caracas]: exp(1)
R> as_expr(lim_f)
#> [1] 2.72
```

We can also tell **caracas** not to evaluate the limit (with the `doit = FALSE` argument) but only set up the symbol for later evaluation and/or for additional algebraic manipulations:

```
R> lim_f_sym <- lim(f, n, Inf, doit = FALSE)
R> lim_f_sym
#> [caracas]:          n
#>             /    1\
#>          lim |1 + -|
#>         n->oo\    n/
```

By default **caracas** uses UTF-8 printing, but in this paper we have used pretty ASCII printing which can be set globally by `options(caracas.print.prettyascii = TRUE)`.

The unevaluated symbol can be evaluated as follows:

```
R> lim_f <- doit(lim_f_sym)
R> lim_f
#> [caracas]: exp(1)
```

Hence, three **caracas** symbols have been created above:  $f$ ,  $\lim\_f\_sym$  and  $\lim\_f$ . Objects can be printed in  $\text{\TeX}$  form using `tex()`, e.g.

```
R> tex(lim_f_sym)
#> [1] "\\lim_{n \\to \\infty} \\left(1 + \\frac{1}{n}\\right)^{n}"
```

This can be used in a  $\text{\TeX}$  environment as e.g.

```
\[
`r tex(f)`, \quad `r tex(lim_f_sym)`, \quad `r tex(lim_f)`.
\]
```

giving

$$\left(1 + \frac{1}{n}\right)^n, \quad \lim_{n \rightarrow \infty} \left(1 + \frac{1}{n}\right)^n, \quad e.$$

### Differentiation and integration

Consider this function (taken from a vignette for the **mosaicCalc** package (Kaplan et al., 2020)). Using the **Deriv** package, the derivative can be found as follows:

```
R> f <- function(x){
+   a * x + b * x^2 + c * sin(x^2)
+ }
R> Deriv::Deriv(f, "x")
#> function (x)
#> a + x * (2 * (c * cos(x^2)) + 2 * b)
```

The anti-derivative, however, is not easily obtained in R. Using **caracas** we get derivative and anti-derivative as:

```
R> f_c <- as_sym("a * x + b * x^2 + c * sin(x^2)")
R> def_sym(x) # To get handle on x in R
R> D_f <- der(f_c, x) # Or: der(f_c, "x")
R> aD_f <- int(f_c, x) %>% simplify()
```

$$D_f = a + 2bx + 2cx \cos(x^2), \quad aD_f = \frac{ax^2}{2} + \frac{bx^3}{3} + \frac{\sqrt{2}\sqrt{\pi}cS\left(\frac{\sqrt{2}x}{\sqrt{\pi}}\right)}{2}$$

Above,  $S()$  is the Fresnel integral  $S(z) = \int_0^z \sin\left(\frac{\pi}{2}t^2\right) dt$ . Evaluation in R requires a definition of `fresnels()`:

```
R> as_expr(aD_f) # Evaluation requires user-defined fresnels()
#> expression(a * x^2/2 + b * x^3/3 + sqrt(2) * sqrt(pi) * c * fresnels(sqrt(2) *
#> x/sqrt(pi))/2)
```

### Exact and numerical evaluations

We can make exact as well as numerical evaluations as follows:

```
R> def_sym(x)
R> f <- exp(x^2)
R> subs(f, x, "1/3")
#> [caracas]: exp(1/9)
R> subs(f, x, 1/3)
#> [caracas]: 1.11751906874186
```

In the first case,  $1/3$  is regarded as a fraction. In the second case,  $1/3$  is evaluated numerically in R before `caracas` gets the value. As a consequence we have:

```
R> subs(f, x, "1/3 + 1/4")
#> [caracas]: / 49\
#> exp|---|
#> \144/
R> subs(f, x, 1/3 + 1/4)
#> [caracas]: 1.40533790799144
```

An exact evaluation can be evaluated numerically afterwards:

```
R> subs(f, x, "1/3 + 1/4") %>% as_expr()
#> [1] 1.41
R> subs(f, x, "1/3 + 1/4") %>% N(30) # Exact representation up to 30 decimals
#> [caracas]: 1.40533790799143890537847414768
```

We can also convert the `caracas` symbol to an R expression that is subsequently evaluated:

```
R> f %>% as_expr()
#> expression(exp(x^2))
R> f %>% as_expr() %>% eval(list(x = 1/3 + 1/4))
#> [1] 1.41
```

### Taylor expansion

We perform a fourth order Taylor expansion of  $f(x) = \cos(x)$  around  $x = 0$ :

```
R> def_sym(x)
R> f <- cos(x)
R> ft_with_0 <- taylor(f, x0 = 0, n = 4+1); ft_with_0
#> [caracas]: 2 4
#> x x / 5.0\
#> 1 - -- + -- + 0\ x /
#> 2 24
```

The order term can be removed:

```
R> ft <- drop_remainder(ft_with_0); ft
#> [caracas]: 4 2
#> x x
#> -- - -- + 1
#> 24 2
R> ft %>% as_expr()
```

```
#> expression(x^4/24 - x^2/2 + 1)
```

## Matrix algebra

We briefly demonstrate the use matrices in **caracas** (see also <https://r-cas.github.io/caracas/>):

```
R> A <- matrix_(c("a", "b", "c", "d"), nrow = 2, ncol = 2) # Note the '_' postfix
R> # Or: matrix(c("a", "b", "c", "d"), nrow = 2, ncol = 2) %>% as_sym()
```

Note that `rbind()` and `cbind()` also works on **caracas** (vector) symbols:

```
R> c1 <- as_sym(c("a", "b"))
R> c2 <- as_sym(c("c", "d"))
R> A <- cbind(c1, c2); A
#> [caracas]: [a c]
#>           [  ]
#>           [b d]
R> D <- diag_(c("e1", "e2")); D # Note the '_' postfix
#> [caracas]: [e1 0 ]
#>           [  ]
#>           [0 e2]
```

Some routines are demonstrated below:

```
R> detA <- det(A)
R> Ai <- inv(A) # Shorthand for solve_lin(A)
R> AD <- A %*% D
```

$$\det A = ad - bc, \quad A_i = \begin{bmatrix} \frac{d}{ad-bc} & -\frac{c}{ad-bc} \\ -\frac{b}{ad-bc} & \frac{a}{ad-bc} \end{bmatrix}, \quad AD = \begin{bmatrix} ae_1 & ce_2 \\ be_1 & de_2 \end{bmatrix}$$

```
R> evec <- eigenvec(A)
R> evec1 <- evec[[1]]$eigvec %>% simplify()
R> eval <- eigenval(A)
R> eval1 <- eval[[1]]$eigval %>% simplify()
```

$$\text{evec1} = \begin{bmatrix} -\frac{2c}{a-d+\sqrt{a^2-2ad+4bc+d^2}} \\ 1 \end{bmatrix}, \quad \text{eval1} = \frac{a}{2} + \frac{d}{2} - \frac{\sqrt{a^2-2ad+4bc+d^2}}{2}.$$

```
R> B <- matrix_(c("b", "0", "0", "1"), nrow = 2, ncol = 2)
R> qr_res <- QRdecomposition(B)
R> Q <- qr_res$Q
R> R <- qr_res$R
```

$$Q = \begin{bmatrix} \frac{b}{|b|} & 0 \\ 0 & 1 \end{bmatrix}, \quad R = \begin{bmatrix} |b| & 0 \\ 0 & 1 \end{bmatrix}.$$

## Lagrange multiplier and maximizing a likelihood

Here we illustrate how to maximize a multinomial likelihood using Lagrange multiplier. Consider a multinomial model with three categories with probabilities  $p_1, p_2$  and  $p_3$  such that  $p_1 + p_2 + p_3 = 1$ . We then observe counts  $y_1, y_2$  and  $y_3$  of each category. The multinomial log-likelihood for this model is

$$l(p) = y_1 \log(p_1) + y_2 \log(p_2) + y_3 \log(p_3). \quad (1)$$

We wish to maximize  $l(p)$  under the constraint that  $p_1 + p_2 + p_3 = 1$ . This can be achieved using Lagrange multiplier where we instead solve the unconstrained optimization problem  $\max_p L(p)$  where

$$L(p) = -l(p) + \lambda g(p) \quad \text{under the constraint that} \quad (2)$$

$$g(p) = p_1 + p_2 + p_3 - 1 = 0. \quad (3)$$

The function  $L$  can be expressed in **caracas** as follows where we create character vectors in R and convert them to a **caracas** symbol using `as_sym()`:

```
R> p <- as_sym(paste0("p", 1:3))
```

```
R> y <- as_sym(paste0("y", 1:3))
R> def_sym(a)
R> l <- sum(y * log(p))
R> L <- -l + a * (sum(p) - 1); L
#> [caracas]: a*(p1 + p2 + p3 - 1) - y1*log(p1) - y2*log(p2) - y3*log(p3)
```

To solve the unconstrained optimization problem we find the critical points and afterwards check the eigenvalues of the Hessian (at the critical points). The critical points are found as follows by first finding the gradient with `der()` (for derivative) and then equating the gradient to zero:

```
R> gL <- der(L, list(p, a))
```

Hence, `caracas` computes the gradient to be

$$\nabla L(p_1, p_2, p_3, a) = \begin{bmatrix} a - \frac{y_1}{p_1} & a - \frac{y_2}{p_2} & a - \frac{y_3}{p_3} & p_1 + p_2 + p_3 - 1 \end{bmatrix}.$$

Next we solve  $\nabla L(p_1, p_2, p_3, a) = 0$ :

```
R> sols <- solve_sys(gL, list(p, a)) # takes an RHS argument which defaults to zero
R> sols
#> Solution 1:
#>   p1 =      y1
#>   -----
#>   y1 + y2 + y3
#>   p2 =      y2
#>   -----
#>   y1 + y2 + y3
#>   p3 =      y3
#>   -----
#>   y1 + y2 + y3
#>   a  = y1 + y2 + y3
```

One critical point is found. (Notice that in general it is difficult to know how many critical points a function has. We will not go into details about this aspect of the problem.) Next we verify that we have found a minimum: We find the Hessian as a symbol and evaluate it in the critical point:

```
R> H <- der2(l, p) # der2(...) is shorthand for calling der() twice
R> H_sol <- subs_lst(H, sols[[1]]) # Substitute solution into H
```

$$H = \begin{bmatrix} -\frac{y_1}{p_1^2} & 0 & 0 \\ 0 & -\frac{y_2}{p_2^2} & 0 \\ 0 & 0 & -\frac{y_3}{p_3^2} \end{bmatrix}, \quad H_{\text{sol}} = \begin{bmatrix} -\frac{(y_1+y_2+y_3)^2}{y_1} & 0 & 0 \\ 0 & -\frac{(y_1+y_2+y_3)^2}{y_2} & 0 \\ 0 & 0 & -\frac{(y_1+y_2+y_3)^2}{y_3} \end{bmatrix}$$

We verify that the solution is indeed a minimum: As  $H_{\text{sol}}$  is a diagonal matrix, its eigenvalues are the diagonal entries. (In general, eigenvalues/eigenvectors can be found using `eigenval()/eigenvec()`.) Provided that all  $y_i > 0$ , all eigenvalues are negative and the likelihood reached a maximum.

### Extending `caracas` – calling SymPy functions directly

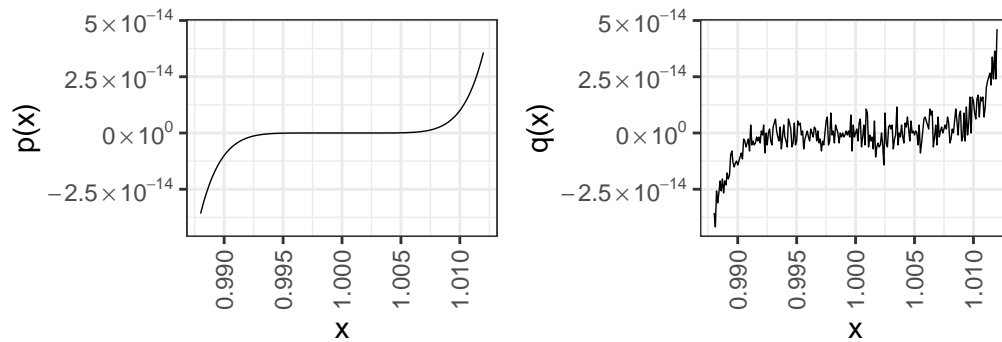
The `caracas` can be extended as it is possible to call SymPy functions directly with the `sympy_func()` function. Please refer to the SymPy documentation at <https://docs.sympy.org/latest/index.html> for documentation of SymPy functions.

At the time of writing, the SymPy functions `collect()` and `factor()` are not implemented in `caracas`, but they can be invoked as shown in the following. For example, we can collect terms in a polynomial expression:

```
R> def_sym(x, y, z)
R> p <- x*y + x - 3 + 2*x^2 - z*x^2 + x^3
R> p %>% sympy_func("collect", x)
#> [caracas]: 3      2
#>             x  + x*(2 - z) + x*(y + 1) - 3
```

We can also expand and factor a polynomial:

```
R> def_sym(x)
R> p <- (x - 1)^7
R> q <- p %>% expand(); q # or p %>% sympy_func("expand")
```



**Figure 1:** Difference between symbolic and numerical mathematics. Left: Plot of polynomial  $p(x) = (x - 1)^7$ . Right: Plot of expansion of same polynomial.

```
#> [caracas]: 7      6      5      4      3      2
#>           x - 7*x + 21*x - 35*x + 35*x - 21*x + 7*x - 1
R> q %>% sympy_func("factor")
#> [caracas]: 7
#>           (x - 1)
```

In passing we illustrate a difference between symbolic and numerical mathematics: Floating point arithmetic can lead to catastrophic cancellations when nearly identical quantities are subtracted. This can be demonstrated as follows. Evaluate  $p$  and  $q$  on a range of  $x$ -values near 1, and plot the results in Fig. 1.

### Statistics examples

In a linear model setting where  $E(y) = X\beta$ , the least squares estimate of  $\beta$  can be written as  $\hat{\beta} = (X^T X)^{-1} X^T y$ . It is illustrative to use symbolic mathematics for illustrating what is computed in the matrix algebra.

### One-way analysis of variance (one-way ANOVA)

First consider one-way analysis of variance (ANOVA).

```
R> ngrp <- 3 # Number of groups
R> spg <- 2 # Number of subjects per group
R> g <- seq_len(ngrp)
R> f <- factor(rep(g, each = spg))
R> y <- as_sym(paste0("y", seq_along(f)))
R> X <- as_sym(model.matrix(~ f))
```

We compute the usual quantities needed for finding the least squares estimate for the regression coefficients.

```
R> XtX <- t(X) %*% X
R> XtXinv <- inv(XtX) # Shorthand for solve_lin(XtX)
```

$$X = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \quad X^T X = \begin{bmatrix} 6 & 2 & 2 \\ 2 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix}, \quad (X^T X)^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 1 & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} & 1 \end{bmatrix}$$

Likewise,

```
R> Xty <- t(X) %*% y
R> beta_hat <- XtXinv %*% Xty
R> y_hat <- X %*% beta_hat
```

$$X^T y = \begin{bmatrix} y_1 + y_2 + y_3 + y_4 + y_5 + y_6 \\ y_3 + y_4 \\ y_5 + y_6 \end{bmatrix}, \quad \hat{\beta} = \frac{1}{2} \begin{bmatrix} y_1 + y_2 \\ -y_1 - y_2 + y_3 + y_4 \\ -y_1 - y_2 + y_5 + y_6 \end{bmatrix}, \quad \hat{y} = \frac{1}{2} \begin{bmatrix} y_1 + y_2 \\ y_1 + y_2 \\ y_3 + y_4 \\ y_3 + y_4 \\ y_5 + y_6 \\ y_5 + y_6 \end{bmatrix}$$

Hence  $X^T y$  consists of the sum of all observations, the sum of observations in group 2 and the sum of observations in group 3. Similarly,  $\hat{\beta}$  consists of the average in group 1, the average in group 2 minus the average in group 1 and the average in group 3 minus the average in group 1. Fitted values are simply group averages.

Next consider a linear model setting, i.e.  $y \sim N(X\beta, \sigma^2 I)$ . The score function and Hessian matrix can be derived in closed form as follows: Define residuals  $r = y - X\hat{\beta}$  and residual-sum-of-squares as  $RSS = \sum_i r_i^2$ . The log-likelihood based on  $n$  observations is

$$l = -\frac{n}{2}\sigma^2 - \frac{1}{2\sigma^2}RSS.$$

Here we can find critical points of  $l$  for  $RSS$  and  $\sigma^2$  independently, so we ignore  $\sigma^2$  and proceed focusing on  $RSS$  as follows:

```
R> beta <- as_sym(paste0("beta", 1:3))
R> res <- y - X %>% beta
R> RSS <- sum(res^2)
R> logL <- - RSS / 2
```

We find the score function and Hessian matrix by differentiation.

```
R> Score <- der(logL, beta) %>% matlify() # Convert Python list to vector
R> Hessian <- der2(logL, beta) %>% matlify() # Convert Python list to matrix
```

$$\text{Score} = \begin{bmatrix} -6\beta_1 - 2\beta_2 - 2\beta_3 + y_1 + y_2 + y_3 + y_4 + y_5 + y_6 \\ -2\beta_1 - 2\beta_2 + y_3 + y_4 \\ -2\beta_1 - 2\beta_3 + y_5 + y_6 \end{bmatrix}, \quad \text{Hessian} = \begin{bmatrix} -6 & -2 & -2 \\ -2 & -2 & 0 \\ -2 & 0 & -2 \end{bmatrix}$$

Notice the following: The output from `der` and `der2` are lists in Python, and to be able to work with these quantities as we normally do a coercion to matrices is needed. The `matlify()` function does this. We conclude this example by solving the likelihood equations which, fortunately, leads to the same quantity as  $\hat{\beta}$  derived above:

```
R> sol <- solve_sys(Score, beta)
R> sol
#> Solution 1:
#> beta1 = y1 y2
#>      -- + --
#>      2 2
#> beta2 = y1 y2 y3 y4
#>      - -- - -- + -- + --
#>      2 2 2 2
#> beta3 = y1 y2 y5 y6
#>      - -- - -- + -- + --
#>      2 2 2 2
```

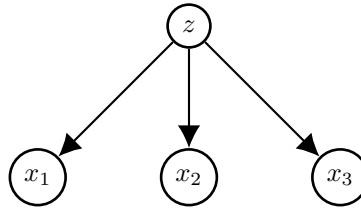
Similar considerations can be done for other linear models, e.g. a (balanced) two-way analysis of variance (two-way ANOVA).

### Probabilistic principal component analysis

A probabilistic principal component analysis (PCA) model arises as follows, see e.g. [Bishop \(2006\)](#), pp. 570: There is a latent vector  $z$  and it is assumed that  $z \sim N(0, I)$ . There is a vector  $x$  of observables and it is assumed that  $x | z \sim N(Wz + \mu, v^2 I)$ . It is not a restriction to assume that  $\mu = 0$  because we center each variable around its average. We can write the model as

$$z = e_z \quad \text{and} \quad x = Wz + e_x, \quad (4)$$





**Figure 2:** A directed acyclic graph (DAG) illustrating probabilistic PCA: The observables  $x = (x_1, x_2, x_3)$  are conditionally independent given  $z$ .

where  $e_z \sim N(0, I)$  and  $e_x \sim N(0, v^2 I)$  are error terms that are assumed independent. The  $W$  matrix is the model matrix of weights that reflects model assumptions about how  $z$  impacts  $x$ .

In a statistical inference setting, the unknown parameters ( $v^2$  and the components of  $W$ ) must be estimated. To do this the covariance matrix and concentration matrix are needed. The first step is to identify the structural form of the covariance matrix  $V = \mathbf{Var}(z, x)$  and concentration matrix  $K = V^{-1}$ , and `caracas` can do this for us. The next step is to use these structural forms in the likelihood function which can then be maximized.

Define

$$V = \mathbf{Var}(z, x) = \begin{pmatrix} V_{zz} & V_{zx} \\ V_{xz} & V_{xx} \end{pmatrix}, \quad K = V^{-1} = \begin{pmatrix} K_{zz} & K_{zx} \\ K_{xz} & K_{xx} \end{pmatrix}, \quad V_e = \mathbf{Var}(e) = \begin{pmatrix} I & 0 \\ 0 & v^2 I \end{pmatrix}.$$

Also define

$$L = \begin{pmatrix} I & 0 \\ -W & I \end{pmatrix} \text{ and note that } L^{-1} = \begin{pmatrix} I & 0 \\ W & I \end{pmatrix}. \quad (5)$$

Isolating error terms in (4) gives

$$e = \begin{pmatrix} e_z \\ e_x \end{pmatrix} = \begin{pmatrix} I & 0 \\ -W & I \end{pmatrix} \begin{pmatrix} z \\ x \end{pmatrix} = L \begin{pmatrix} z \\ x \end{pmatrix}.$$

Hence  $\mathbf{Var}(e) = L\mathbf{Var}(z, x)L^\top$  and therefore

$$V = \mathbf{Var}(z, x) = L^{-1}\mathbf{Var}(e)(L^{-1})^\top \text{ and } K = V^{-1} = L^\top \mathbf{Var}(e)^{-1}L. \quad (6)$$

Since the error terms are independent, a direct calculation gives

$$V = \begin{pmatrix} I & W^\top \\ W & WW^\top + v^2 I \end{pmatrix} \text{ and } K = \begin{pmatrix} I + v^{-2}W^\top W & -v^{-2}W^\top \\ v^{-2}W & v^{-2}I \end{pmatrix} \quad (7)$$

The following observations can be made:

1. First recall a general result on the multivariate normal distribution. Suppose  $U = (U_1, \dots, U_d) \sim N(\mu, V)$ , and let  $K = V^{-1}$ . Then  $K_{ij} = 0$  if and only if  $U_i$  and  $U_j$  are conditionally independent given all other components of  $U$ . Next return to the specific setting. The lower right corner,  $K_{xx}$ , of  $K$  is  $v^{-2}I$  and the fact that this matrix is diagonal reflects that all pairs of observables  $x_u$  and  $x_v$  are conditionally independent given the latent variables  $z$ .
2. The lower right corner,  $V_{xx}$ , of  $V$  is  $WW^\top + v^2 I$  and this matrix is the covariance matrix of observables  $x$ . The inverse of  $WW^\top + v^2 I$  is the concentration matrix of  $x$  (in the marginal distribution of  $x$ ) and this concentration matrix does not in general contain zeros. There are no conditional independencies among the observables alone; conditional independencies arise from conditioning on the latent variables.
3. To estimate the parameters  $W$  and  $v^2$  we can maximize the log-likelihood for the observables with covariance matrix  $V_{obs} = WW^\top + v^2 I$ . This can often be done directly using `optim()`. (Notice that we can just center data to eliminate the parameter  $\mu$ ).

**A simple example** A particularly simple example is the following where  $z$  is one-dimensional and  $x$  is three-dimensional and  $W$  is a  $3 \times 1$  matrix with  $a$  in all entries:

$$x_i = az + e_i, \quad i = 1, \dots, 3, \quad z = u$$

All  $e_1, \dots, e_3$  are  $N(0, v^2)$  distributed,  $u \sim N(0, 1)$  and all error terms are independent. See an illustration of this model in Fig. 2. Let  $e = (e_1, \dots, e_3)$  and  $x = (x_1, \dots, x_3)$ . Hence  $e \sim N(0, v^2 I)$  and  $\text{Var}(u, e)$  is a diagonal matrix,  $V_{ue} = \text{diag}(1, v^2, \dots, v^2)$ . Isolating error terms gives

$$(u, e) = \begin{bmatrix} u \\ e_1 \\ e_2 \\ e_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -a & 1 & 0 & 0 \\ -a & 0 & 1 & 0 \\ -a & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} z \\ x_1 \\ x_2 \\ x_3 \end{bmatrix} = L(z, x), \text{ say.}$$

```
R> N <- 3
R> L <- diag("1", N + 1)
R> L[cbind(1 + (1:N), 1)] <- "-a"
R> Vue <- matrix("0", nrow = N + 1, ncol = N + 1)
R> diag(Vue) <- c("1", rep("v2", N))
```

Following (6) we find  $V$  and  $K$  as:

```
R> V <- inv(L) %%% Vue %%% t(inv(L))
R> K <- t(L) %%% inv(Vue) %%% L
```

$$V = \begin{bmatrix} 1 & a & a & a \\ a & a^2 + v_2 & a^2 & a^2 \\ a & a^2 & a^2 + v_2 & a^2 \\ a & a^2 & a^2 & a^2 + v_2 \end{bmatrix}, \quad K = \begin{bmatrix} \frac{3a^2}{v_2} + 1 & -\frac{a}{v_2} & -\frac{a}{v_2} & -\frac{a}{v_2} \\ -\frac{a}{v_2} & \frac{1}{v_2} & 0 & 0 \\ -\frac{a}{v_2} & 0 & \frac{1}{v_2} & 0 \\ -\frac{a}{v_2} & 0 & 0 & \frac{1}{v_2} \end{bmatrix}$$

**Introducing data** Let  $S$  is the empirical covariance matrix for the observed variables based on  $n$  observations. The observed-data log-likelihood is

$$l = \frac{n}{2} (\log \det(V_{xx}^{-1}) - \text{tr}(V_{xx}^{-1} S)) = \frac{n}{2} (\log \det(K_{xx}) - \text{tr}(K_{xx} S)).$$

Now  $K_{xx} = V_{xx}^{-1}$  can be extracted and used in the likelihood function:

```
R> Vxx_inv <- inv(V[-1, -1])
```

Alternatively,  $K_{xx}$  can be found as

```
R> Kxx <- (K[-1, -1] - K[-1, 1, drop=F] %%%
+ inv(K[1, 1, drop=F]) %%% K[1, -1, drop=F]) %>% simplify
```

$$K_{xx} = \frac{1}{v_2(3a^2 + v_2)} \begin{bmatrix} 2a^2 + v_2 & -a^2 & -a^2 \\ -a^2 & 2a^2 + v_2 & -a^2 \\ -a^2 & -a^2 & 2a^2 + v_2 \end{bmatrix}$$

It remains to be investigated in practice whether it is computationally more efficient to construct  $V_{xx}$  numerically first and then invert  $V_{xx}$  to obtain  $K_{xx}$  numerically instead of finding  $K_{xx}$  symbolically and subsequently evaluating this numerically.

### With a view towards teaching

We have found ANOVA examples (and variants hereof) useful in connection with teaching: Students are often exposed to estimating the vector of regression coefficients as

$$\hat{\beta} = (X^\top X)^{-1} X^\top y.$$

However, in the computer area, students are not always exposed to what is really computed in simple cases: Various group sums and differences of these. It is often illustrative for students to study, for example, the effect of: (1) including/excluding the intercept term in a model, (2) working with different contrasts in the models, and (3) making a design imbalanced.

For the probabilistic PCA example it is illustrative for students (1) to take the step from the symbolic model formulation to estimation (using e.g. `optim()`). (2) It can also be illustrative to realize the interpretation implied by forcing certain elements of  $W$  to be identical (as the case was above). (3) Likewise, it is straight forward to change the conditional variance of  $x$  given  $z$  from  $\sigma^2 I$  to a diagonal matrix  $\Psi$  (which is the case in standard factor analysis). Elaborating further, it is illustrative for students to see for example autoregression and a dynamic linear model formulated in similar way.

## Discussion

We have presented the `caracas` package and argued that the package extends the functionality of R significantly with respect to symbolic mathematics. One practical virtue of `caracas` is that the package integrates nicely with `Rmarkdown`, Allaire et al. (2021), (e.g. with the `tex()` functionality) and thus supports creating of scientific documents and teaching material. As for the usability in practice we await feedback from users.

## Acknowledgements

We would like to thank the R foundation for financial support for creating the `caracas` package, users for pin pointing points that can be improved in `caracas` and Ege Rubak (Aalborg University, Denmark) and Malte Bødkergaard Nielsen (Aalborg University, Denmark) for comments on this manuscript.

## Bibliography

- J. Allaire, Y. Xie, J. McPherson, J. Luraschi, K. Ushey, A. Atkins, H. Wickham, J. Cheng, W. Chang, and R. Iannone. *rmarkdown: Dynamic Documents for R*, 2021. URL <https://github.com/rstudio/rmarkdown>. R package version 2.7. [p11]
- M. M. Andersen and S. Højsgaard. Ryacas: A computer algebra system in R. *Journal of Open Source Software*, 4(42), 2019. URL <https://doi.org/10.21105/joss.01763>. [p1]
- S. M. Bache and H. Wickham. *magrittr: A Forward-Pipe Operator for R*, 2020. URL <https://CRAN.R-project.org/package=magrittr>. R package version 2.0.1. [p2]
- C. M. Bishop. *Pattern Recognition and Machine Learning*. Springer, New York, USA, 2006. [p8]
- D. T. Kaplan, R. Pruim, and N. J. Horton. *mosaicCalc: Function-Based Numerical and Symbolic Differentiation and Antidifferentiation*, 2020. URL <https://CRAN.R-project.org/package=mosaicCalc>. R package version 0.5.1. [p3]
- A. Meurer, C. P. Smith, M. Paprocki, O. Čertík, S. B. Kirpichev, M. Rocklin, A. Kumar, S. Ivanov, J. K. Moore, S. Singh, T. Rathnayake, S. Vig, B. E. Granger, R. P. Muller, F. Bonazzi, H. Gupta, S. Vats, F. Johansson, F. Pedregosa, M. J. Curry, A. R. Terrel, v. Roučka, A. Saboo, I. Fernando, S. Kulal, R. Cimrman, and A. Scopatz. Sympy: symbolic computing in python. *PeerJ Computer Science*, 3: e103, Jan. 2017. ISSN 2376-5992. doi: 10.7717/peerj-cs.103. URL <https://doi.org/10.7717/peerj-cs.103>. [p1]
- A. Pinkus, S. Winnitzky, and G. Mazur. Yacas - yet another computer algebra system. Technical report, 2016. URL <https://yacas.readthedocs.io/en/latest/>. [p1]
- A. Z. Pinkus and S. Winitzki. YACAS: A Do-It-Yourself Symbolic Algebra Environment. In *Proceedings of the Joint International Conferences on Artificial Intelligence, Automated Reasoning, and Symbolic Computation*, AISC '02/Calculemus '02, pages 332–336, London, UK, UK, 2002. Springer-Verlag. ISBN 3-540-43865-3. doi: 10.1007/3-540-45470-5\_29. URL [http://doi.org/10.1007/3-540-45470-5\\_29](http://doi.org/10.1007/3-540-45470-5_29). [p1]
- R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2021. URL <http://www.R-project.org/>. ISBN 3-900051-07-0. [p1]
- United Nations General Assembly. Sustainable development goals, 2015. <https://sdgs.un.org/>. [p1]
- K. Ushey, J. Allaire, and Y. Tang. *reticulate: Interface to 'Python'*, 2020. URL <https://CRAN.R-project.org/package=reticulate>. R package version 1.18. [p1]

## Appendix: Technicalities

To avoid confusion we elaborate on the construction of symbols in the following:

- `as_sym()` converts an R object (or string) to symbol.
- `symbol()` declares a symbol by string, and allows for assumptions.
- `def_sym()` declares a symbol (either by string or non-standard evaluation) and assigns to an R variable with same name.

The behaviour of `def_sym()` can be obtained by both `symbol()` and `as_sym()`, but the two latter require an explicit assignment. Thus the following three statements are equivalent:

```
R> a <- as_sym("a")
R> a <- symbol("a")
R> def_sym(a)
```

To elaborate, consider a vector in R: Using `symbol` - the following fails because `a` is an object and not a string:

```
R> a <- c(-1, 1); a
#> [1] -1 1
R> a <- symbol(a)
#> Error in verify_variable_name(x): The name must have length 1
```

On the other hand, `as_sym` works as expected. Using `def_sym` also works, but not as the user expects: A new variable `a` is created and the old `a` (the vector) is no longer bound to a variable:

```
R> a2 <- as_sym(a); t(a2)
#> [caracas]: [-1 1]
R> a ## a is unchanged
#> [1] -1 1
R> def_sym(a); a
#> [caracas]: a
```

## Appendix: Assumptions

It is sometimes required to impose assumptions on variables. There is currently (limited) support for this in [caracas](#):

```
R> x <- symbol("x")
R> sol <- solve_sys(x^2 + 1, x); sol
#> Solution 1:
#> x = -I
#> Solution 2:
#> x = I
```

Requiring `x` to be real:

```
R> x <- symbol("x", real = TRUE)
R> ask(x, 'real')
#> [1] TRUE
R> sol <- solve_sys(x^2 + 1, x); sol
#> No solutions
```

Requiring `x` to be positive:

```
R> x <- symbol("x", positive = TRUE)
R> ask(x, 'positive')
#> [1] TRUE
R> sol <- solve_sys(x^2 - 1, x); sol
#> Solution 1:
#> x = 1
```

*Mikkel Meyer Andersen*  
*Department of Mathematical Sciences, Aalborg University, Denmark*  
*Skjernvej 4A*  
*9220 Aalborg Ø, Denmark*

[mikl@math.aau.dk](mailto:mikl@math.aau.dk)

*Søren Højsgaard*  
*Department of Mathematical Sciences, Aalborg University, Denmark*  
*Skjernvej 4A*  
*9220 Aalborg Ø, Denmark*

[sorenh@math.aau.dk](mailto:sorenh@math.aau.dk)