GPoM : 1 Conventions

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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 integration[1].

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"
```

[1]Mangiarotti 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.

```
##  [2,] "0"   "X3 "
##  [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 system[2] 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 decribed 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
##
```

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

```
## dX2/dt = 0.52 X2  + 1 X1
##
## dX3/dt = 2  -4 X3  + 1 X1 X3
```

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)
```

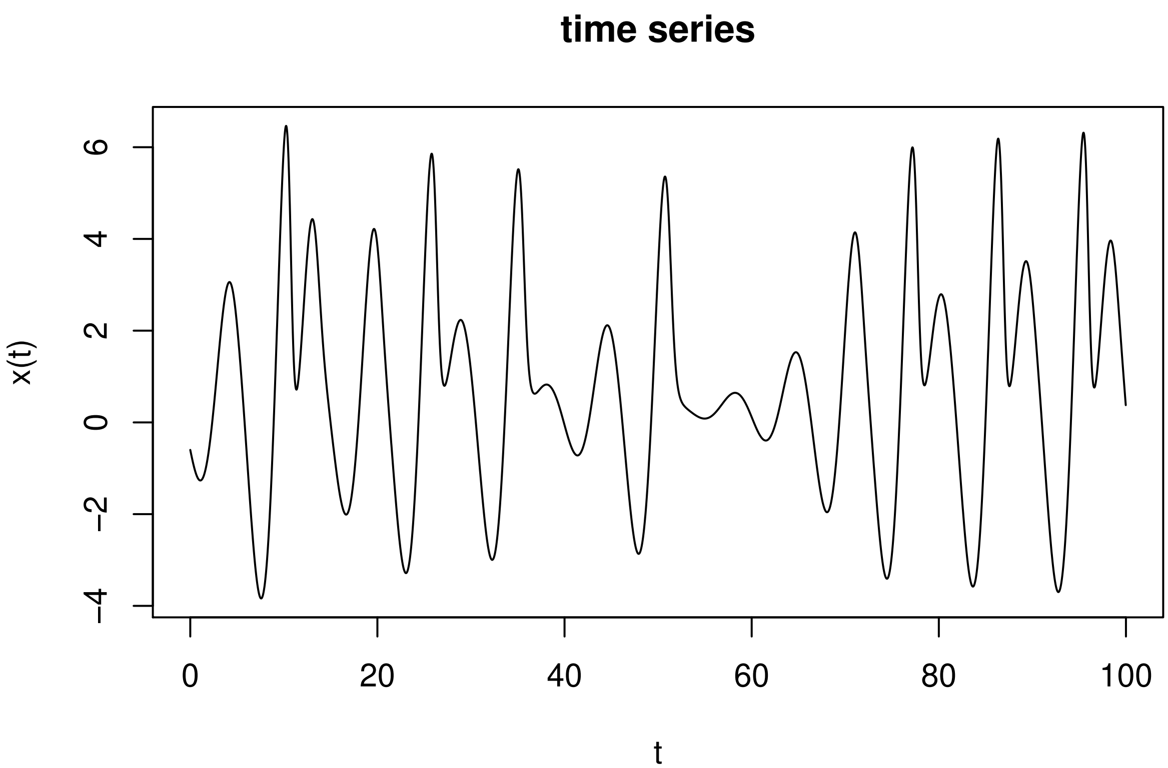
and (2) the simulations `$reconstr`. This matrix has `nVar + 1` columns. The first one is the time, the other ones correspond to the variables of the system $(X1, X2, X3, \ldots)$ (or (x, y, z) to keep the formulation used previously in the text).

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]
```

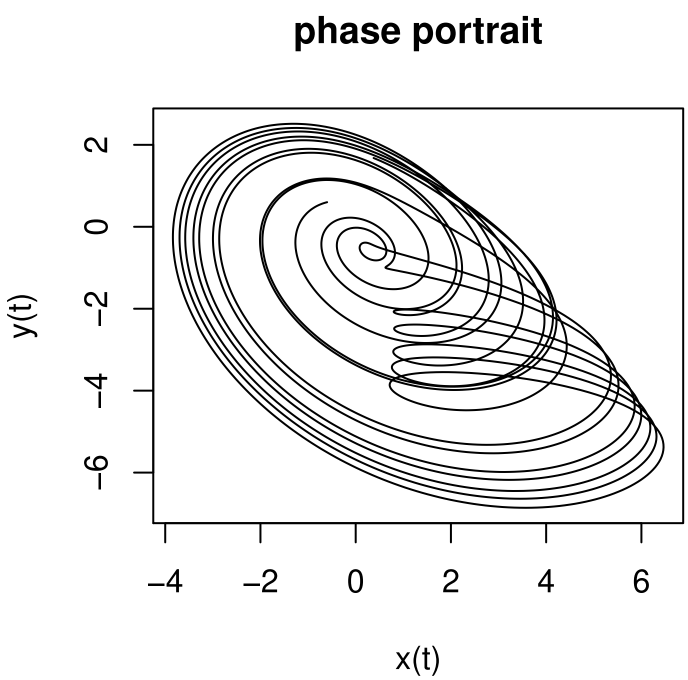
The simulated time series can be plotted as follows:

```
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)')
```



Next steps

The aim of the GPoM package is to retreive 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`.