The statistical model behind simmr (and SIAR)

Andrew Parnell
andrew.parnell@mu.ie

Maynooth University
National University of Ireland Maynooth

Learning outcomes:

- Understand the statistical model behind simmr/SIAR
- Know how to run a model in simmr/SIAR and check that it works
- Be able to follow the technical details of the 2010 SIAR Plos ONE paper

Our simple SIMM

- In the last class we had a simple SIMM defined via:

$$y_i \sim N\left(\sum_{k=1}^{2} p_k s_k, \sigma^2\right)$$

  with $s_k \sim N(\mu_{s_k}, \sigma^2_{s_k})$, $p_1 \sim U(0,1)$ and $\sigma \sim U(0,100)$
- Here y_i is the isotope value, s are the source values, p are the dietary proportions, and σ is the residual standard deviation
- The goal is to estimate the p and its uncertainty. The other parameters can be considered nuisance parameters

Expanding the simple SIMM

- This SIMM is currently too simplistic. We need to expand it by:
    - increasing the number of food sources
    - including trophic enrichment factors (TEFs)
    - including concentration dependence
    - allowing for multiple isotopes
    - allowing for richer source sampling by consumers
- If we include all of these factors we end up with the simmr/SIAR model
- We will take them in turn and add them into our JAGS code

Reminder: the SIAR geese data

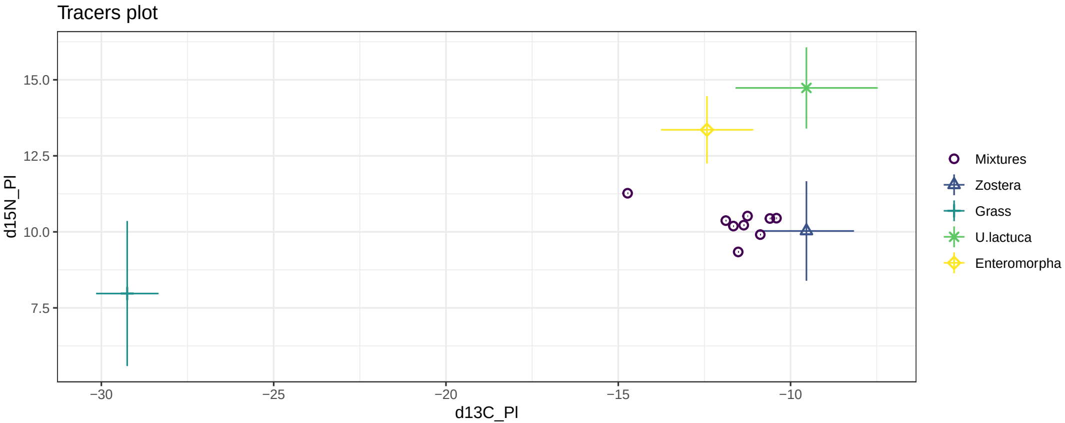
```
data(geese_data_day1)
str(geese_data_day1)
```

```
## List of 8
##  $ mixtures           : num [1:9, 1:2] -11.4 -11.9 -10.6 -11.2 -11.7 ..
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr [1:2] "d13C_Pl" "d15N_Pl"
##  $ tracer_names       : chr [1:2, 1] "d13C_Pl" "d15N_Pl"
##  $ source_names       : chr [1:4] "Zostera" "Grass" "U.lactuca" "Entero
##  $ source_means       : num [1:4, 1:2] -11.17 -30.88 -11.17 -14.06 6.49
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
##   .. ..$ : chr [1:2] "meand13CPl" "meand15NPl"
##  $ source_sds         : num [1:4, 1:2] 1.215 0.641 1.959 1.172 1.459 ..
##   ..- attr(*, "dimnames")=List of 2
##   .. ..$ : NULL
```

Plotting the data

A plot in isotope space:

```
plot(simmr_in)
```



Including multiple sources

- Adding in multiple sources to the likelihood means having more terms in the sum:

$$y_i \sim N\left(\sum_{k=1}^{K} p_k s_k, \sigma^2\right)$$

- In the above we have K sources and hence K dietary proportions
- We also now need K source prior distributions
- The tricky part about adding in multiple proportions is the prior distribution

Priors for constrained dietary proportions

- We must have $\sum_{k=1}^{K} p_k = 1$ so any prior distribution we place on the ps must satisfy this restriction
- (You will often hear values restricted in sum referred to as a *simplex*)
- Luckily there is a distribution known as the *Dirichlet* which is suitable for restricted sum parameters
- The Dirichlet has one parameter for each proportion $\alpha_1, \ldots, \alpha_K$. The larger the α value the larger prior weight that dietary proportion will be given
- Setting all the α values to 1 is equivalent to the simplex uniform distribution, i.e. a prior assumption that all sources are consumed equally

JAGS SIMM with a Dirichlet prior

```
model_code ='
model {
  for(i in 1:N) { y[i] ~ dnorm(inprod(p,s),sigma^-2) }
  p ~ ddirch(alpha)
  for(k in 1:K) { s[k] ~ dnorm(s_mean[k],s_sd[k]^-2) }
  sigma ~ dunif(0,100)
}
'
data=with(geese_data_day1,
          list(y=mixtures[,1],
               s_mean=source_means[,1],
               s_sd=source_sds[,1],
          N = nrow(mixtures),K=nrow(source_means),
          alpha=rep(1,nrow(source_means))))
set.seed(123)
model_run = jags(data = data,
                 parameters.to.save = c("p", "sigma"),
                 model.file = textConnection(model_code))
```

Results

- We can explore/plot results with `summary(output)`, `plot(output)`, and also run multiple chains, form predictive distributions, check convergence, etc
- One important thing to note is that the fitting method (MCMC) produces a joint posterior distribution of the dietary proportions. This means that each set of samples will sum to 1:

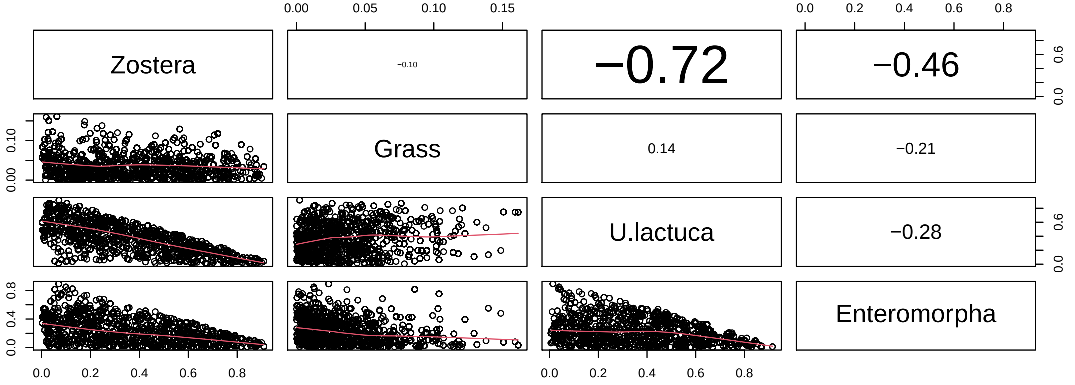
```
head(model_run$BUGSoutput$sims.matrix,4)
```

```
##      deviance      p[1]        p[2]      p[3]       p[4]    sigma
## [1,] 38.24013 0.2931735 0.037865208 0.6128807 0.05608053 2.666854
## [2,] 29.94426 0.2925945 0.049061414 0.4754383 0.18290585 1.237191
## [3,] 29.19475 0.3280195 0.051608762 0.4583445 0.16202724 1.385694
## [4,] 29.35735 0.5883123 0.004139584 0.1634236 0.24412454 1.037509
```

- The key implication of this is that, aside from exploring the *marginal* posterior distributions (with means, sds, etc) we can explore the *joint* uncertainty of the dietary proportions

A joint plot of the posterior dietary proportions

```
out_2 = model_run$BUGSoutput$sims.list$p
colnames(out_2) = geese_data_day1$source_names
pairs(out_2, lower.panel = panel.smooth,
      upper.panel = panel.cor)
```



Trophic enrichment factors and concentration dependence

- Trophic enrichment factors (c) and concentration dependence (q) represent adjustments to the source values to account for various measurement effects
- We can include them by expanding the likelihood:

$$y_i \sim N\left(\frac{\sum_{k=1}^{K} p_k q_k (s_k + c_k)}{\sum_{k=1}^{K} p_k q_k}, \sigma^2\right)$$

- The extra part on the denominator is needed so that the dietary proportions still sum to 1
- The prior for c_k comes from external data and are given normal distributions like the source values
- In SIAR the concentration dependencies must be less than 1 (given as proportions) and are treated as fixed. You could use a strong Dirichlet prior on these instead

Including TEFs and CD - JAGS model

```
model_code ='
model {
  for(i in 1:N) {
    y[i] ~ dnorm(inprod(p*q,s+c)/inprod(p,q),sigma^-2)
  }
  p ~ ddirch(alpha)
  for(k in 1:K) {
    s[k] ~ dnorm(s_mean[k],s_sd[k]^-2)
    c[k] ~ dnorm(c_mean[k],c_sd[k]^-2)
  }
  sigma ~ dunif(0,100)
}
'
data=with(geese_data_day1,
          list(y=mixtures[,1], s_mean=source_means[,1],
               s_sd=source_sds[,1], c_mean = correction_means[,1],
               c_sd = correction_sds[,1], q = concentration_means[,1],
          N = nrow(mixtures),K=nrow(source_means),
          alpha=rep(1,length(source_names))))
model_run = jags(data = data
```

Notes on the TEF and CD model

- If you run this, you'll find that convergence isn't quite as neat and it starts to get a bit slower
- Although it's a nuisance parameter, saving `sigma` is often a good idea because a large value indicates a poorly fitting model (usually also seen in the iso-space plot)
- The model will also create posterior distributions for s and c, though these are usually pretty similar to the prior, as there isn't much information about their values in the data

Adding extra isotopes

- If we have extra isotopes we can just list the likelihood twice, once for each value of the isotope. Only the dietary proportions are 'shared' between the isotopes
- Now write y_{ij} as the consumer values for observation i on *isotope* j, where $j = 1, \ldots, J$
- We now have source values s_{jk}, TEF values c_{jk}, concentration dependencies q_{jk}, and each isotope has its own residual standard deviation σ_j
- The likelihood is now:

$$y_{ij} \sim N\left(\frac{\sum_{k=1}^{K} p_k q_{jk}(s_{jk} + c_{jk})}{\sum_{k=1}^{K} p_k q_{jk}}, \sigma_j^2 \right)$$

Richer source sampling

- The model we've been fitting up to now assumes that all individuals sample the same source value s_k for each source and isotope. This is unrealistic
- A better model has each individual sampling a different source value from the source prior distribution, i.e. we now have s_{ik} (or s_{ikj} with multiple isotopes)
- The JAGS code becomes:

```
for(k in 1:K) {
  for(i in 1:N) {
    s[i,k] ~ dnorm(s_mean[k],s_sd[k]^-2)
  }
}
```

- We can do the same with the concentration dependence values
- In fact with a bit of clever maths we can remove (*marginalise over*) the s_{ik} values to get a simpler model with fewer parameters.

The full simmr/SIAR model

- Using the trick mentioned on the last slide, we end up with a full model which looks like this:

$$y_{ij} \sim N\left(\frac{\sum_{k=1}^{K} p_k q_{jk}(\mu_{s,jk} + \mu_{c,jk})}{\sum_{k=1}^{K} p_k q_{jk}}, \frac{\sum_{k=1}^{K} p_k^2 q_{jk}^2 (\sigma_{s,jk}^2 + \sigma_{c,jk}^2)}{(\sum_{k=1}^{K} p_k q_{jk})^2} + \sigma_j^2 \right)$$

- This model has a more complicated likelihood, but removes the extra s and c parameters

Full SIAR model: JAGS code

```
model_code ='
model {
  for (i in 1:N) {
    for (j in 1:J) {
      y[i,j] ~ dnorm(inprod(p*q[,j], s_mean[,j]+c_mean[,j]) /
        inprod(p,q[,j]), var_y[j]^-1)
    }
  }
  p ~ ddirch(alpha)
  for(j in 1:J) {
    var_y[j] <- inprod(pow(p*q[,j],2),s_sd[,j]^2+c_sd[,j]^2)/pow(inprod(p,q[,j]),
      + pow(sigma[j],2)
  }
  for(j in 1:J) { sigma[j] ~ dunif(0,100) }
}
'
```

Full simmr/SIAR model: R code

```
data=with(geese_data_day1,
          list(y=mixtures,s_mean=source_means,
          s_sd=source_sds,
          c_mean=correction_means,c_sd=correction_sds,
          q=concentration_means,N=nrow(mixtures),
          J=ncol(mixtures),alpha=rep(1,length(source_names))))
model_run = jags(data = data,
                 parameters.to.save = c("p", "sigma"),
                 model.file = textConnection(model_code),
                 DIC = FALSE)
```

Summary of posterior dietary proportions

```
out_2 = model_run$BUGSoutput$sims.matrix
colnames(out_2) = c(geese_data_day1$source_names,'SD1','SD2')
t(round(apply(out_2,2,quantile,probs=c(0.025,0.5,0.975)),2))
```

```
##              2.5%  50% 97.5%
## Zostera      0.43 0.61  0.80
## Grass        0.03 0.07  0.12
## U.lactuca    0.01 0.14  0.35
## Enteromorpha 0.01 0.15  0.46
## SD1          0.05 0.86  2.45
## SD2          0.02 0.36  1.40
```

Some of these proportions are quite imprecise: perhaps see better with matrix plot?

Running SIAR/simmr

- The SIAR/simmr R packages run exactly this model with a few extra tweaks
- It contains a slightly optimised algorithm as JAGS sometimes gets a bit stuck on harder data sets. It's also much faster than JAGS for complicated problems
- It allows for direct plotting of the data in isotope space and *p*-space (i.e. dietary proportion space - `pairs` plots)
- It allows for changing the α values to put in proper prior information
- It includes convergence checking
- Most of this was covered in the practical yesterday

simmr version

- simmr is a much more elegantly written version of SIAR with neater plots and many more features
- Four steps to run a simmr model
  1. Call simmr_load to load in the data
  2. Call plot to see the iso-space plot
  3. Call simmr_mcmc to run the model
  4. Call plot or summary to access the output
- simmr has further features to combine sources and to compare dietary proportions

simmr code

```
# Load
data("geese_data_day1")
simmr_in = with(geese_data_day1,
                simmr_load(mixtures = mixtures,
                      source_names = source_names,
                      source_means = source_means,
                      source_sds = source_sds,
                      correction_means = correction_means,
                      correction_sds = correction_sds,
                      concentration_means = concentration_means))
# Iso-space plot
plot(simmr_in)
# MCMC run
simmr_out = simmr_mcmc(simmr_in)
# Box-plots
plot(simmr_out, type = 'boxplot')
```

Summary

- The simmr and SIAR models are just complicated versions of linear regression
- The response is multivariate and the prior distributions on some of the parameters have to be constrained to sum to 1
- It used to be the case that JAGS was slow and couldn't run SIMM-type models. This is no longer true. You can fit much richer models in JAGS (and now MixSIAR) than with SIAR/simmr
- The MixSIAR is an order of complexity again as it uses ideas from generalised linear models to include covariates on the dietary proportions