02 - Very first example

2019-04-30

This vignette gives a basic first introduction to estimating transmission flows with the `phyloflows` package. Please read the sections "Our Job" and "Our Solution" on the main page before you go ahead here.

Input data

phyloflows expects input data in a specific format.

- `dobs` a data.frame of observed transmission counts within and between population groups.
- `dprior` a data.frame that summarises prior information on how population groups were sampled.

To get you started, **phyloflows** comes with a small simulated example data set of transmission counts and sampling information between two population groups, denoted by "1" and "2":

```
#   required R packages
require(phyloflows)
require(ggplot2)
require(bayesplot)
require(data.table)
require(coda)

#
#   load transmission flow data "twoGroupFlows1"
data(twoGroupFlows1, package="phyloflows")
#   observed transmission counts
dobs <- twoGroupFlows1$dobs
#   sampling information
dprior <- twoGroupFlows1$dprior
```

Input data: observed transmission flows

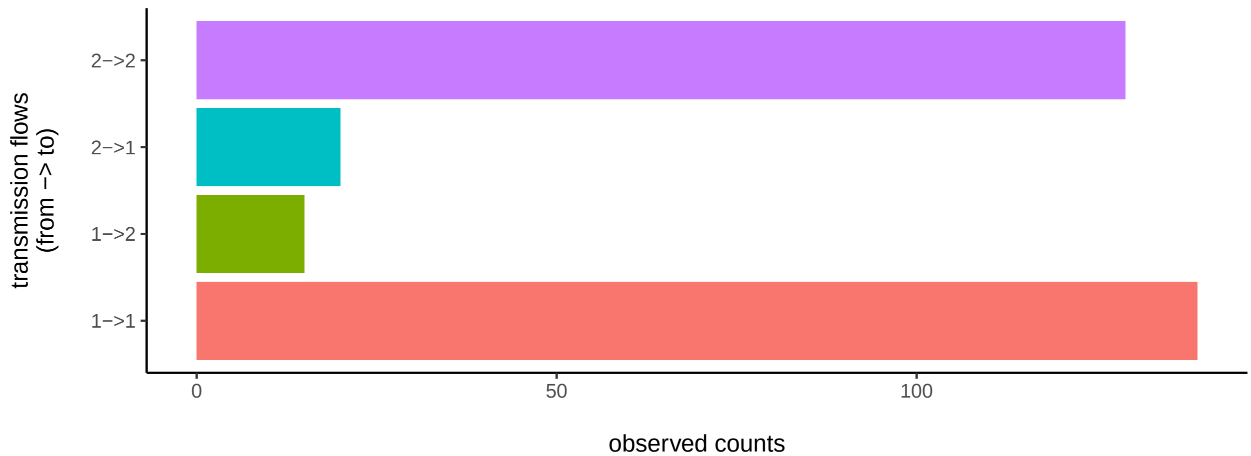
```
dobs
#>    REC_TRM_CATEGORY TR_TRM_CATEGORY TR_SAMPLING_CATEGORY
#> 1:                1               1                    1
#> 2:                2               1                    1
#> 3:                1               2                    2
#> 4:                2               2                    2
#>    REC_SAMPLING_CATEGORY TRM_OBS TRM_CAT_PAIR_ID
#> 1:                     1     139               1
#> 2:                     2      15               2
#> 3:                     1      20               3
#> 4:                     2     129               4
```

`dobs` specifies observed counts of transmissions from a transmitter group to a recipient group. It must contain the following columns:

- *TR_TRM_CATEGORY* name of transmitter group.
- *REC_TRM_CATEGORY* name of recipient group.
- *TRM_CAT_PAIR_ID* identifier of transmitter-recipient pair

- *TRM_OBS* observed transmission counts

Let us look at the data. The first row contains counts of transmission flows from group “1” to group “1”, and there are 139 of them. The next row contains counts of transmission flows from group “1” to group “2”, and there are 15 of them. Here is a barplot of our input data:



Input data: sampling information

`dobs` also must contain information about how each group was sampled. This is stored in the following columns:

- *TR_SAMPLING_CATEGORY* sampling strata of transmitter group
- *REC_SAMPLING_CATEGORY* sampling strata of recipient group

Each transmitter/recipient group is associated to a sampling category. This can be “sampling group a” for both “1” and “2”, or “a” and “b” respectively for “1” and “2”. In our little data set, we gave the same name to transmitter/recipient and sampling groups.

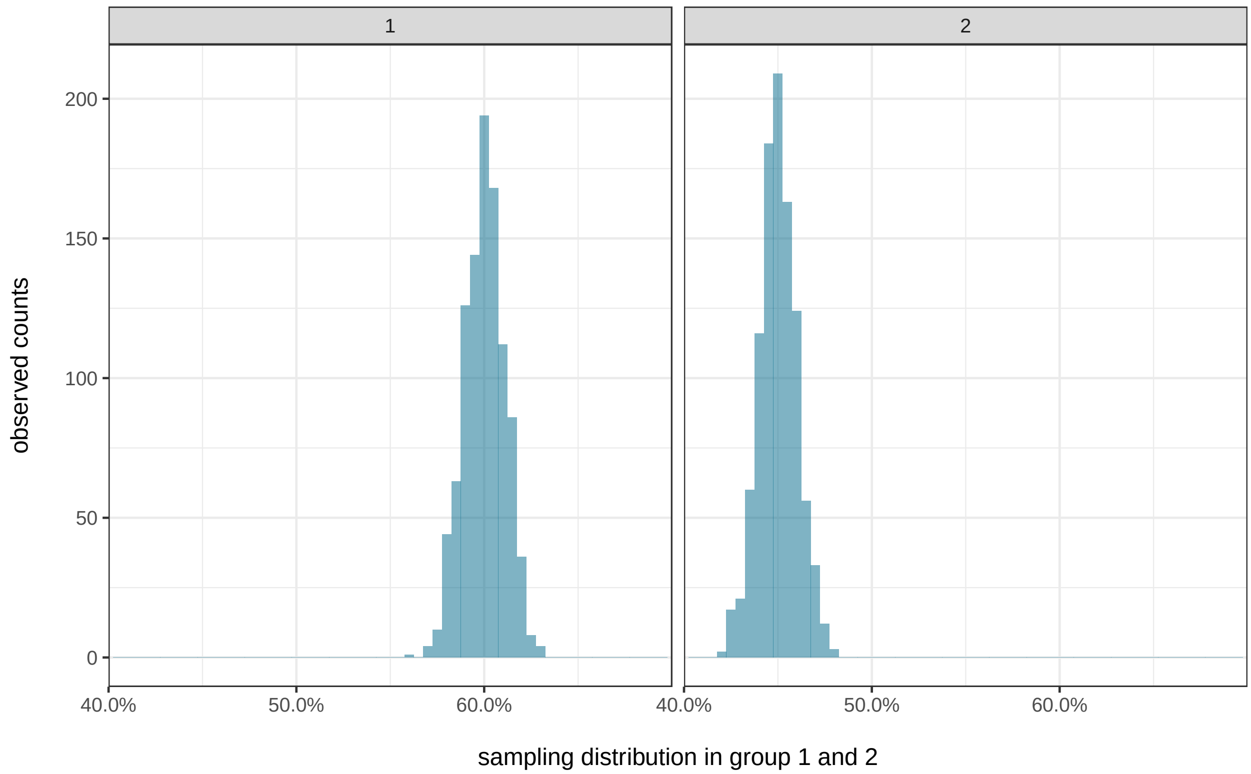
`dprior` specifies the probability of sampling an individual from each sampling group. To keep this as flexible as possible, samples from the sampling distribution, rather than say the mean and standard deviation, need to be given. This information is stored in the following columns:

- *SAMPLING_CATEGORY* name of sampling strata
- *SAMPLE* identifier of sample from the sampling distribution
- *P* sampling probability
- *LP* log density of the sampling probability under the sampling distribution.

Let us look at the sampling information:

```
head(dprior)
#>    SAMPLING_CATEGORY         P SAMPLE       LP
#> 1:                 1 0.5824160      1 2.318750
#> 2:                 1 0.6184042      2 2.168504
#> 3:                 1 0.6033518      3 3.548540
#> 4:                 1 0.6015475      4 3.585452
#> 5:                 1 0.5918721      5 3.321375
#> 6:                 1 0.6034198      6 3.546614
```

Here is a histogram of the sampling distribution from sampling groups “1” and “2”. Notice that in our example, the probability of sampling individuals in group “1” is higher than that among individuals in group “2”.



phyloflows MCMC algorithm

Statistical model

`phyloflows` uses a Bayesian approach to estimate the proportion of transmissions between the two population groups,

$$\pi = (\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22}).$$

The model can be motivated as follows. Suppose the actual, unobserved number of transmissions from group i to group j are z_{ij}. Denote the vector of actual transmission counts by

$$z = (z_{11}, z_{12}, z_{21}, z_{22}).$$

The likelihood of the actual transmission counts is then given by

$$p(z|Z, \pi) = Multinomial(z; Z, \pi),$$

where Z is the total number of transmissions, $Z = \sum_{kl} z_{kl}$, if we assume that transmission events occurred independently of each other. Next, we specify a model for observing one actual transmission event. This is given by

$$p(n_{ij}|z_{ij}, s_i, s_j) = Binomial(n_{ij}; z_{ij}, s_i * s_j),$$

where s_i is the probability of sampling an individual from group i, and similary for s_i. The free parameters of the model are

$$\theta = (z, Z, \pi, s),$$

and the posterior distribution of the free parameters is given by

$$\begin{aligned} p(\theta|n) &\propto p(n|\theta)p(\theta) \\ &= \prod_{ij} Bin(n_{ij}; z_{ij}, s_i * s_j) Multin(z; Z, \pi) p(Z) p(\pi) p(s). \end{aligned}$$

In general we specify for

- $p(\pi)$ an uninformative prior distribution (Dirichlet distribution with parameters 0.8/4);
- $p(s)$ a strongly informative prior distribution, based on available data (as illustrated above);
- $p(Z)$ a strongly informative prior distribution, based on available data (Poisson distribution with mean set to the expected number of actual transmissions).

MCMC: syntax

Now that we understand the input data, we are ready to estimate the transmission flows within and between the two population groups,

$$\pi = (\pi_{11}, \pi_{12}, \pi_{21}, \pi_{22}).$$

We just need to specify a seed, number of iterations of the Markov Chain Monte Carlo algorithm, a flag for verbose output, and an output file name if you like to have the results written to an *.rda* file.

```
control <- list(seed=42, mcmc.n=500, verbose=0)
ans <- phyloflows:::source.attribution.mcmc(dobs, dprior, control)
#>
#> Setting seed to 42
#> Number of parameters:     17
#> Dimension of PI:  4
#> Sweep length:     5
#> Number of sweeps:     100
#> Number of iterations:     500
#> Number of transmission pair categories updated per iteration, and their frequencies:
#>
#> 2
#> 4
#>
#> Sweeps done:  100
```

MCMC: messages

Let s have a look at the messages first.

- The total number of unknown parameters in **phyloflows** MCMC is the length of π plus the length of the latent transmission flows z plus the length of the pairwise sampling probabilities ξ, $\xi_{ij} = s_i * s_j$, plus twice the length of the sampling probabilities s, plus 1 for Z. This makes $4+4+4+2*2+1 = 17$ in our very first example.
- The MCMC updates all these parameters in a certain number of MCMC iterations, and this number is called a sweep. A sweep is always twice the length of the sampling probabilities plus 1 for updating the values of π. This makes $2*2+1$ in our very first example.
- The total number of sweeps is determined from `control[['mcmc.n']]`. In our case, it is $50/5 = 10$. If we had set `control[['mcmc.n']]<- 51`, then the total number of sweeps would have been 11.
- The total number of iterations is the length of a sweep times the total number of sweeps. In our example, $5*10 = 50$. If we had set `control[['mcmc.n']]<- 51`, then the total number of iterations would have been $5*11 = 55$.
- Finally, we have the number of transmission pair categories updated per iteration. These numbers are important to assess the likely performance of the MCMC. The algorithm proceeds by updating the sampling probabilities for the transmitter groups, then those for the recipient groups, and finally one update for the values of π. If we update s_1 for the transmitter groups, we also need to update all pairwise sampling probabilities that contain s_1 for the transmitter groups. These are $\xi_{11} = s_1 * s_1$ and $\xi_{12} = s_1 * s_2$, so we have two pairwise sampling probabilities to update. In our very first example, this is

always the case: if we update any of the 4 s_i for either the transmitter and recipient groups, we always have to update 2 pairwise sampling probabilities. This is what you see printed, before the algorithm gets cranking. In general, the fewer pairwise sampling probabilities need to be updated, the better, because the MCMC acceptance rates take a huge hit when many parameters need to be updated at once. Set up your model so that you have at most 4-6 joint parameter updates at any MCMC iteration.

MCMC: output

Let us have a look at the output:

```
str(ans)
#> List of 12
#>  $ with.sampling: logi TRUE
#>  $ time         : 'difftime' num 0.39043402671814
#>   ..- attr(*, "units")= chr "secs"
#>  $ dlu          :Classes 'data.table' and 'data.frame':  4 obs. of  3 variables:
#>   ..$ WHO              : Factor w/ 2 levels "TR_SAMPLING_CATEGORY",..: 1 1 2 2
#>   ..$ SAMPLING_CATEGORY: num [1:4] 1 2 1 2
#>   ..$ UPDATE_ID        : int [1:4] 1 2 3 4
#>   ..- attr(*, ".internal.selfref")=<externalptr>
#>   ..- attr(*, "sorted")= chr "UPDATE_ID"
#>  $ dl           :Classes 'data.table' and 'data.frame':  8 obs. of  4 variables:
#>   ..$ WHO              : Factor w/ 2 levels "TR_SAMPLING_CATEGORY",..: 1 1 1 1 2 2 2 2
#>   ..$ SAMPLING_CATEGORY: num [1:8] 1 1 2 2 1 1 2 2
#>   ..$ UPDATE_ID        : int [1:8] 1 1 2 2 3 3 4 4
#>   ..$ TRM_CAT_PAIR_ID  : int [1:8] 1 2 3 4 1 3 2 4
#>   ..- attr(*, ".internal.selfref")=<externalptr>
#>   ..- attr(*, "sorted")= chr "UPDATE_ID"
#>  $ dlt          :Classes 'data.table' and 'data.frame':  4 obs. of  4 variables:
#>   ..$ TRM_CAT_PAIR_ID: int [1:4] 1 2 3 4
#>   ..$ TR_UPDATE_ID   : int [1:4] 1 1 2 2
#>   ..$ REC_UPDATE_ID  : int [1:4] 3 4 3 4
#>   ..$ TRM_OBS        : int [1:4] 139 15 20 129
#>   ..- attr(*, ".internal.selfref")=<externalptr>
#>   ..- attr(*, "sorted")= chr "TRM_CAT_PAIR_ID"
#>  $ nprior       : int 1000
#>  $ sweep        : int 5
#>  $ nsweep       : num 100
#>  $ n            : num 500
#>  $ pars         :List of 9
#>   ..$ LAMBDA: num [1, 1:4] 0.2 0.2 0.2 0.2
#>   ..$ XI    : num [1:101, 1:4] 0.603 0.603 0.591 0.591 0.591 ...
#>   ..$ XI_LP : num [1:101, 1:4] 3.56 3.56 3.24 3.24 3.24 ...
#>   ..$ S     : num [1:101, 1:4] 0.368 0.368 0.36 0.355 0.355 ...
#>   ..$ S_LP  : num [1:101, 1:4] 6.74 6.74 6.42 6.82 6.82 ...
#>   ..$ Z     : int [1:101, 1:4] 366 366 381 361 361 345 345 333 333 333 ...
#>   ..$ NU    : num 1102
#>   ..$ N     : int [1:101, 1] 1226 1113 1183 1113 1104 1088 1100 1154 1108 1108 ...
#>   ..$ PI    : num [1:101, 1:4] 0.303 0.299 0.337 0.305 0.316 ...
#>  $ it.info      :Classes 'data.table' and 'data.frame':  501 obs. of  7 variables:
#>   ..$ IT       : int [1:501] 0 1 2 3 4 5 6 7 8 9 ...
#>   ..$ PAR_ID   : int [1:501] 0 1 2 3 4 NA 1 2 3 4 ...
#>   ..$ BLOCK    : chr [1:501] "INIT" "S-Z-N" "S-Z-N" "S-Z-N" ...
```

```
#>   ..$ MHRATIO  : num [1:501] 1 0.012701 1 0.000414 0.000642 ...
#>   ..$ ACCEPT   : int [1:501] 1 0 1 0 0 1 1 1 0 0 ...
#>   ..$ LOG_LKL  : num [1:501] -26.7 -26.7 -23.5 -23.5 -23.5 ...
#>   ..$ LOG_PRIOR: num [1:501] 29 29 35.2 35.2 35.2 ...
#>   ..- attr(*, ".internal.selfref")=<externalptr>
#>  $ curr.it      : int 501
```

We are mostly interested in the joint posterior distribution

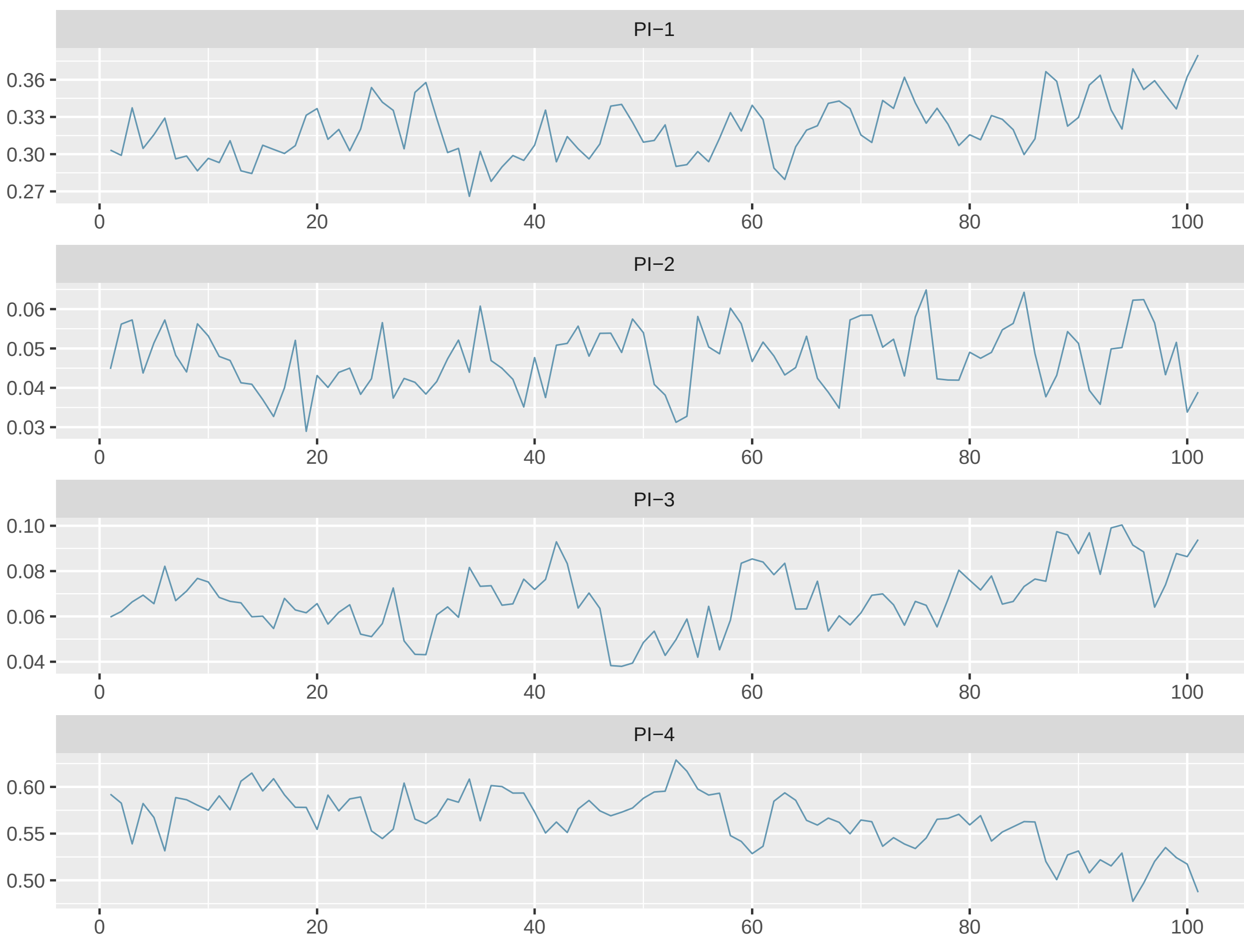
$$p(\pi|n),$$

which is just a component of the entire posterior distribution of all parameters

$$p(\pi, z, Z, \xi, s|n).$$

So let us look at just this component in the output, and make a trace plot:

```
post.pi <- ans[['pars']][['PI']]
colnames(post.pi) <- paste0('PI-',1:ncol(post.pi))
bayesplot:::mcmc_trace(post.pi, pars=colnames(post.pi), facet_args = list(ncol = 1), n_warmup=0)
```



Ok, fab. Of course we would like many more iterations, perhaps $10,000$ sweeps are a good number. We can do that. But what really are *PI-1*, *PI-2*, *PI-3*, *PI-4*? The numbers 1-4 are just the values of the transmission pair IDs in `dobs`, `dobs$TRM_CAT_PAIR_ID`. So we can associate more interpretable names to the output as follows:

```r
post.pi <- ans[['pars']][['PI']]
setkey(dobs, TRM_CAT_PAIR_ID) #order by pair IDs
post.pi.colnames <- paste0('PI ',dobs$TR_TRM_CATEGORY,'->',dobs$REC_TRM_CATEGORY)
colnames(post.pi) <- post.pi.colnames
bayesplot:::mcmc_trace(post.pi, pars=colnames(post.pi), facet_args = list(ncol = 1), n_warmup=0)
```

That's it for now. Use your usual R wizadry to process the output further, and have a look at the other vignettes.