ToxLim : Incorporating Ecological Data and Uncertainty in Bioaccumulation Modeling

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Abstract

Rpackage **ToxLim** (De˜Laender and Soetaert 2010) contains the OMEGA model to estimate the estimates the bioaccumulation of a nonbiotransforming chemical through a food web.

It also contains several food web examples.

The methodology was described in the paper by (De˜Laender, Van˜Oevelen, Middelburg, and Soetaert 2009). Please cite this paper when using this package.

Keywords:˜ toxicity, food webs, linear inverse models, R .

1. Introduction

R-package **ToxLim** , accompanying the paper (De˜Laender *et˜al.* 2009) models the bioaccumulation of a nonbiotransforming chemical through a food web.

It contains an implementation of the `OMEGA` model (Hendriks, van˜der Linde, Cornelissen, and Sijm 2001), as extended for multiple food sources by (De˜Laender *et˜al.* 2009), and three food web examples: the pelagic food web of the Barents Sea, and two food webs of freshwater (lake) enclosures.

For background on inverse modelling, we refer to the documents of the **LIM** package (van Oevelen, van˜den Meersche, Meysman, Soetaert, Middelburg, and Vezina 2010), or the **limSolve** package (Soetaert, den Meersche, and van Oevelen 2009).

Also see (Van˜den Meersche, Soetaert, and Van˜Oevelen 2009) for running a constrained monte carlo.

The **LIM** package also contains many other food web examples.

2. The example food webs

Three food webs are included in the package.

2.1. LIMbarents

The Barents Sea food web was published in (De˜Laender, Van˜Oevelen, Middelburg, and Soetaert 2010a) and the bioaccumulation model applied to it in (De˜Laender, Van˜Oevelen, S, Middelburg, and Soetaert 2010b).

It consists of the linear inverse model specification for the Southern Barents Sea.

The food web compartments for the area are dissolved organic carbon (DOC), detritus, bacteria, heterotrophic flagellates and ciliates, phytoplankton (pico- and nanoplankton, diatoms and Phaeocystis sp.), mesozooplankton (copepods), macrozooplankton (krill and chaetognaths), cod (Gadus morhua), herring (Clupea harengus) and capelin (Mallotus villosus). Adult cod (> 3 yrs) and young cod (< 3 yrs) were considered as two different populations.

First the food web is solved:

```
> plotweb(Flowmatrix(LIMbarents),main="Barents Sea Food Web",
+   sub="gC/m2/day")
```

Then the ranges of flows and variables are calculated and plotted:

```
> pm <- par(mfrow=c(1,2))
> Plotranges(LIMbarents,lab.cex=0.7,xlab="gC/m2/d",
+    main="Flows")
> #
> Plotranges(LIMbarents,type="V",lab.cex=0.7,xlab="gC/m2/d",
+    main="variables")
> mtext(outer=TRUE,"Southern Barents Sea food web",side=3,line=-1,cex=1.5)
> par(mfrow=pm)
```

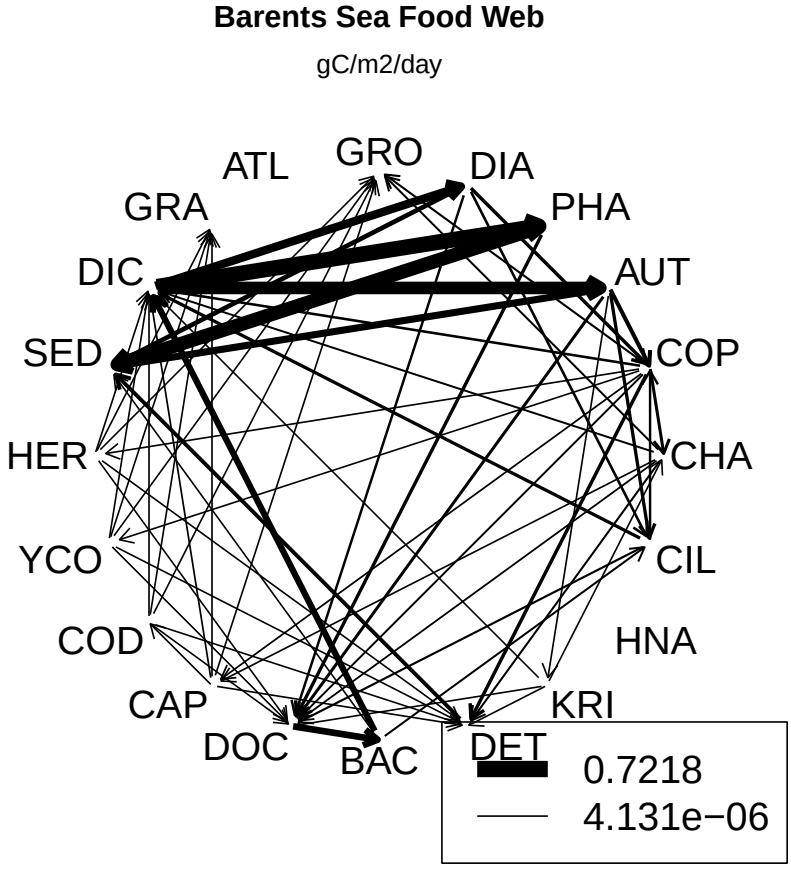

Figure 1: The Barents Sea food web

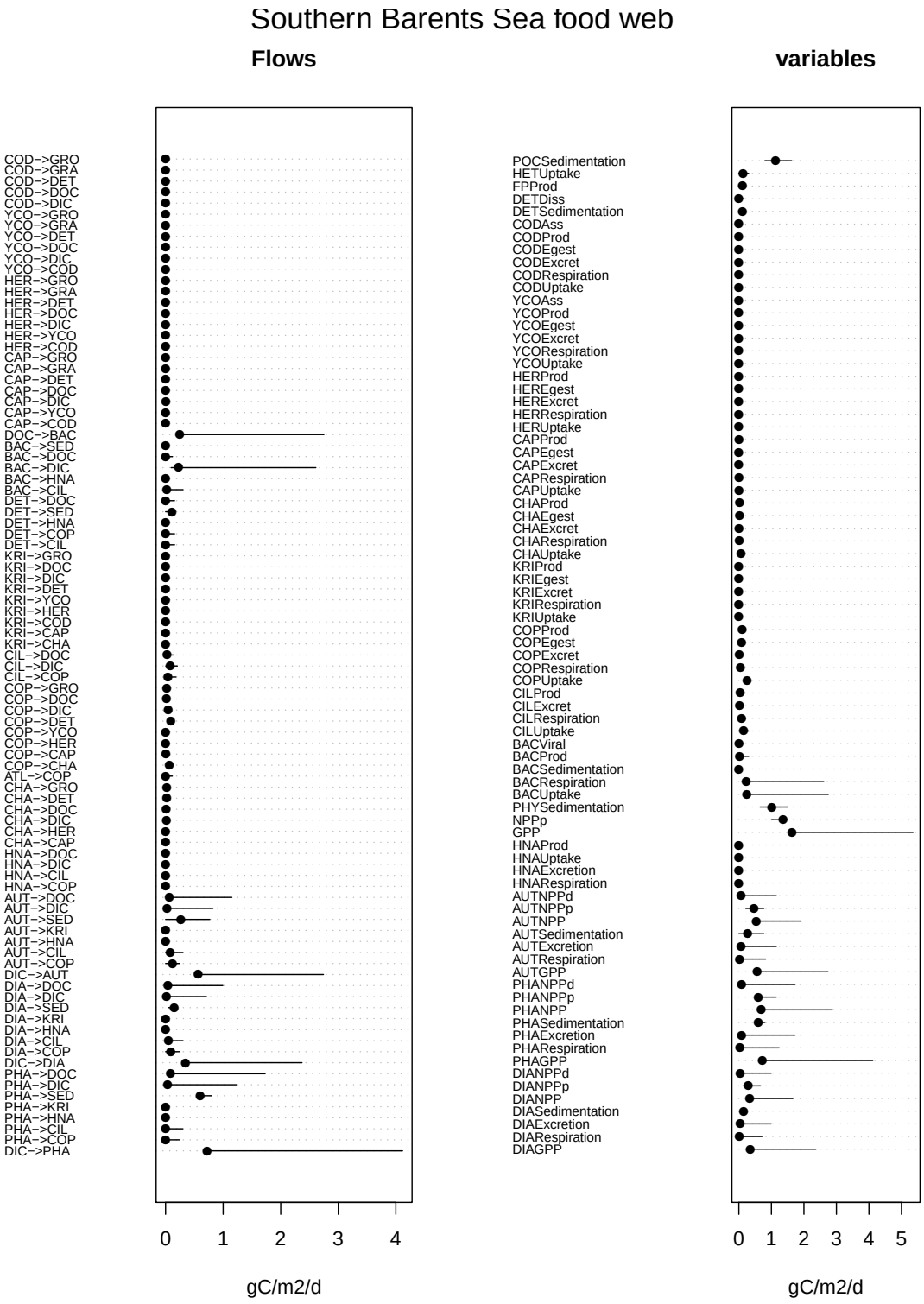

Figure 2: The Barents Sea food web ranges of flows and variables

2.2. LIMlake and LIMlakeFish

This includes the Linear inverse model specification for two freshwater lake enclosures (Lac Croche, Canada), (Ridal, Mazumder, and Lean 2001), used as demonstration example in (De˜Laender *et˜al.* 2009).

Food web compositions in the enclosures were manipulated by additions of planktivorous fish and/or nutrients giving four types of food webs: planktonic, planktonic with nutrient addition, planktonic with planktivorous fish, and planktonic with planktivorous fish and nutrient additions. The trophic links in the mass-balances of each LIM are identical, except that the fish compartment is only present in F and FN.

`LIMlake` is the linear inverse model for the food web without fish and without nutrient addition. `LIMlakeFish` has fish, but also no nutrients were added.

First the food web is solved:

```
> pm <- par(mfrow=c(1,2))
> lake <- Flowmatrix(LIMlake)
> plotweb(lake,main="Lake enclosure food web",sub="gC/m2/day")
> plotweb(Flowmatrix(LIMlakeFish),main="Lake enclosure food web + FISH",
+   sub="gC/m2/day")
```

Then the ranges of flows and variables are calculated and plotted:

```
> # ranges of flows
> Plotranges(LIMlake,lab.cex=0.7,xlab="gC/m2/d",
+    main="Flows")
> # ranges of variables
> Plotranges(LIMlake,type="V",lab.cex=0.7,xlab="gC/m2/d",
+    main="variables")
> mtext(outer=TRUE,"Lake enclosure food web",side=3,line=-1,cex=1.5)
> par(mfrow=pm)
```

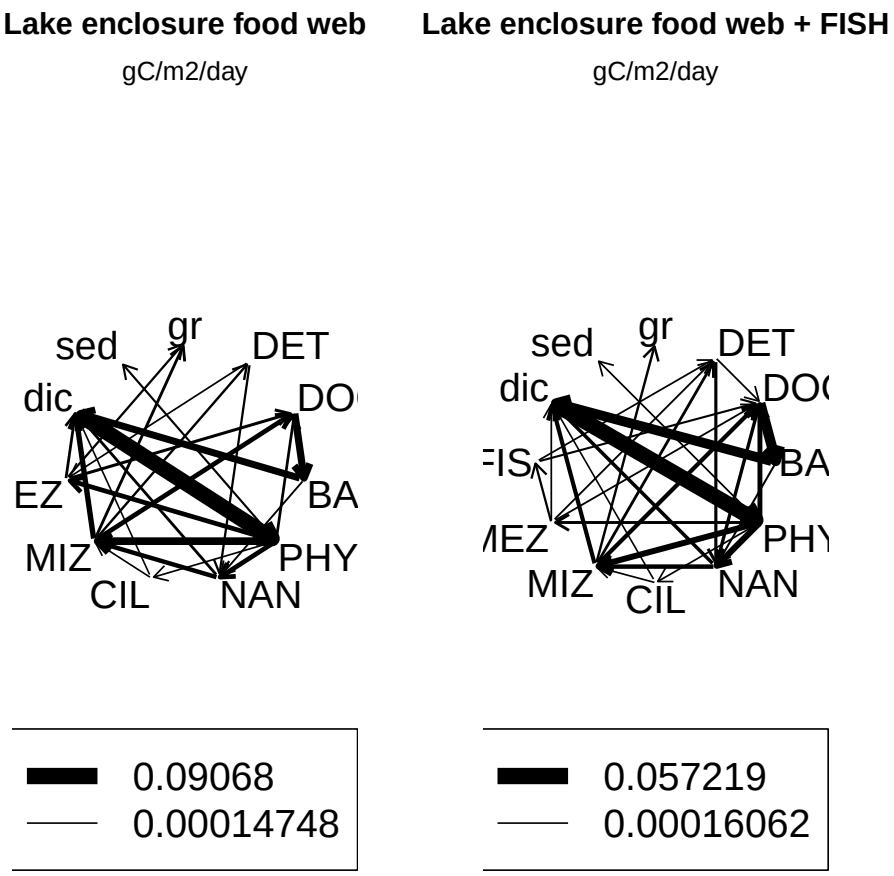

Figure 3: The Limlake food web with and without fish

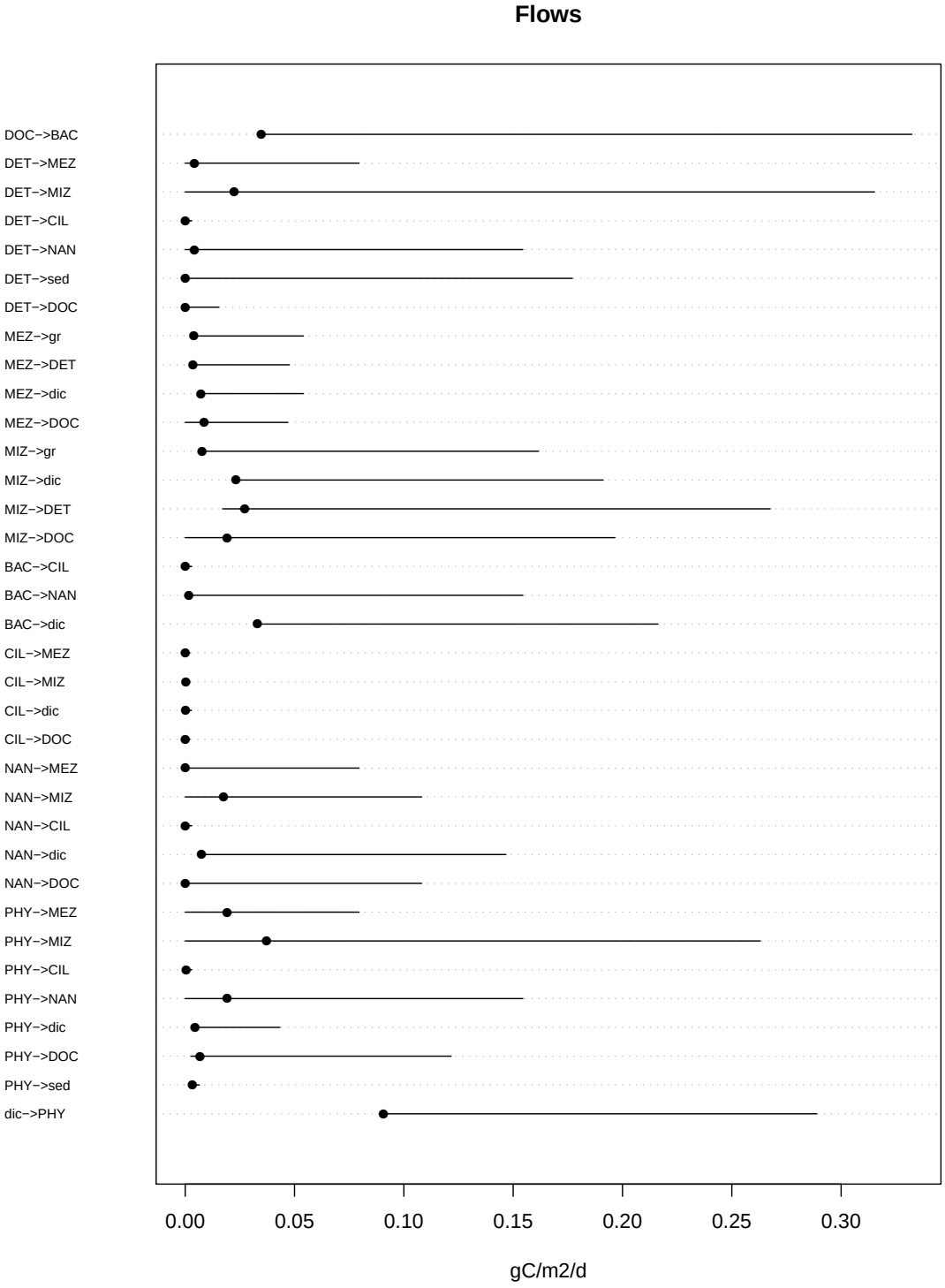

Figure 4: The Limlake food web ranges of flows and variables

3. The LimOmega function

The `OMEGA` model (Hendriks *et˜al.* 2001) estimates the rate of change of the concentration Ci of a nonbiotransforming chemical in compartment i by taking into account the chemical uptake rates through feeding and directly from water, the chemical dilution rate through production and the rates of egestion with faeces and excretion to water.

While `OMEGA` initially was developed to represent food chains, it was extended with multiple food sources in (De˜Laender *et˜al.* 2009).

The set of differential equations for all m compartments in a food web was cast in matrix notation as:

$$\frac{dC}{dt} = K_{up,food} \cdot C + K_{up,water} \cdot Cwater - K_{out+dil} \cdot C$$

where C is the internal concentration vector, $\frac{dC}{dt}$ is the rate of change of the internal concentration vector, $K_{up,food}$ is a m * m matrix with chemical uptake rates through feeding (d-1), containing elements $k_{up,food,ji}$ on row i, column j, $K_{up,water}$ the uptake rates directly from water ($L˜kg^{-1}˜d^{-1}$) is a column vector with m elements and $K_{out+dil}$ the chemical dilution rate through production, the rates of egestion with faeces and excretion to water (d^{-1}), a m * m diagonal matrix with elements $k_{out,eg,i} + k_{dil,pr,i} + k_{out,water,i}$.

Expressions for rate coefficients ($k_{up,food,ji}$; $k_{up,water,i}$; $k_{out,eg,i}$; $k_{dil,pr,i}$; $k_{out,water,i}$) that regulate chemical uptake and loss processes and how these relate to the carbon flows predicted by the **LIM** framework can be found in Table S1 of the Supporting Information (SI) of (De˜Laender *et˜al.* 2009).

Internal concentrations in small particles such as microzooplankton, phytoplankton, detritus, protozoa, and bacteria (collectively termed `INST` in this package), are assumed to be in rapid equilibrium with the water phase and may be calculated as

$$C^*_{INST} = Cwater \cdot OC_{INST} \cdot K_{OC}$$

where C^*_{inst} denotes the concentration vector for model compartments that are in instant equilibrium with the surrounding water (microg kg-1 wet weight), OC_{inst} their organic carbon fraction (-), and K_{OC}, the organic carbon-water partition coefficient ($L˜kg^{-1}$), calculated as 0.41KOW, with KOW the octanol-water partition coefficient.

3.1. The bioaccumulation model applied to the three example food webs

First we apply the bioaccumulation model to the three food webs, and using the default values (e.g. a `logKoW` of 6):

The lake food web,

```
> LimOmega (lim = LIMlake,
+           INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+           KINE= "MEZ", EXPO=c("sed","gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=7.596535e-08, SS_KINE=0.079508)
```

```
$BAF_LC
    MEZ
1073583

$BCF_OC
   DET    DOC    BAC    PHY    NAN    CIL    MIZ
410000 410000 410000 410000 410000 410000 410000
```

The lake food web with fish:

```
> LimOmega (lim = LIMlakeFish,
+           INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+           KINE=c("MEZ","FIS"), EXPO=c("sed","gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=c(1.85e-08,1.7e-3),
+           SS_KINE=c(0.00514800,0.26))

$BAF_LC
    MEZ     FIS
 943609 1051809

$BCF_OC
   DET    DOC    BAC    PHY    NAN    CIL    MIZ
410000 410000 410000 410000 410000 410000 410000
```

The Barents Sea example:

```
> LimOmega (lim = LIMbarents,
+           INST=c("DIA","PHA","AUT","CIL","HNA","DET","BAC"),
+           KINE=c("COP","CHA","KRI","CAP","COD","YCO","HER"),
+           EXPO=c("SED","GRA","GRO"),
+           DOC="DOC", DET="DET", DIC="DIC",
+           WW_KINE=c(0.000001,8e-05,0.00006,10e-3,3,1,20e-3),
+           LIPID_KINE=c(0.01,0.01,0.01,0.03,0.03,0.03,0.03),
+           LIPID_INST=0.04,
+           SS_KINE=c(1.79,0.6965,0.003,0.38,0.053,0.006,0.055))

$BAF_LC
      COP       CHA       KRI       CAP       COD       YCO       HER
 887935.9 1003297.5  467057.2  958170.3 1657017.9  780377.1 1160962.6

$BCF_OC
   DIA    PHA    AUT    CIL    HNA    DET    BAC
410000 410000 410000 410000 410000 410000 410000
```

3.2. A monte carlo run on food web structure

First we take `niter` random samples from all possible solutions using a Markow Chain Monte Carlo approach (Van˜den Meersche *et˜al.* 2009)

```
>   X0       <- Lsei(LIMlake)$X
>   niter <- 50
>   SolXS    <- Xsample(LIMlake, iter=niter, type = "mirror",
+                       jmp=NULL, x0=X0, fulloutput = FALSE)
>   BAFlc_all  <- NULL
```

Then, for each of these samples the flowmatrix is created and LimOmega applied:

```
>   for (i in 1:niter) {
+    flowmat <- Flowmatrix(LIMlake, SolXS[i,])
+    LO<- LimOmega (flowmatrix=flowmat,
+           INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+           KINE=c("MEZ"), EXPO=c("sed","gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=7.596535e-08, SS_KINE=0.079508,
+           Growth=0, k=0.25, Q=1)
+
+    BAFlc_all <- c(BAFlc_all,LO$BAF_LC)
+   }
```

Show results

```
> hist(BAFlc_all)
```

Now the same food web structure is used with different chemical parameters:

```
>   niter <- 100
```

We create a normally distributed sample of log kow:

```
>   lkw <- rnorm(niter,mean=6,sd=0.4)
>   BAFlc_all  <- NULL
>   BCFoc_all  <- NULL
```

We also use the `LIMlake` foodweb:

```
>   flowmat <- Flowmatrix(LIMlake)
```

and run the `LimOmega` model for each value of log kow:

```
>   for (i in 1:niter) {
+    LO<- LimOmega (flowmatrix=flowmat,
+           INST=c("DET","DOC","BAC","PHY","NAN","CIL","MIZ"),
+           KINE=c("MEZ"), EXPO=c("sed","gr"),
+           DOC="DOC", DET="DET", DIC="dic",
+           WW_KINE=7.596535e-08, SS_KINE=0.079508,
+           Growth=0, k=0.25, Q=1, logKow = lkw[i])
+
+    BAFlc_all <- c(BAFlc_all,LO$BAF_LC)
+    BCFoc_all <- c(BCFoc_all,LO$BCF_OC[1])
+   }
```

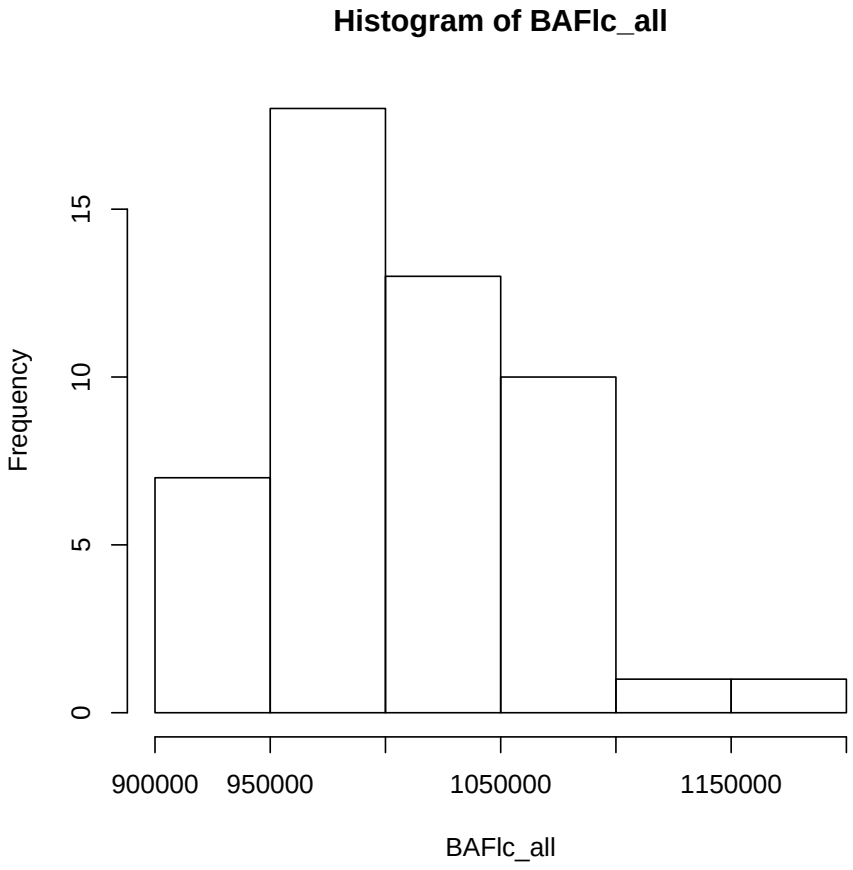

Figure 5: The LimOmega model, applied 50 times, to the lake food web

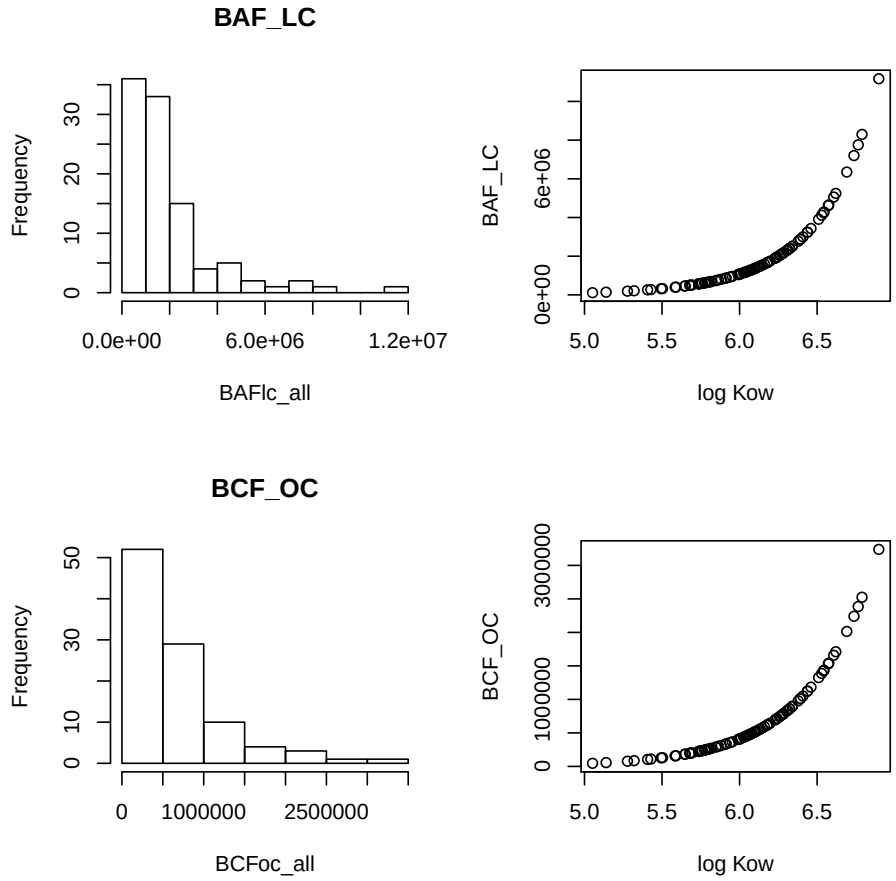

Figure 6: The LimOmega model, applied with different values of log kow

Finally, we plot the results:

```
> pm <- par(mfrow=c(2,2))
> hist(BAFlc_all,main="BAF_LC")
> plot(lkw,BAFlc_all,xlab="log Kow",ylab="BAF_LC")
> hist(BCFoc_all,main="BCF_OC")
> plot(lkw,BCFoc_all,xlab="log Kow",ylab="BCF_OC")
> par(mfrow=pm)
```

4. Finally

This vignette was made with Sweave (Leisch 2002).

References

De˜Laender F, Soetaert K (2010). *ToxLim: Incorporating Ecological Data and Associated Uncertainty in Bioaccumulation Modeling*. R package version 1.0.

De˜Laender F, Van˜Oevelen D, Middelburg J, Soetaert K (2009). "Incorporating Ecological Data and Associated Uncertainty in Bioaccumulation Modeling: Methodology Development and Case Study." *Environmental Science and Technology*, **43 No. 7**, 2620–2626.

De˜Laender F, Van˜Oevelen D, Middelburg J, Soetaert K (2010a). "Carbon transfer in herbivore- and microbial loop-dominated pelagic food webs in the southern Barents Sea during spring and summer." *Marine Ecology Progress Series*, **398**, 93 – 107.

De˜Laender F, Van˜Oevelen D, S F, Middelburg J, Soetaert K (2010b). "Seasonal PCB Bioaccumulation in an Arctic Marine Ecosystem: A Model Analysis Incorporating Lipid Dynamics, Food-Web Productivity and Migration." *Environmental Science and Technology*, **44**, 356 – 361.

Hendriks A, van˜der Linde A, Cornelissen G, Sijm D (2001). "The power of size. 1. Rate constants and equilibrium ratios for accumulation of organic substances related to octanol-water partition ratio and species weight." *Environ. Toxicol. Chem.*, **20**, 1399 – 1420.

Leisch F (2002). "Sweave: Dynamic Generation of Statistical Reports Using Literate Data Analysis." In W˜Härdle, B˜Rönz (eds.), "Compstat 2002 — Proceedings in Computational Statistics," pp. 575–580. Physica Verlag, Heidelberg. ISBN 3-7908-1517-9, URL http://www.stat.uni-muenchen.de/~leisch/Sweave.

Ridal JJ, Mazumder A, Lean D (2001). "Effects of nutrient loading and planktivory on the accumulation of organochlorine pesticides in aquatic food chains." *Environ. Toxicol. Chem.*, **20**, 1312 – 1319.

Soetaert K, den Meersche KV, van Oevelen D (2009). *limSolve: Solving Linear Inverse Models*. R package version 1.5.1, URL http://CRAN.R-project.org/package=limSolve.

Van˜den Meersche K, Soetaert K, Van˜Oevelen D (2009). "xsample(): An R Function for Sampling Linear Inverse Problems." *Journal of Statistical Software*, **30**, 1–15.

van Oevelen D, van˜den Meersche K, Meysman F, Soetaert K, Middelburg JJ, Vezina AF (2010). "Quantifying Food Web Flows Using Linear Inverse Models." *Ecosystems*, **13**, 32–45. doi:10.1007/s10021-009-9297-6. URL http://www.springerlink.com/content/4q6h4011511731m5/fulltext.pdf.

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