RCaN

Supplementary Material

Hilaire Drouineau[1], Benjamin Planque[2], and Christian Mullon[3]

[1]INRAE, Bordeaux, France
[2]HI, Tromsoe, Norway
[3]IRD, MARBEC, Sete, France

March 30, 2021

1 Introduction

1. Goals: an example of a RCaN study : a sequence of RCaN-commands, their input, their output and their interpretation.
2. The case study: the Barents sea (main text).
3. The RCaN file has been previously built. It is attached.
4. All following commands in joined R script.
5. A first run with all main steps.
6. A second run after removing some constraints
7. Comparisons between both runs and interpretation

2 Preliminary: R Environment

A few libraries are to be loaded.

```
> library(RCaN) #the main package
> library(ggplot2) #to draw results
> library(coda) #to explore mcmc
> library(dplyr) #to manipulate data frame
```

```
> library(xtable) #to create latex tables
> library(xlsx) # to import excel files
```

3 The RCaN file

Parameters, observations and constraints have been gathered in an Excel file with a specific structure.

```
> setwd('/Users/christianmullon/gitC/article_supporting')
> # NAMEFILE <- 'BarentsSeaReconstructions_01_02_21.xlsx'
> NAMEFILE <- 'CaN_template_miniS.xlsx'
>
```

3.1 Components

	Component	Inside	AssimilationE	Digestibility	OtherLosses
1	PhytoAndBacteria	0.00		0.65	
2	HerbZooplankton	1.00	1.00	0.90	8.40
3	OmniZooplankton	1.00	1.00	0.90	5.50
4	Fishery	0.00			

Table 1: Components

3.2 Fluxes

	Flux	From	To	Trophic
1	PhytoAndBacteria_HerbZooplankton	PhytoAndBacteria	HerbZooplankton	1.00
2	PhytoAndBacteria_OmniZooplankton	PhytoAndBacteria	OmniZooplankton	1.00
3	HerbZooplankton_OmniZooplankton	HerbZooplankton	OmniZooplankton	1.00
4	OmniZooplankton_Fishery	OmniZooplankton	Fishery	0.00

Table 2: Fluxes

3.3 Observations

	Year	HerbZooplankton_Biomass	OmniZooplankton_Biomass	Benthos_Biomass	PelagicFish
1	1988.00	16608.00	16864.00	105000.00	
2	1989.00	27872.00	13616.00	105000.00	
3	1990.00	23504.00	7696.00	105000.00	
4	1991.00	21776.00	14640.00	105000.00	
NA					
NA.1					
NA.2					
NA.3					
NA.4					
NA.5					

Table 3: Observations

3.4 Constraints

	Id	Constraint
1	C01	PhytoAndBacteria_HerbZooplankton+PhytoAndBacteria_OmniZooplankton<=PrimaryProdu
2	C02	-(PhytoAndBacteria_HerbZooplankton+PhytoAndBacteria_OmniZooplankton)<=-PrimaryPr
3	C03	OmniZooplankton_Fishery=OmniZooplankton_Landings
NA		
NA.1		
NA.2		
NA.3		

Table 4: Constraints

4 Building polytope

```
> begin <- Sys.time()
> POLYTOPE <- buildCaN(NAMEFILE)
> end <- Sys.time()
> end-begin

Time difference of 1.036968 secs

> summary(POLYTOPE)

                  Length Class      Mode
components_param  10     data.frame list
species            2     -none-     character
fluxes_def         4     data.frame list
flow               4     -none-     character
series            13     data.frame list
ntstep             1     -none-     numeric
data_series_name  12     -none-     character
constraints        5     data.frame list
H                  4     -none-     numeric
N                  8     -none-     numeric
A                972     dgCMatrix  S4
AAll             972     dgCMatrix  S4
C                 72     dgCMatrix  S4
CAll              72     dgCMatrix  S4
v                  4     -none-     numeric
vAll               4     -none-     numeric
L                144     dgCMatrix  S4
b                 54     -none-     numeric
bAll              54     -none-     numeric
symbolic_enviro   56     -none-     environment
```

5 Structure of polytope

The polytope is defined by two pairs of a matrix and and a vector. F being the vector of all flows at all timesteps, first one (A, b) is an equality $A.F = b$, second one (C, v) is an eqality $C.F \leq v$. For the Barents sea, we have: :

```
> dim(POLYTOPE$A)

[1] 54 18

> length(POLYTOPE$b)

[1] 54

> dim(POLYTOPE$C)
```

```
[1]  4 18
```

```
> length(POLYTOPE$v)
```

```
[1] 4
```

6 Checking polytope

As it is defined in the RCaN file for the Barents' sea, the polytope is non-empty and bounded:

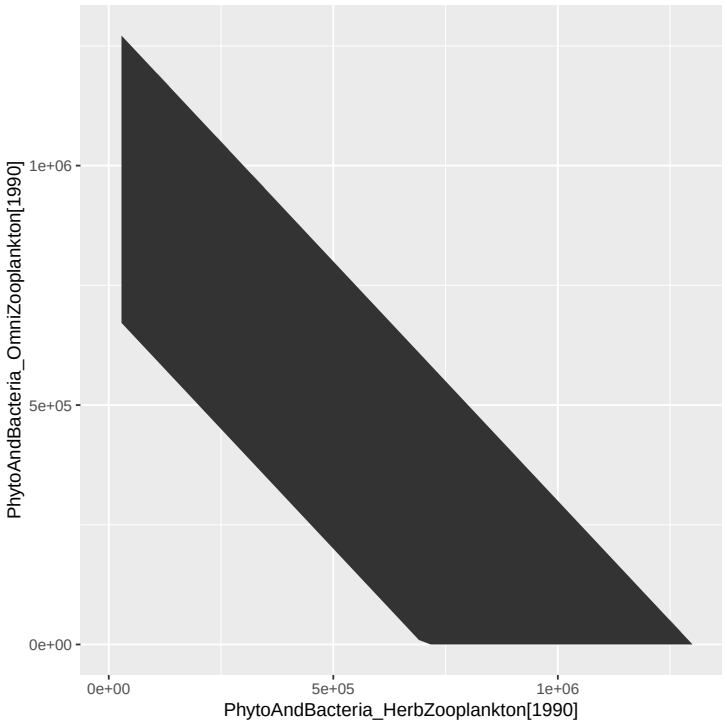
```
> checkPolytopeStatus(POLYTOPE)

[1] "polytope ok"
```

Limits of the Barents' sea polytope in all dimensions are obtained with getAllBoundsParam:

```
> BOUNDS <- getAllBoundsParam(POLYTOPE, progressBar = FALSE)
> summary(BOUNDS)

    param             lowerbound        upperbound
 Length:18          Min.   :   0.00   Min.   :       49
 Class :character   1st Qu.:   0.00   1st Qu.:   843805
 Mode  :character   Median :  24.34   Median :  1298552
                    Mean   : 296.54   Mean   : 21517685
                    3rd Qu.: 144.85   3rd Qu.:  1300000
                    Max.   :1884.94   Max.   :364556692
```

Function plotPolytope2DCaNmod allows seeing the polytope in the plane defined by two parameters. In its first two dimensions, for the second 1990, the Barents sea polytope dimensions appears as.

```
> fluxX <- paste(FLUXES[1,1],'[1990]',sep="")
> fluxY <- paste(FLUXES[2,1],'[1990]',sep="")
> plotPolytope2D(POLYTOPE, c(fluxX, fluxY), progressBar=FALSE)
```


1e+06
5e+05
0e+00
PhytoAndBacteria_OmniZooplankton[1990]
0e+00
5e+05
1e+06
PhytoAndBacteria_HerbZooplankton[1990]

7 Sampling polytope

7.1 Sampling

```
> begin = Sys.time()
> SAMPLE <- sampleCaN(POLYTOPE,
+                       N=100,thin=100,
+                       nchain=2,
+                       ncore=2)
> end=Sys.time()
> end-begin

Time difference of 6.5403 secs
```

7.2 Convergence

```
> nchain(SAMPLE$mcmc)
```

```
[1] 2
```

```
> # summary(SAMPLE$mcmc)
```

Gelman diagnostics

```
> fluxY <- paste(FLUXES[2,1],'[1990]',sep="")
> gelman.diag(SAMPLE$mcmc[,fluxY])
```

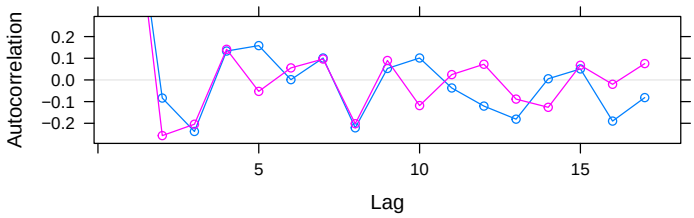
```
Potential scale reduction factors:

     Point est. Upper C.I.
[1,]       1.01       1.07
```

Autocorrelation function

```
> fluxZ <- paste(FLUXES[3,1],'[1990]',sep="")
> thinned_SAMPLE <- window(SAMPLE$mcmc,thin=2)
> thin(thinned_SAMPLE)
```

```
[1] 2
```

```
> acfplot(thinned_SAMPLE[,fluxZ])
```



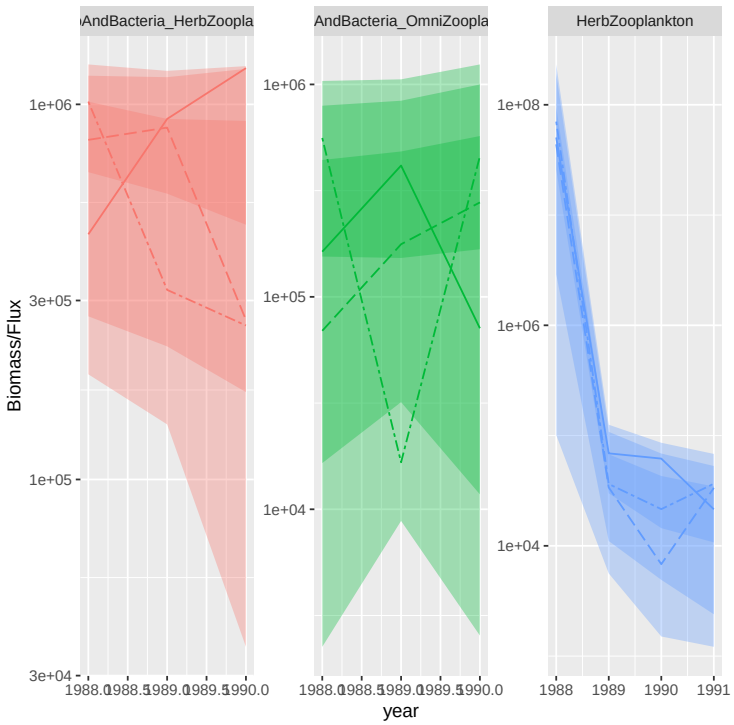
7.3 Dynamics

For several variables or flux, plots of sampled dynamics.

```
> fluxX <- FLUXES[1,1]
> fluxY <- FLUXES[2,1]
> compA <- COMPONENTS[2,1]
> compB <- COMPONENTS[3,1]
> c(fluxX,fluxY,compA)
```

```
[1] "PhytoAndBacteria_HerbZooplankton" "PhytoAndBacteria_OmniZooplankton"
[3] "HerbZooplankton"
```

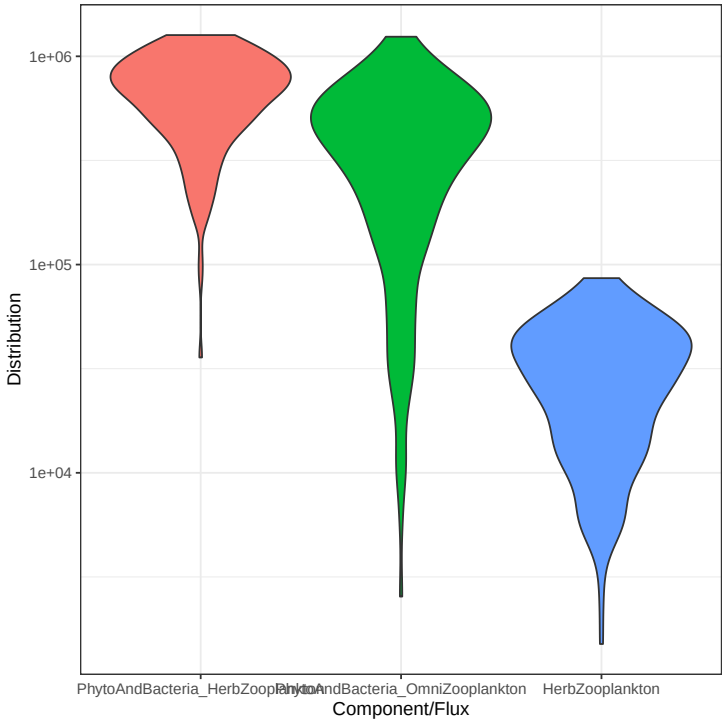
```
> g <- ggSeries(SAMPLE, c(fluxX,fluxY,compA), TRUE)
> g + scale_y_log10() + guides(color = FALSE, fill = FALSE)
```



7.4 Distribution

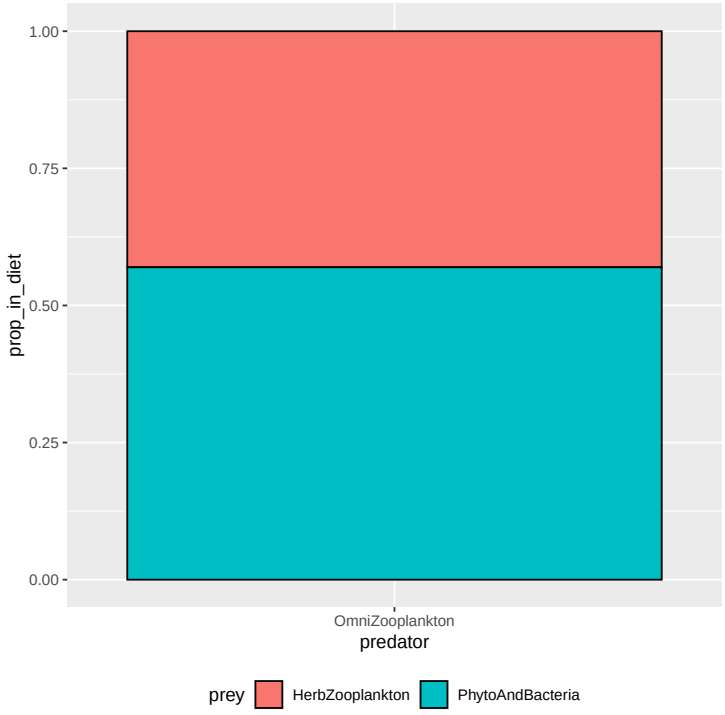
For a component or a flux, for a year, the distribution of sampled values.

```
> ggViolin(SAMPLE,c(fluxX,fluxY,compA),year=1990,TRUE)
```



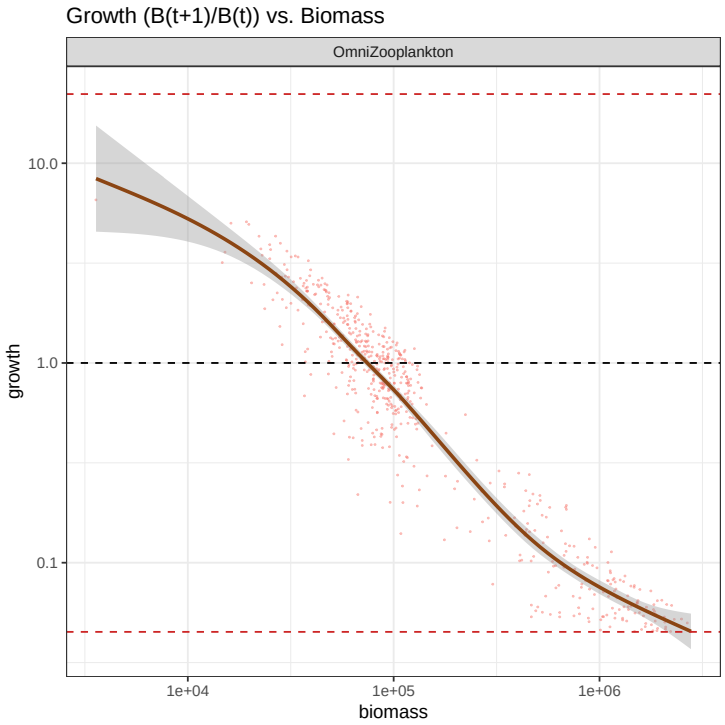
7.5 Diet relationships

```
> ggDiet(SAMPLE, compB)
```



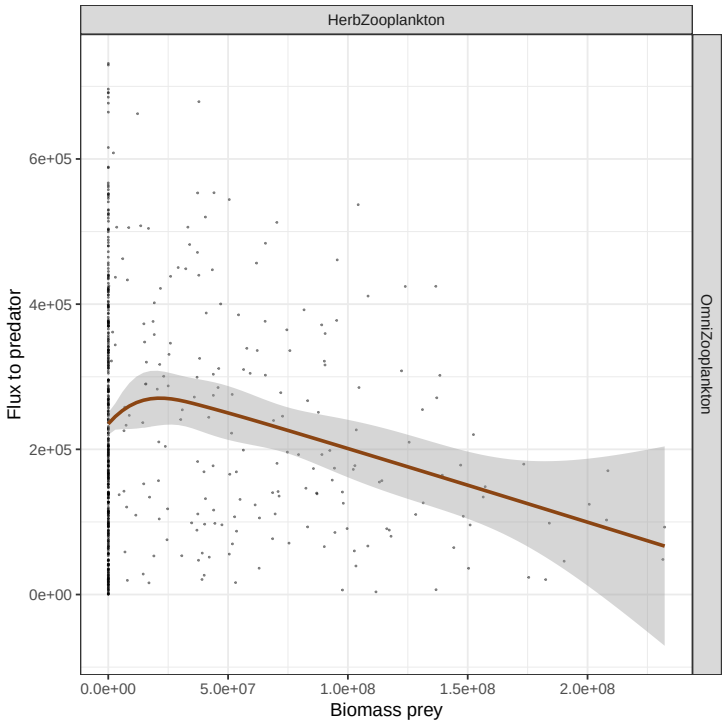
7.6 Growth

```
> ggGrowth(SAMPLE, compB)
```



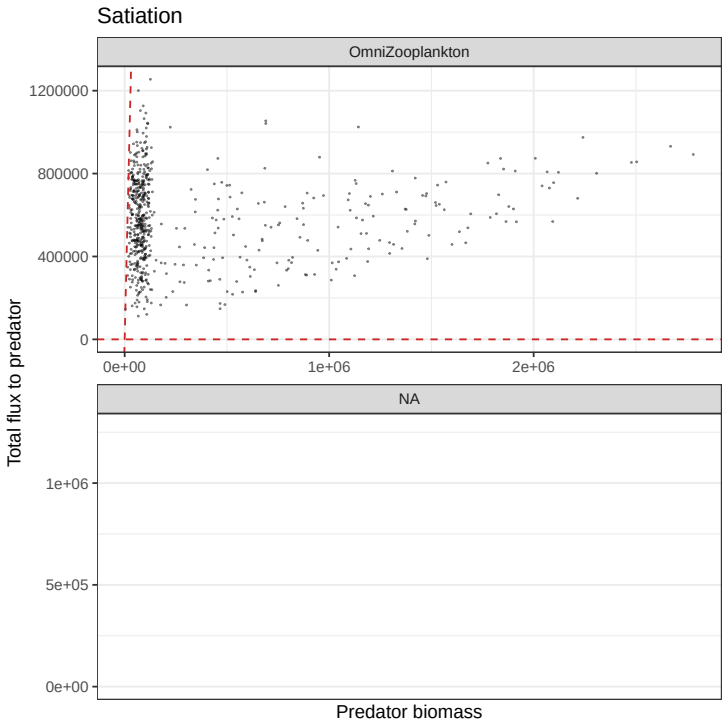
7.7 Trophic relation

```
> ggTrophicRelation(SAMPLE)
> # ggTrophicRelation(SAMPLE, compB)
```



7.8 Satiation

```
> ggSatiation(SAMPLE, compB)
```



8 Try and errors

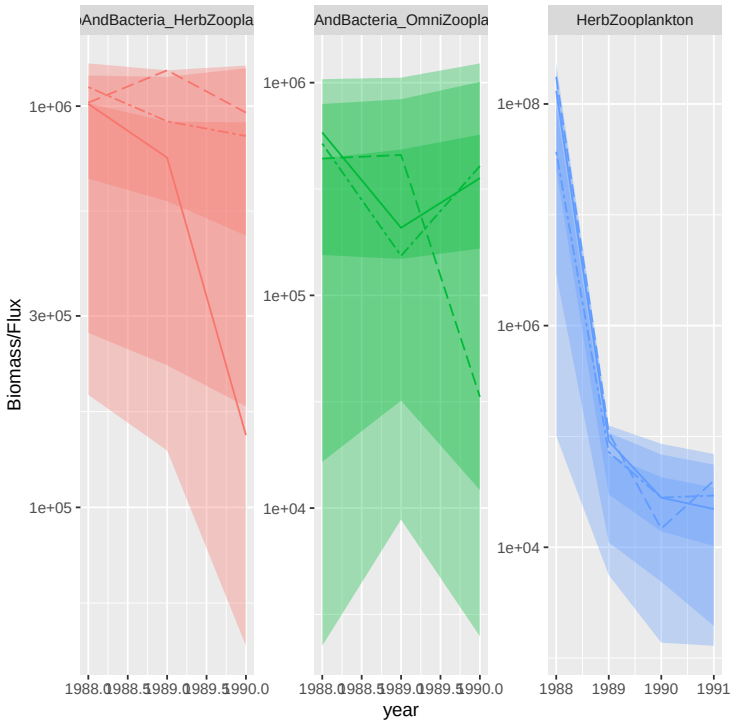
8.1 Activating and desactivating constraint

```
> #disactivate constraints CO2
> constA = CONSTRAINTS[2,1]
> constA

[1] "CO2"

> POLYTOPEA <- toggleConstraint(POLYTOPE, constA)

[1] "disactivate inequality CO2 : 1988" "disactivate inequality CO2 : 1989"
[3] "disactivate inequality CO2 : 1990" "disactivate inequality CO2 : 1991"

> #disactivate constraints CO2 for year 1991
> constYearA = paste(constA, "1991", sep = " : ")
> POLYTOPEB <- toggleConstraint(POLYTOPE, constYearA)

[1] "disactivate inequality CO2 : 1991"

> checkPolytopeStatus(POLYTOPEA)
```

```
[1] "polytope ok"

> checkPolytopeStatus(POLYTOPEB)

[1] "polytope ok"
```

8.2 Building and analyzing sample

```
> begin = Sys.time()
> SAMPLEB <- sampleCaN(POLYTOPEB,
+                      N=100,thin=100,
+                      nchain=2,
+                      ncore=2)
> end=Sys.time()
> end-begin

Time difference of 6.61147 secs

> fluxX <- FLUXES[1,1]
> fluxY <- FLUXES[2,1]
> compA <- COMPONENTS[2,1]
> compB <- COMPONENTS[3,1]
> c(fluxX,fluxY,compA)

[1] "PhytoAndBacteria_HerbZooplankton" "PhytoAndBacteria_OmniZooplankton"
[3] "HerbZooplankton"

> g <- ggSeries(SAMPLEB, c(fluxX,fluxY,compA), TRUE)
> g + scale_y_log10() + guides(color = FALSE, fill = FALSE)
```


AndBacteria_HerbZoopla
AndBacteria_OmniZoopla
HerbZooplankton
Biomass/Flux
1e+06
3e+05
1e+05
1e+04
1e+08
1988.0
1988.5
1989.0
1989.5
1990.0
1988
1989
1990
1991
year