

GPoM : 1 Conventions

Sylvain Mangiarotti & Mireille Huc

2023-06-15

The Generalized Global Polynomial Modelling (GPoM) package allows a generic formulation of any Ordinary Differential Equations (ODEs) in polynomial form. The aim of the present vignette **1 Conventions** is to introduce briefly the way to describe a set of polynomial ODEs with GPoM and to show how to perform its numerical integration¹.

Conventions used to describe a polynomial

The polynomial description is based on a convention defined by the function `regOrd` that provides the order of the polynomial terms. This convention depends on the model dimension (that is the number `nVar` of state variables), and on the maximum polynomial degree used for the formulation (defined by the parameter `dMax`). This order can be visualized using the `poLabs` function. For instance, for `nVar = 3` and `dMax = 2`, the convention used to formulate a polynomial will be:

```
nVar = 3
dMax = 2
poLabs(nVar = nVar, dMax = dMax)

## [1] "ct"      "X3 "      "X3^2 "    "X2 "      "X2 X3 "   "X2^2 "    "X1 "      "X1 X3 "
## [9] "X1 X2 "   "X1^2 "
```

This formulation has `pMax = 10` terms:

```
pMax = d2pMax(nVar, dMax)
```

Based on this convention, one single ordinary differential equation (ODE) in polynomial form with `nVar` variables and of maximum polynomial degree `dMax` can be formulated as one single vector using the convention given by `regOrd(nVar, dMax)`. As an example, the equation :

$$dX_1/dt = 1 + 2X_1 - 3X_1X_3 + 4X_2^2$$

has the three variables X_1 , X_2 and X_3 (it thus requires at least `nVar = 3`) and is of maximum polynomial degree two due to terms X_1X_3 and X_2^2 (it thus requires at least `dMax = 2`). Following the convention defined by `poLabs(nVar = 3, dMax = 2)`, it will require the definition of the following vector of parameters:

```
param <- c(1, 0, 0, 0, 0, 4, 2, -3, 0, 0)
```

Indeed:

```
nVar = 3
dMax = 2
cbind(param, poLabs(nVar, dMax))
```

```
##      param
## [1,] "1"   "ct"
## [2,] "0"   "X3 "
```

¹Mangiarotti S, Le Jean F, Chassan M, Drapeau L, Huc M. 2018. GPoM: Generalized Polynomial Modelling. Version 1.1. *Comprehensive R Archive Network*. <https://cran.r-project.org/package=GPoM>.

```
## [3,] "0" "X3^2 "
## [4,] "0" "X2 "
## [5,] "0" "X2 X3 "
## [6,] "4" "X2^2 "
## [7,] "2" "X1 "
## [8,] "-3" "X1 X3 "
## [9,] "0" "X1 X2 "
## [10,] "0" "X1^2 "
```

The same convention will be used for any other equation. Note that, by default, the notation used for the variables is X1, X2, etc. However, to facilitate the analysis, alternative notations may also be used using the optional parameter `Xnote`:

```
poLabs(3, 2, Xnote = 'y')
```

```
## [1] "ct" "y3 " "y3^2 " "y2 " "y2 y3 " "y2^2 " "y1 " "y1 y3 "
## [9] "y1 y2 " "y1^2 "
```

or for a full choice of the notation:

```
poLabs(3, 2, Xnote = c('x', 'W', 'y'))
```

```
## [1] "ct" "y " "y^2 " "W " "W y " "W^2 " "x " "x y " "x W " "x^2 "
```

Definition of a set of polynomial ODE

A set of N equations will require the definition of N parameter vectors and will thus be represented by a matrix of `pMax` lines by `nVar` columns. For example, the Rössler system² is defined by a set of three equations

$$dx/dt = -y - z$$

$$dy/dt = x + ay$$

$$dz/dt = b + z(x - c).$$

For ($a = 0.52, b = 2, c = 4$), this system can be described by three vectors (one for each equation)

```
# parameters
a = 0.52
b = 2
c = 4
# equations
Eq1 <- c(0, -1, 0, -1, 0, 0, 0, 0, 0, 0)
Eq2 <- c(0, 0, 0, a, 0, 0, 1, 0, 0, 0)
Eq3 <- c(b, -c, 0, 0, 0, 0, 0, 1, 0, 0)
```

The model formulation is obtained by concatenating the vectors of the three equations into one single matrix `K` containing all the coefficients of the model:

```
K = cbind(Eq1, Eq2, Eq3)
```

The corresponding model equations can be edited in a mathematical form using the function `visuEq()`

```
visuEq(K)
```

```
## dX1/dt = -1 X3 -1 X2
```

```
## dX2/dt = 0.52 X2 + 1 X1
```

```
## dX3/dt = 2 -4 X3 + 1 X1 X3
```

²O. Rössler, An Equation for Continuous Chaos, *Physics Letters*, **57A**(5), 1976, 397-398

By default, the notation used in `visuEq` for the variables is `X` with an indicative number, such as `X1`, `X2`, etc. Alternative notation can be used to edit the equations with the `visuEq` function using the optional parameter `substit`. For `substit = 1`, single letters are automatically chosen such as

```
visuEq(K, substit = 1)
```

```
## dx/dt = -1 z -1 y
## dy/dt = 0.52 y + 1 x
## dz/dt = 2 -4 z + 1 x z
```

The notation can be defined also manually, such as:

```
visuEq(K, substit = c("U", "V", "W"))
```

```
## dU/dt = -1 W -1 V
## dV/dt = 0.52 V + 1 U
## dW/dt = 2 -4 W + 1 U W
```

Numerical integration

The numerical integration of the model defined by matrix `K` can be done using the `numicano` function. It requires the use of the external package `deSolve`. The following parameters are required as input:

```
# The initial conditions of the system variables
v0 <- c(-0.6, 0.6, 0.4)
# the model formulation K (see former section)
# the number of integration steps `Istep`
nIstep <- 5000
# the time step length `onestep`
onestep = 1/50
# the model dimension `nVar`
nVar = 3
# the maximum polynomial degree `dMax`
dMax = 2
```

The numerical integration is launched as follows:

```
outNumi <- numicano(nVar, dMax, Istep = nIstep, onestep = onestep, KL = K, v0 = v0)
```

The output of the function `numicano` is a list that contains (1) a memory `$KL` of the model parameters

```
outNumi$KL
```

from which `nVar` and `dMax` (required to reformulate the equations) can be retrieved

```
# nVar
dim(outNumi$K)[2]
# dMax
pMax <- dim(outNumi$K)[1]
p2dMax(nVar, pMaxKnown = pMax)
```

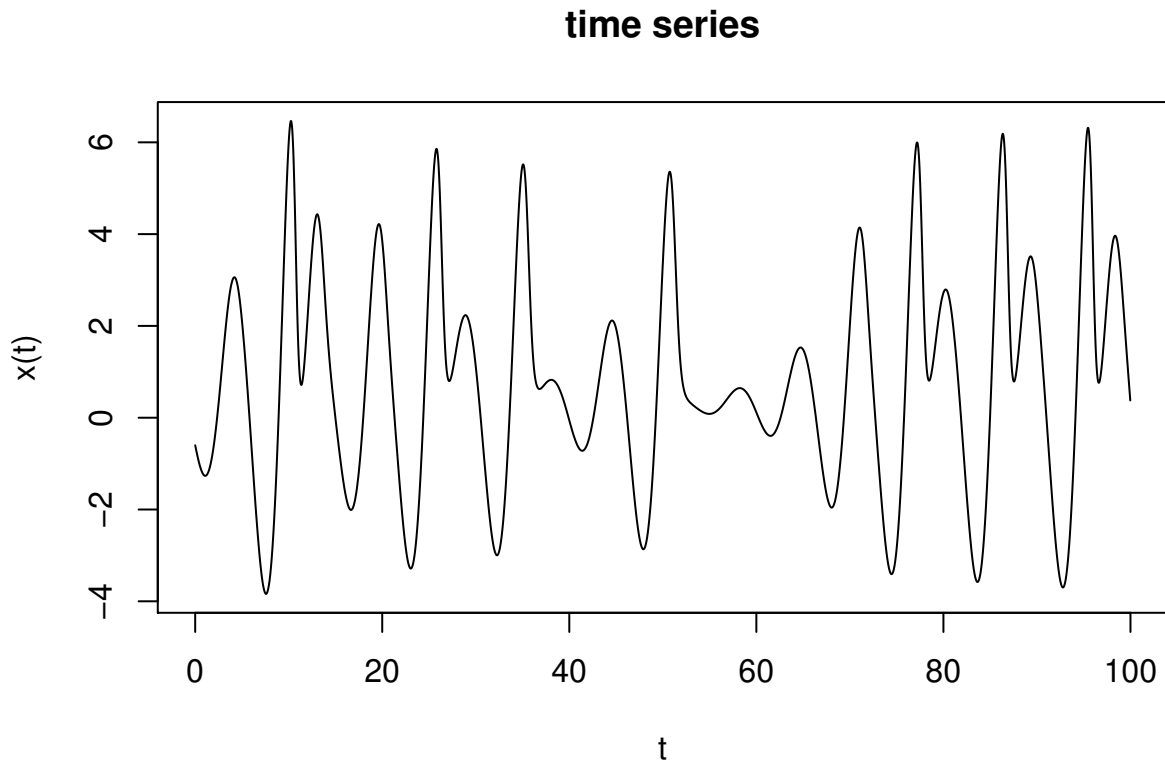
and (2) the simulations `$reconstr`. This matrix has `nVar + 1` columns. The first one is the time, the other ones correspond to the variables of the system (`X1`, `X2`, `X3`, ...) (or (x, y, z) to keep the formulation used previously in the text).

Note that all the other input parameters used in `numicano` can be retrieved from the outputs:

```
# initial conditions
head(outNumi$reconstr, 1)[2:(nVar+1)]
# time step
diff(outNumi$reconstr[1:2,1])
# number of integration time step
dim(outNumi$reconstr)[1]
```

The simulated time series can be plotted as follows:

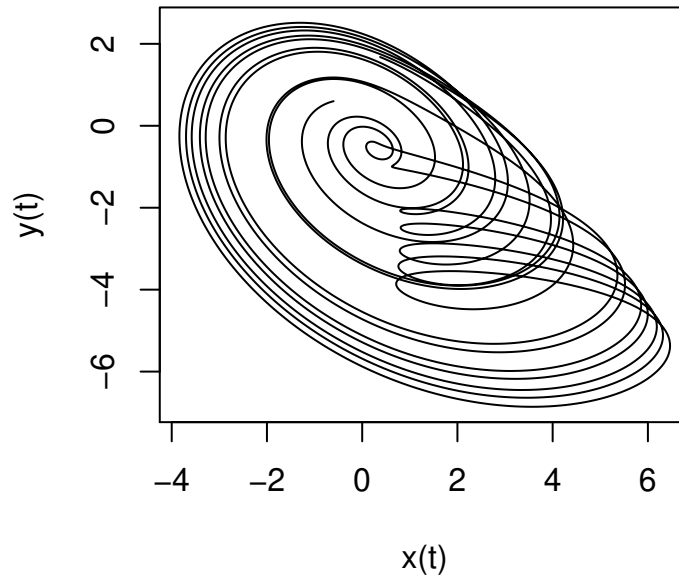
```
plot(outNumi$reconstr[,1], outNumi$reconstr[,2], type='l',
      main='time series', xlab='t', ylab = 'x(t)')
```



and the plot of the phase portrait as well:

```
plot(outNumi$reconstr[,2], outNumi$reconstr[,3], type='l',
      main='phase portrait', xlab='x(t)', ylab = 'y(t)')
```

phase portrait



Next steps

The aim of the GPoM package is to retrieve ODEs from time series using global modelling. Such type of modelling may require a careful data preprocessing. Simple examples of preprocessing will be given in the next vignette 2 **Preprocessing**. Examples for applying global modelling to time series will then be presented in vignette 3 **Modelling**.