

## **Instruction Manual**

# **EEMS: a method to visualize patterns of non-stationary isolation by distance**

**Version 0.0.0.9000**

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EEMS is a program to analyze and visualize spatial population structure from geo-referenced genetic samples. EEMS uses the concept of *effective migration* to model the relationship between genetics and geography, and it outputs an estimated *effective migration* surface (hence EEMS) – a visual representation of population structure that highlights regions of higher-than-average and lower-than-average historic gene flow.

## 1 Building the EEMS program

There are two versions of EEMS: `runeems_snps` for SNP data and `runeems_sats` for microsatellite data. The data input format and the EEMS model are somewhat different for SNPs and microsatellites, hence the two versions. However, both versions are compiled with `make`. It takes a slightly different syntax to link a program to the dynamic Boost libraries on a Mac and a Linux machine, so build `runeems_xxxx` by typing `make darwin` on a Mac, or `make linux` on a Linux machine, inside the `src` directory which contains the source code.

### 1.1 Requirements

The EEMS model is implemented in C++ using Eigen for linear algebra computations and Boost for random number generation and the habitat geometry. The Eigen template library can be downloaded from <http://eigen.tuxfamily.org> and the Boost libraries can be downloaded from <http://www.boost.org>. EEMS has been tested with Eigen 3.2.2 and Boost 1\_57.

After downloading Eigen (it does not need installation) and installing Boost, update the variables `EIGEN_INC`, `BOOST_INC`, `BOOST_LIB` in the Makefile.

### 1.2 `runeems_snps`

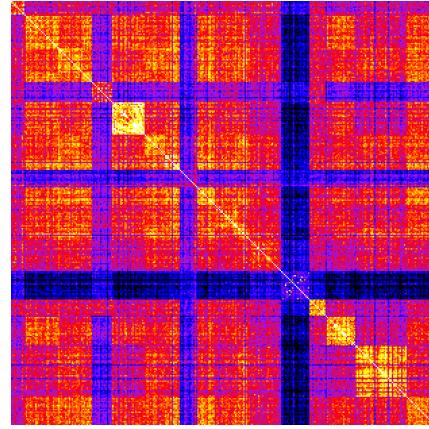
The program `runeems_snps` implements the EEMS method for analyzing spatial population structure. This version uses the pairwise genetic dissimilarity matrix computed from SNP data. The sub-directory `src` contains the C++ source code, which needs to be compiled; `data` contains simulated data generated with `ms` [Hudson, 2002] to illustrate the input file format. The program requires three data input files that have the same file name but different extension. The description below assumes that `datopath` is the full path + the file name (but without the extension).

`datopath.diffs` is the matrix of average pairwise genetic dissimilarities. This can be computed with `bed2diffs` (also available on GitHub) from genetic data in plink binary format. See Figure 1(a). The dissimilarity matrix is nonnegative, symmetric, with 0s on the main diagonal. These conditions are necessary but not sufficient for `diffs` to be a valid dissimilarity matrix. Mathematically, `diffs` should be conditionally negative definite.

`datopath.coord` are the sample coordinates, two coordinates per sample, one sample per line. See Figure 1(b).

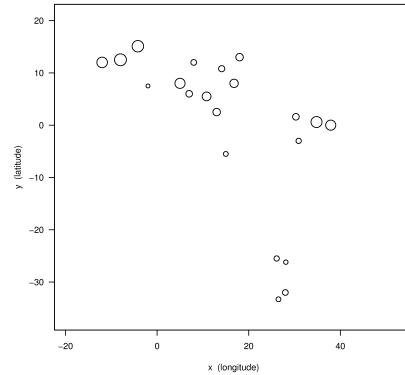
`datopath.outer` are the habitat coordinates, as a sequence of vertices that form a closed polygon. See Figure 1(c).

0	0.656010	0.666522	...
0.656010	0	0.661998	...
0.666522	0.661998	0	...
0.662323	0.652633	0.651595	...
0.675922	0.668446	0.668843	...
...	...	...	...



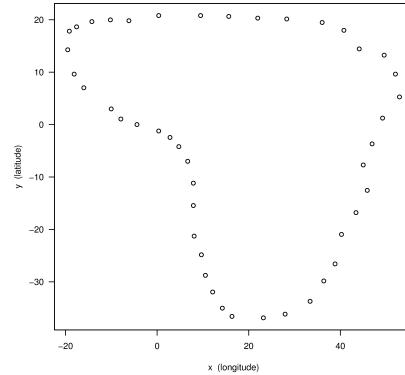
(a) The observed genetic dissimilarity matrix: the top left corner of datapath.diffs on the left and the entire matrix as a heatmap on the right.

30.9	-3.0
30.9	-3.0
30.9	-3.0
30.9	-3.0
30.9	-3.0
...	...



(b) The sample coordinates: the top 5 lines in datapath.coord on the left and the complete sampling scheme on the right. A bigger circle means that more samples are taken from that location.

-18.1	9.6
-16.0	7.0
-10.0	3.0
...	...
-19.2	17.8
-19.5	14.3
-18.1	9.6



(c) The habitat polygon: the top and bottom lines in datapath.outer on the left and the entire habitat outline on the right.

**Figure 1** EEMS requires three data input files. **(a)** datapath.diffs is the observed genetic dissimilarity matrix. There is a lot of population structure in this example and the rows/columns can be ordered to emphasize the pattern further. The ordering, however, is irrelevant to EEMS. **(b)** The sampling locations in datapath.coord should be given in the same order as the rows and columns of the dissimilarity matrix. **(c)** The habitat vertices in datapath.outer should be listed *counterclockwise* and the first vertex should also be the last vertex, so that the outline is a *closed ring*. Otherwise, EEMS attempts to “correct” the polygon and prints a warning message.

### **1.3 `runeems_sats`**

The program `runeems_sats` implements the EEMS method for analyzing spatial population structure. This version uses raw microsatellite data. `runeems_sats` also requires three data input files that have the same file name but different extension.

`datapath.sites` is the matrix of allele copies; missing alleles are specified by any negative number. For  $n$  individuals at  $L$  loci, the `sites` matrix is  $n \times L$  for  $L$  haploid markers and  $n \times 2L$  for  $L$  diploid markers.

`datapath.coord`, `datapath.outer` are the sample and habitat coordinates as described above for SNP data.

## 2 Running the EEMS program

This example shows how to run EEMS on a small simulated dataset (one of the “barrier to migration” datasets used for Figure 2 in the EEMS paper.)

First, copy/create the three input parameter files. All input parameters are the same, except for the output directory `mcmcpath`. Running `runeems_snps` three times will sample – independently – three MCMC chains from the same target distribution: the posterior distribution of the EEMS model parameters.

Here is the first parameter file `params-chain1.ini`:

```
1 datapath = ../data/barrier-schemeZ-nIndiv300-nSites3000
2 mcmcpath = ../data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-nDemes200-chain1
3 nIndiv = 300
4 nSites = 3000
5 nDemes = 200
6 diploid = false
7 numMCMCIter = 2000000
8 numBurnIter = 1000000
9 numThinIter = 9999
```

Then run EEMS (on the command line) with three different random seeds. The argument `--seed` is optional; it can be specified in the parameter file as well, and if not specified, the seed is randomly assigned.

```
1 ./runeems_snps --params params-chain1.ini --seed 123
2 ./runeems_snps --params params-chain2.ini --seed 456
3 ./runeems_snps --params params-chain3.ini --seed 789
```

### 2.1 The EEMS program arguments

There are a number of program parameters that can be set by the user. First, there are several parameters that have to be specified (they have no default values):

- `datapath`: path to the input data. For SNP data, EEMS expects three files: a matrix of average pairwise differences, `datapath.diffs`; a list of sample coordinates, `datapath.coord`; a list of habitat boundary points, `datapath.outer`. For microsatellite data, EEMS also expects three files: a matrix of allele copies, `datapath.sites`; a list of sample coordinates, `datapath.coord`; a list of habitat boundary points, `datapath.outer`.
- `mcmcpath`: path to the output directory. EEMS creates this directory and saves all results there. There is an accompanying R package which parses the output files and generates several figures to visualize the EEMS results. See Section 3.
- `nIndiv` and `nSites`: number of samples and number of markers. For SNP data, the `diffs` matrix is  $n\text{Indiv} \times n\text{Indiv}$  but the input data files do not otherwise contain information about `nSites`. For microsatellite data, the `sites` matrix is  $n\text{Indiv} \times n\text{Sites}$  if the species is haploid, and  $n\text{Indiv} \times 2n\text{Sites}$  if the species is diploid.

- `numMCMCIter`, `numBurnIter`, `numThinIter`: number of MCMC iterations, number of burn-in iterations to discard at the start, and number of iterations to thin between two writing steps.
- `nDemes`: the (approximate) number of demes in the population graph. If the habitat is irregular, the actual number of demes in the grid might not be exactly equal to the specified number of demes. See Figure 3. Alternatively, instead of `nDemes`, specify `gridpath` where the file `gridpath.demes` is a list of demes, the file `gridpath.edges` is a list of edges and `gridpath.ipmap` is a mapping which assigns samples to demes. See Section 2.2.

EEMS assumes that the samples come from a diploid species [`diploid = true`, which is the default] or a haploid species [`diploid = false`]. The difference is only in how the matrix of expected genetic dissimilarity is scaled. See Section S1.2 in the supplement of the EEMS paper.

Further, there are several extra parameters that can be specified optionally (they have default values but modifying those values could improve convergence).

- Variances for the proposal distributions of migration parameters:
  - `mEffctProposals2`: proposal variance for the migration cell effects,  $e_1, \dots, e_{C_m}$ . Defaults to 0.1.
  - `mSeedsProposals2`: proposal variance for the migration cell locations,  $s_1, \dots, s_{C_m}$ . Defaults to 0.01.
  - `mrateMuProposals2`: proposal variance for the overall migration rate  $\mu$  (on the  $\log_{10}$  scale). Defaults to 0.01.
- Variances for the proposal distributions of diversity parameters:
  - `qEffctProposals2`: proposal variance for the diversity cell effects,  $f_1, \dots, f_{C_q}$ . Defaults to 0.001.
  - `qSeedsProposals2`: proposal variance for the diversity cell locations,  $t_1, \dots, t_{C_q}$ . Defaults to 0.1.
- Variance for the proposal distribution on the degrees of freedom:
  - `dfProposals2`: only relevant for SNP data and thus only used in `runeems_snps`. The default value is the square root of the number of markers `nSites`. For microsatellite data, the degrees of freedom are equal to the number of loci.
- Hyperparameters:
  - `mrateShape`, `mrateScale`: (inverse gamma) hyperparameters for the variance  $\omega_m^2$  of the migration effects. Default to 0.001 and 1, respectively.
  - `qrateShape`, `qrateScale`: (inverse gamma) hyperparameters for the variance  $\omega_q^2$  of the diversity effects. Default to 0.001 and 1, respectively.
  - `s2locShape`, `s2locShape`: (inverse gamma) hyperparameters for the scale parameters  $\sigma_1^2, \dots, \sigma_p^2$ . Default to 0.001 and 1, respectively.
  - `negBiSize`: number of failures for the Negative-Binomial prior on the number of Voronoi tiles. Defaults to 10.

- negBiProb: success probability for the Negative-Binomial prior on the number of Voronoi tiles.  
Defaults to 0.67.

For all datasets analyzed in the EEMS paper, we used the default hyperparameter values and we tuned the proposal variances. Choosing values for the proposal variances is something of a dark art – the goal is to choose the parameters so that proposals are accepted about 20% – 30% of the time. In practice, it seems to be sufficient to choose the variances so that proposals are not accepted too rarely (less than 10% of the time) or too often (more than 40% of the time).

Suppose that we run EEMS (say, with the default values for all proposal distributions) and at the end EEMS reports the following information about the frequency of accepting proposals of different types.

```

1 (2050/2593) = 79.06% for type "qTileRate"          ## change the rate of one tile in the diversity tessellation
2 (1414/2478) = 57.06% for type "qTileMove"        ## move the seed of one tile in the diversity tessellation
3 (1047/2494) = 41.98% for type "qBirthDeath"       ## add/remove one tile in the diversity tessellation
4 (20625/47530) = 43.39% for type "mTileRate"       ## change the rate of one tile in the migration tessellation
5 (15486/50098) = 30.91% for type "mMeanRate"        ## change the overall log10 migration rate
6 (22352/47532) = 47.03% for type "mTileMove"        ## move the seed of one tile in the migration tessellation
7 (26305/47275) = 55.64% for type "mBirthDeath"      ## add/remove one tile in the migration tessellation

```

It seems that the qTileRate and qTileMove are accepted too often. So it might be a good idea to increase qEffectProposals2 and qSeedsProposals2. [If the proposal variance is higher, then bigger changes/moves will be proposed and hence the updates will be accepted less often.]

Finally, the parameter qVoronoiPr specifies how often to propose updating the diversity Voronoi tessellation. Its default value is 0.05, which means that about 5% of the time the proposals are about the diversity tessellation and about 95% of the time the proposals are about the migration tessellation.

## 2.2 Specifying the population grid

The population graph is a triangular grid contained entirely inside the habitat. The user specifies its density as a number of demes, nDemes, and EEMS constructs a grid with about the same number of demes which fills the habitat. This procedure is not necessarily optimal (i.e., it might not cover as much area as possible near the boundaries) and it might be helpful to iterate between refining the habitat specification and the density argument nDemes, to choose a satisfactory grid. [Or even better, since the assignment of samples to demes changes with the grid, run EEMS with slightly different grids to investigates how/whether this changes the results.] See Figure 3 for an illustration. Furthermore, there exists a convenient online tool to draw polygons with Google Maps API, available at <http://www.birdtheme.org/useful/v3tool.html>, that might be useful for outlining an irregularly shaped habitat, in longitude and latitude coordinates.

Alternatively, EEMS can read in the population graph. In this case, there are three necessary files:

- gridpath.demes: list of demes, two coordinates per deme, one deme per row.
- gridpath.edges: list of connected pairs of demes, two indices per edge, one edge per row. Demes are indexed from 1 to  $d$  (where  $d$  is the number of demes in the grid), in the order implied by gridpath.demes, i.e., the deme with index 1 has the coordinates on the 1st row in gridpath.demes.

- `gridpath.ipmap`: list of deme indices which indicate the deme each sample is assigned to. There should be  $n$  rows (where  $n$  is the number of samples), with one row for each sample in `datapath.coord`, in the same order.

The stepping-stone model which generated the simulated data is a  $12 \times 8$  regular triangular grid.

```

1 datapath = ./data/barrier-schemeZ-nIndiv300-nSites3000
2 gridpath = ./data/barrier-schemeZ-nIndiv300-nSites3000
3 mcmcpath = ./data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-true_grid-chain1
4 nIndiv = 300
5 nSites = 3000
6 diploid = false
7 numMCMCIter = 2000000
8 numBurnIter = 1000000
9 numThinIter = 9999

```

The sample and habitat coordinates can be specified either latitude first or longitude first as long as the files `datapath.coord` and `datapath.outer` use the same convention. However, the ordering of the coordinates must be specified when plotting the results; see Section 3.

Finally, the vertices of the population graph (the demes) fall inside the habitat by construction. However, EEMS does not check that the sampling locations fall inside the habitat – instead, each sample is assigned to the closest deme. Therefore, the user should specify a habitat that is sufficiently large to cover all sampling locations.

## 2.3 Restarting the MCMC sampler

Suppose that `runeems_snps` (or `runeems_sats`, if the data is microsatellites) has finished running but the MCMC chain has not converged, as indicated by the posterior trace plot. [Section 3 describes how to generate this plot as well as two other diagnostic figures.]

Rather than initializing the parameter state randomly, the user can restart EEMS from the final parameter state in a previous run, by providing the path to an existing EEMS output directory `prevpath`. The required arguments remain the same. The `datapath`, `nIndiv`, `nSites` are fixed as they describe the dataset, but new values can be chosen for all other arguments, e.g., no burn-in (`numBurnIter = 0`) or a denser grid (with more `nDememes`).

If `mcmcpath` is the same as `prevpath`, then the previous results will be overwritten.

```

1 datapath = ./data/barrier-schemeZ-nIndiv300-nSites3000
2 prevpath = ./data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-nDememes200-chain1
3 mcmcpath = ./data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-nDememes200-chain1
4 nIndiv = 300
5 nSites = 3000
6 nDememes = 200
7 diploid = false
8 numMCMCIter = 1000000
9 numBurnIter = 0

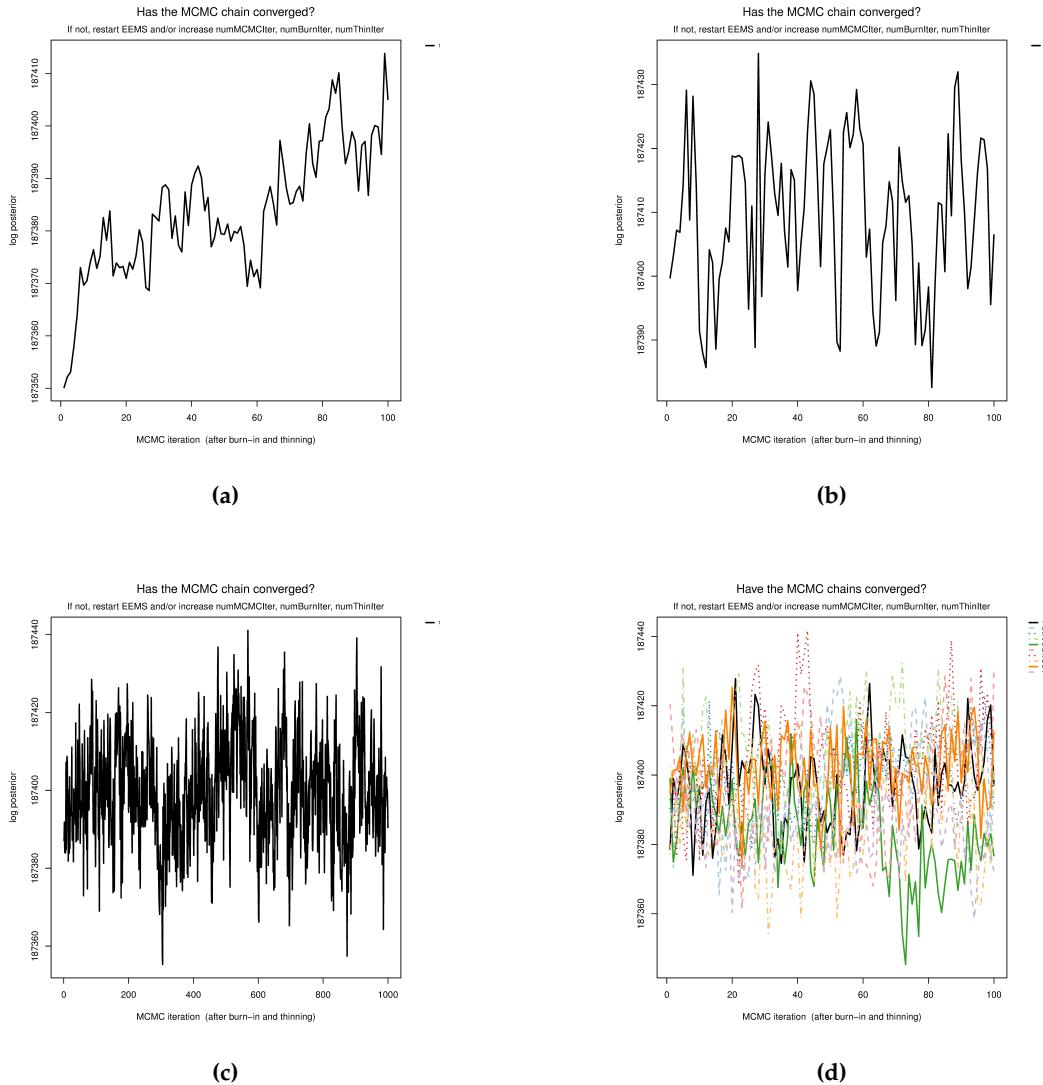
```

```
10 numThinIter = 9999
```

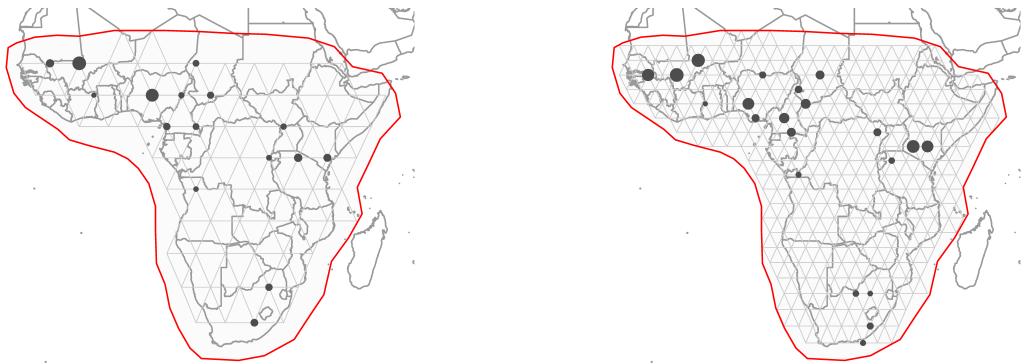
If `mcmcpath` is different from `prevpath`, then the previous results will not be overwritten.

```
1 datapath = ../data/barrier-schemeZ-nIndiv300-nSites3000
2 prevpath = ../data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-nDemes200-chain1
3 mcmcpath = ../data/barrier-schemeZ-nIndiv300-nSites3000-EEMS-nDemes200-chain1.1
4 nIndiv = 300
5 nSites = 3000
6 nDemes = 200
7 diploid = false
8 numMCMCIter = 1000000
9 numBurnIter = 0
10 numThinIter = 9999
```

After running EEMS (either `runeems_snps` for SNP data or `runeems_sats` for microsatellite data), the next step to visualize the results.

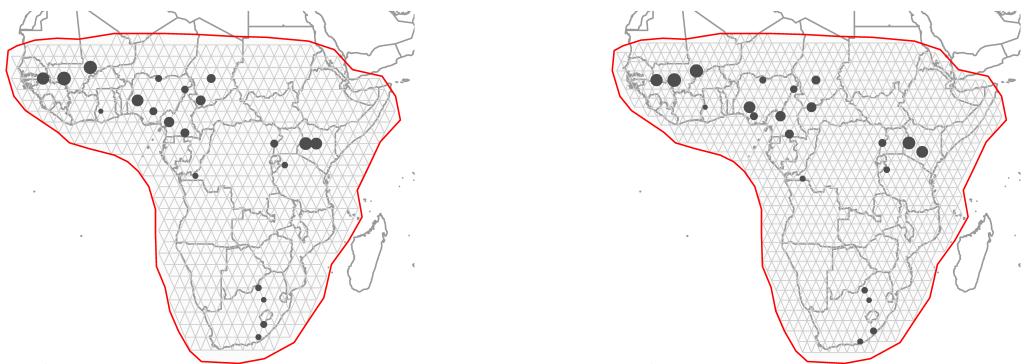


**Figure 2** The `eems.plots` function in the `rEEMSpplots` package generates a posterior trace plot. **(a)** This MCMC chain obviously has not converged. **(b)** There is no indication that the MCMC chain has not converged. This is not quite the same as there is evidence that the MCMC chain has converged. **(c)** To be confident that EEMS has converged, we can run the MCMC sampler for more iterations. **(d)** Alternatively, to be confident that EEMS has converged, we can run the MCMC sampler several times, each time starting from a different randomly initialized parameter state.



(a) nDemes = 100 (There are 75 vertices.)

(b) nDemes = 400 (There are 358 vertices.)



(c) nDemes = 700 (There are 651 vertices.)

(d) nDemes = 1000 (There are 927 vertices.)

**Figure 3** Given the grid density parameter, nDemes, EEMS automatically generates a triangular grid, which is contained entirely inside the habitat. Then EEMS assigns each sample to its closest deme. Here the habitat is outlined in red. [The outline was created, as a “polyline”, with a convenient online tool from Google, available at <http://www.birdtheme.org/useful/v3tool.html>.] A higher value for nDemes produces a denser grid, and a denser grid means a more flexible EEMS model because, with more vertices and edges, there are more rate parameters in the model. However, the computational cost of running EEMS increases as well.

### 3 Plotting the EEMS results

First install the R package `rEEMSpots` which provides the function `eems.plots`. It is not on CRAN, so install it from source instead.

```
1 ## Check that the current directory contains the rEEMSpots source directory (from GitHub)
2 if (dir.exists("rEEMSpots")) {
3   install.packages("rEEMSpots", repos = NULL, type = "source")
4 } else {
5   stop("Move to the directory that contains the rEEMSpots source to install the package.")
6 }
```

`rEEMSpots` provides one main function, with a variety of options. I will use an example to demonstrate those options.

```
1 # Use the provided example or supply the path to your own EEMS run.
2 exdata_path <- system.file("exdata", package = "rEEMSpots")
3 eems_results <- file.path(exdata_path, "EEMS-example")
4 name_figures <- file.path(path.expand("~/"), "EEMS-example")
5
6 if (!file.exists(eems_results)) {
7   stop("Check that the rEEMSpots package is installed without errors.")
8 }
```

You can see all these examples in the documentation of the `eems.plots` by typing

```
1 library("rEEMSpots")
2 ?eems.plots
```

in the R console.

#### 3.1 Required arguments

1. `mcmcpath` is a list of EEMS output directories, for the same dataset. It can be a single directory but it is better to run EEMS several times, randomly initializing the MCMC chain each time. [In other words, it is a good idea to simulate several realizations of the Markov chain, each realization starting with a different value of the EEMS parameters.] Warning: There is minimal checking that all directories in the list are for the same dataset.
2. `plotpath` is the full path + the file name for the graphics to be generated. There are several output figures:
  - `plotpath- $\text{mrates}$ 01` is a contour plot of estimated effective migration rates.
  - `plotpath- $\text{qrates}$ 01` is a contour plot of estimated effective diversity rates.
  - `plotpath- $\text{rdist}$ 01` is a scatter plot of observed vs fitted genetic dissimilarities between demes.
  - `plotpath- $\text{rdist}$ 02` is a scatter plot of observed vs fitted genetic dissimilarities within demes.
  - `plotpath- $\text{rdist}$ 03` is a scatter plot of genetic dissimilarities vs geographic distances between demes.
  - `plotpath- $\text{pilog}$ 01` is a posterior probability trace plot.

The contour plots visualize the estimated effective migration and diversity rates and provide insight into spatial patterns of genetic variation. The diagnostic scatter plots are useful for checking whether the EEMS model fits the data well; see Figure 14. The posterior trace plot is helpful for checking whether the MCMC sampler has converged; see Figure 2.

3. `longlat` specifies whether coordinates are given as pairs (longitude, latitude) or (latitude, longitude). In the former case, `longlat = TRUE`, and in the latter case, `longlat = FALSE`. [More generally, the coordinates are ordered pairs of numbers. Almost all plotting options are valid for general coordinates, except for the options to specify the projection and to add the geographic map.] Compare Figures 5 and 7 for the difference between `longlat = TRUE` and `longlat = FALSE`.

I will use a geo-referenced dataset of African elephant samples that were collected and genotyped as part of a large collaborative study to develop assignment methods for determining the geographic origin of elephant samples from across Sub-Saharan Africa [Wasser et al., 2004, Wasser et al., 2008, Wasser et al., 2015].

Figure 5 shows the figures produced by `eems.plots` when only the three required arguments are specified.

```
1 ## Produce the five EEMS figures, with default values for all optional parameters.
2 eems.plots(mcmcpath = eems_results,
3             plotpath = paste0(name_figures, "-default"),
4             longlat = TRUE)
```

Passing `longlat = FALSE` instead of `longlat = TRUE` has the effect of flipping the *x*-axis and the *y*-axis – compare Figures 5(a) and 5(b) to Figures 7(a) and 7(b). It is particularly important to specify this argument correctly if adding a geographic map to the migration and diversity contour plots. [That's why `longlat` is a required, not an optional argument.]

```
1 ## Flip the x and y axis, i.e., assume that the x coordinate is the latitude
2 ## and the y coordinate is the longitude.
3 eems.plots(mcmcpath = eems_results,
4             plotpath = paste0(name_figures, "-axes-flipped"),
5             longlat = FALSE)
```

## 3.2 Optional arguments about the graphics format

`eems.plots` generates output graphics as either PNGs (the default) or PDFs. [PNGs are generated with the `bitmap` function which requires `ghostscript`.]

- `plot.height/plot.width`: dimensions of the display region, in inches.
- `out.png`: TRUE or FALSE, specifies whether to generate PNGs or PDFs.
- `res`: resolution, in dots per inch, only relevant if the output is PNG graphics. The default is 600.

```
1 ## Generate PNG figures with height 9 inches, width 8 inches
2 ## and resolution 600 dots per inch.
3 eems.plots(mcmcpath = eems_results,
```

```

4     plotpath = paste0(name_figures, "-output-PNGs"),
5     longlat = TRUE,
6     plot.height = 8,
7     plot.width = 7,
8     res = 600,
9     out.png = TRUE)
10
11 ## Generate PDF figures with height 9 inches and width 8 inches.
12 ## The resolution option, res, is ignored.
13 eems.plots(mcmcpath = eems_results,
14             plotpath = paste0(name_figures, "-output-PDFs"),
15             longlat = TRUE,
16             plot.height = 8,
17             plot.width = 7,
18             res = 600,
19             out.png = FALSE)

```

### 3.3 Optional arguments about the population grid

- add.grid: TRUE or FALSE, specifies whether to add the population grid or not.
  - col.grid: the color of the grid (default is gray80)
  - lwd.grid: the line width (default is 1)
- add.outline: TRUE or FALSE, specifies whether to add the habitat outline or not.
  - col.outline: the color of the outline (default is white)
  - lwd.outline: the line width (default is 2)
- add.demes: TRUE or FALSE, specifies whether to add the observed demes or not.
  - col.demes: the color of the demes (default is black)
  - pch.demes: the symbol/character used for plotting the demes (default is 19)
  - min.cex.demes: the minimum size of the deme symbol/character (default is 1)
  - max.cex.demes: the maximum size of the deme symbol/character (default is 3)

The unusual options are `min.cex.demes` and `max.cex.demes`. If `max.cex.demes > min.cex.demes`, then demes with more samples also have bigger size: the deme with the fewest samples has size `min.cex.demes` and the deme with the most samples has size `max.cex.demes`. So if the sampling is uneven, then `max.cex.demes > min.cex.demes` underlines this fact. See Figure 8 for an example.

```

1 ## Choose somewhat impractical colors and shapes for the outline, the grid and the demes.
2 eems.plots(mcmcpath = eems_results,
3             plotpath = paste0(name_figures, "-demes-and-edges"),
4             longlat = TRUE,
5             add.grid = TRUE,

```

```

6     col.grid = "gray90",
7     lwd.grid = 2,
8     add.outline = TRUE,
9     col.outline = "blue",
10    lwd.outline = 5,
11    add.demes = TRUE,
12    col.demes = "red",
13    pch.demes = 5,
14    min.cex.demes = 0.5,
15    max.cex.demes = 1.5)

```

### 3.4 Optional arguments about the cartographic projection

If we know the projection of the input coordinates and the R package `rgdal` is installed, then we can plot the effective migration and diversity surfaces in another projection. See Figure 9 for an example.

- `projection.in`: input projection, as a valid PROJ.4 string.
- `projection.out`: output projection, as a valid PROJ.4 string.

```

1 library("rgdal")
2 projection_none <- "+proj=longlat +datum=WGS84"
3 projection_mercator <- "+proj=merc +datum=WGS84"
4
5 ## Produce contour plots in the Mercator projection (used by Google Maps)
6 eems.plots(mcmcpath = eems_results,
7             plotpath = paste0(name_figures, "-cartographic-projections"),
8             longlat = TRUE,
9             projection.in = projection_none,
10            projection.out = projection_mercator)

```

### 3.5 Optional arguments about the geographic map

If we know the projection of the input coordinates and the R packages `rgdal`, `rworldmap`, `rworldxtra` are installed, then we can add a geographic map to the two contour plots. See Figure 10 for an example.

- `add.map`: TRUE or FALSE, specifies whether to add a geographic map or not.
- `col.map`: the color of the map (default is gray60)
- `lwd.map`: the line width (default is 2)

```

1 library("rworldmap")
2 library("rworldxtra")
3
4 ## Add a high-resolution geographic map

```

```

5 eems.plots(mcmcpath = eems_results,
6   plotpath = paste0(name_figures, "-geographic-map"),
7   longlat = TRUE,
8   projection.in = projection_none,
9   projection.out = projection_mercator,
10  add.map = TRUE,
11  col.map = "black",
12  lwd.map = 5)

```

### 3.6 Optional arguments about the color scheme

Finally, we can also specify the color palette as a vector of colors, `eems.plot`, ordered from low to high. See Figure 11 for an example.

```

1 library("RColorBrewer")
2
3 ## Use a divergent Red to Blue color scheme from the RColorBrewer package
4 ## instead of the default DarkOrange to Blue color scheme.
5 eems.plots(mcmcpath = eems_results,
6   plotpath = paste0(name_figures, "-new-eems-colors"),
7   longlat = TRUE,
8   eems.colors = brewer.pal(11, "RdBu"))

```

### 3.7 Add arbitrary graphical elements (points, lines, etc)

We can add an arbitrary collection of graphical elements on top of the contour plot. See Figure 12 for an example.

- `m.plot.xy`: add to migration plot.
- `q.plot.xy`: add to diversity plot.

Important note: Those elements should be in the same projection as the migration/diversity surfaces.

```

1 library("rgdal")      ## Defines functions to transform spatial elements
2 library("rworldmap") ## Defines world map
3
4 projection_none <- "+proj=longlat +datum=WGS84"
5 projection_mercator <- "+proj=merc +datum=WGS84"
6
7 ## Add the map of Africa explicitly by passing the shape file
8 map_world <- getMap()
9 map_africa <- map_world[which(map_world@data$continent == "Africa"), ]
10 eems.plots(mcmcpath = eems_results,
11   plotpath = paste0(name_figures, "-shapefile"),
12   longlat = TRUE,
13   m.plot.xy = { plot(map_africa, col = NA, add = TRUE) },

```

```

14     q.plot.xy = { plot(map_africa, col = NA, add = TRUE) })
15
16 ## Apply the Mercator projection and add the map of Africa
17 ## Don't forget to apply the same projection to the map as well
18 map_africa <- spTransform(map_africa, CRSobj = CRS(projection_mercator))
19 eems.plots(mcmcpath = eems_results,
20             plotpath = paste0(name_figures, "-shapefile-projected"),
21             longlat = TRUE,
22             projection.in = projection_none,
23             projection.out = projection_mercator,
24             m.plot.xy = { plot(map_africa, col = NA, add = TRUE) },
25             q.plot.xy = { plot(map_africa, col = NA, add = TRUE) })
26
27 ## Similarly we can add points, lines, labels, etc.
28 ## Here is how to add a set of colored "labels" on top of the
29 ## migration/diversity rates and the Africa map
30 coords <- matrix(c(-10, 10,
31                     10, 10,
32                     30, 0,
33                     40, -10,
34                     30, -20), ncol = 2, byrow = TRUE)
35 colors <- c("red", "green", "blue", "purple", "orange")
36 labels <- LETTERS[1:5]
37 coords_merc <- sp::spTransform(SpatialPoints(coords, CRS(projection_none)),
38                                 CRS(projection_mercator))
39 ## `coords_merc` is a SpatialPoints structure
40 ## but we only need the coordinates themselves
41 coords_merc <- coords_merc@coords
42
43 eems.plots(mcmcpath = eems_results,
44             plotpath = paste0(name_figures, "-labels-projected"),
45             longlat = TRUE,
46             projection.in = projection_none,
47             projection.out = projection_mercator,
48             m.plot.xy = { plot(map_africa, col = NA, add = TRUE);
49                         text(coords_merc, col = colors, pch = labels, font = 2); },
50             q.plot.xy = { plot(map_africa, col = NA, add = TRUE);
51                         text(coords_merc, col = colors, pch = labels, font = 2); })

```

### 3.8 A test function to generate Voronoi diagrams

Given one EEMS output directory, the function `eems.voronoi.samples`, also available in the `rEEMSplots` package, produces Voronoi diagrams drawn from the posterior distribution of the rate parameters: there is one series of tessellations for the effective migration rates and another series for the effective diversity rates. Both series contain one figure for each saved MCMC iteration, after burn-in and thinning. Warning: `eems.voronoi.samples` potentially generates a large number of figures. See Figure 13 for a small example.

```
1 # Use the provided example or supply the path to your own EEMS run.
2 extdata_path <- system.file("extdata", package = "rEEMSpLOTS")
3 eems_results <- file.path(extdata_path, "EEMS-example")
4 name_figures <- file.path(path.expand("~/"), "EEMS-example")
5
6 library("deldir")
7
8 ## Plot a series of Voronoi diagrams for the EEMS model parameters:
9 ## the effective migration rates (m) and the effective diversity rates (q).
10 eems.voronoi.samples(mcmcpath = eems_results,
11                       plotpath = paste0(name_figures, "-voronoi-diagrams"),
12                       longlat = TRUE, post.draws = 10)
```

## 4 Observed vs fitted dissimilarities

EEMS aims to model the genetic differentiation between individuals in space. To achieve this, EEMS constructs a triangular grid, assigns each sample to its closest vertex (deme) and estimates a migration rate for every edge and a diversity rate for every vertex in the grid. See Figures 4(a) and 4(b).

To be specific, consider two different demes  $\alpha$  and  $\beta$ . Suppose that individual  $i$  is assigned to deme  $\alpha$ , which we denote by  $\delta(i) = \alpha$ . Similarly, suppose that  $\delta(i^*) = \alpha$  but  $i$  and  $i^*$  are distinct individuals, that  $\delta(j) = \beta$  and  $\delta(j^*) = \beta$  but  $j$  and  $j^*$  are distinct individuals. Of course,  $i$  and  $j$  are distinct because they come from different demes.

In EEMS, the observed genetic dissimilarity is the average squared genetic difference, across  $p$  markers:

$$D_{ij} = \frac{1}{p} \sum_{k=1}^p (Z_{ik} - Z_{jk})^2, \quad (1)$$

where  $Z_{ik}, Z_{jk}$  are the genotypes of individuals  $i, j$  at marker  $k$ .

EEMS assumes that individuals in the same deme are exchangeable. Since  $\delta(i) = \delta(i^*) = \alpha$  and  $\delta(j) = \delta(j^*) = \beta$ , exchangeability implies that:

$$\mathbb{E}\{D_{ij}\} = \mathbb{E}\{D_{i^*j}\} = \mathbb{E}\{D_{i^*j}\} = \mathbb{E}\{D_{i^*j^*}\} = \Delta_{\alpha\beta}, \quad \mathbb{E}\{D_{ii^*}\} = \Delta_{\alpha\alpha}, \quad \mathbb{E}\{D_{jj^*}\} = \Delta_{\beta\beta}. \quad (2)$$

That is, the expected genetic dissimilarity between two distinct individuals depends only on their locations. In matrix notation, the observed data is the matrix of average squared genetic differences,  $D = (D_{ij})$ , which is modeled by a *block* matrix of expected genetic dissimilarities,  $\Delta = (\Delta_{\delta(i)\delta(j)}) = (\Delta_{\alpha\beta})$ . Both matrices have a main diagonal of 0s because self-dissimilarity is 0.

EEMS is a spatially explicit model and it is consistent with the following idea: We can expect that  $\langle i, j \rangle$  are more dissimilar than either  $\langle i, i^* \rangle$  or  $\langle j, j^* \rangle$  because  $i$  and  $j$  come from different locations. However, in general, we can't expect  $\langle i, i^* \rangle$  to be as dissimilar as  $\langle j, j^* \rangle$  – there might be some differences in local genetic diversity. And to model the genetic dissimilarity due to migration in space we need to take into account any local variation in genetic diversity. For this reason, EEMS decomposes the genetic dissimilarity into two components, between demes and within demes:

$$\Delta_{\alpha\beta} = \underbrace{\Delta_{\alpha\beta} - (\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2}_{\text{between demes}} + \underbrace{(\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2}_{\text{within demes}}. \quad (3)$$

The within-demes component,  $W$ , characterizes the expected genetic dissimilarity between two distinct individuals from the same deme and is a function of the effective diversity rates:

$$W_\alpha = \Delta_{\alpha\alpha} = g(q_\alpha). \quad (4)$$

Here  $q$  is a vector of effective diversity rates and  $q_\alpha$  is the element that corresponds to deme  $\alpha$ . In Figure 4(c), the diversity parameters are visualized as one point for each vertex in the graph and on the  $\log_{10}$  scale, so that blue indicates higher than average diversity and orange – lower than average diversity. The function  $g$  is the identity.

The between-demes component,  $B$ , characterizes the expected genetic dissimilarity between two individuals from distinct demes and is a function of the effective migration rates. It represents dissimilarity that is due to the spatial structure of the population and is not a consequence of the local diversity in the two demes:

$$B_{\alpha\beta} = \Delta_{\alpha\beta} - (\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2 = f(m)_{\alpha\beta}. \quad (5)$$

Here  $m$  is a sparse matrix that represents an undirected, connected, weighted grid, with weights equal to the effective migration rates between adjacent demes. In Figure 4(d), the migration parameters are visualized as one line segment for each edge in the graph and also on the  $\log_{10}$  scale. The function  $f$  returns the effective resistance distances between vertices in the grid, as a dense matrix, and  $f(m)_{\alpha\beta}$  is the element that corresponds to the pair of demes  $\alpha$  and  $\beta$ .

Therefore, EEMS models expected genetic dissimilarity as:

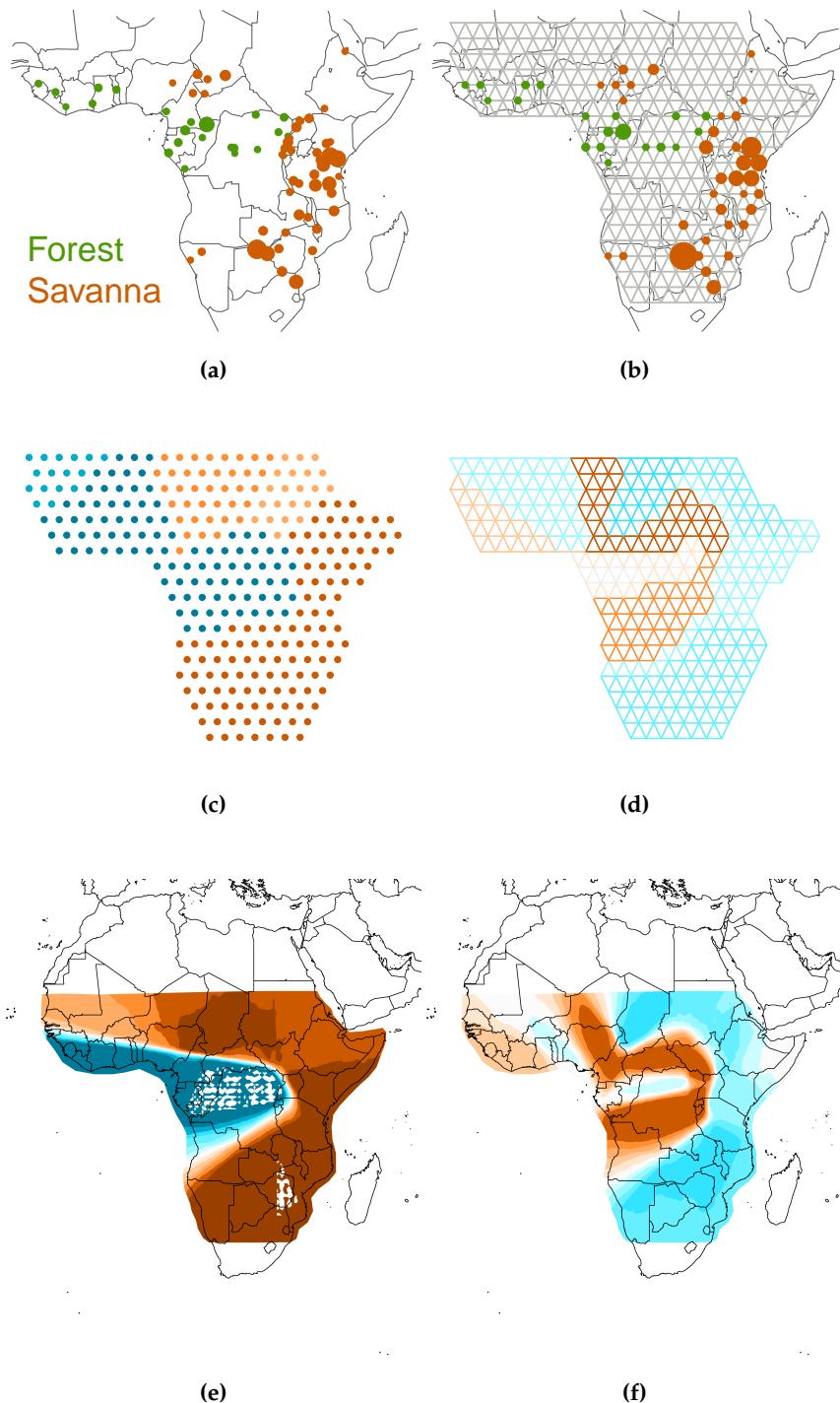
$$\Delta_{\alpha\beta} = \underbrace{\Delta_{\alpha\beta} - (\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2}_{B_{\alpha\beta}} + \underbrace{(\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2}_{(W_\alpha + W_\beta)/2} \quad (6)$$

$$= B_{\alpha\beta} + (W_\alpha + W_\beta)/2. \quad (7)$$

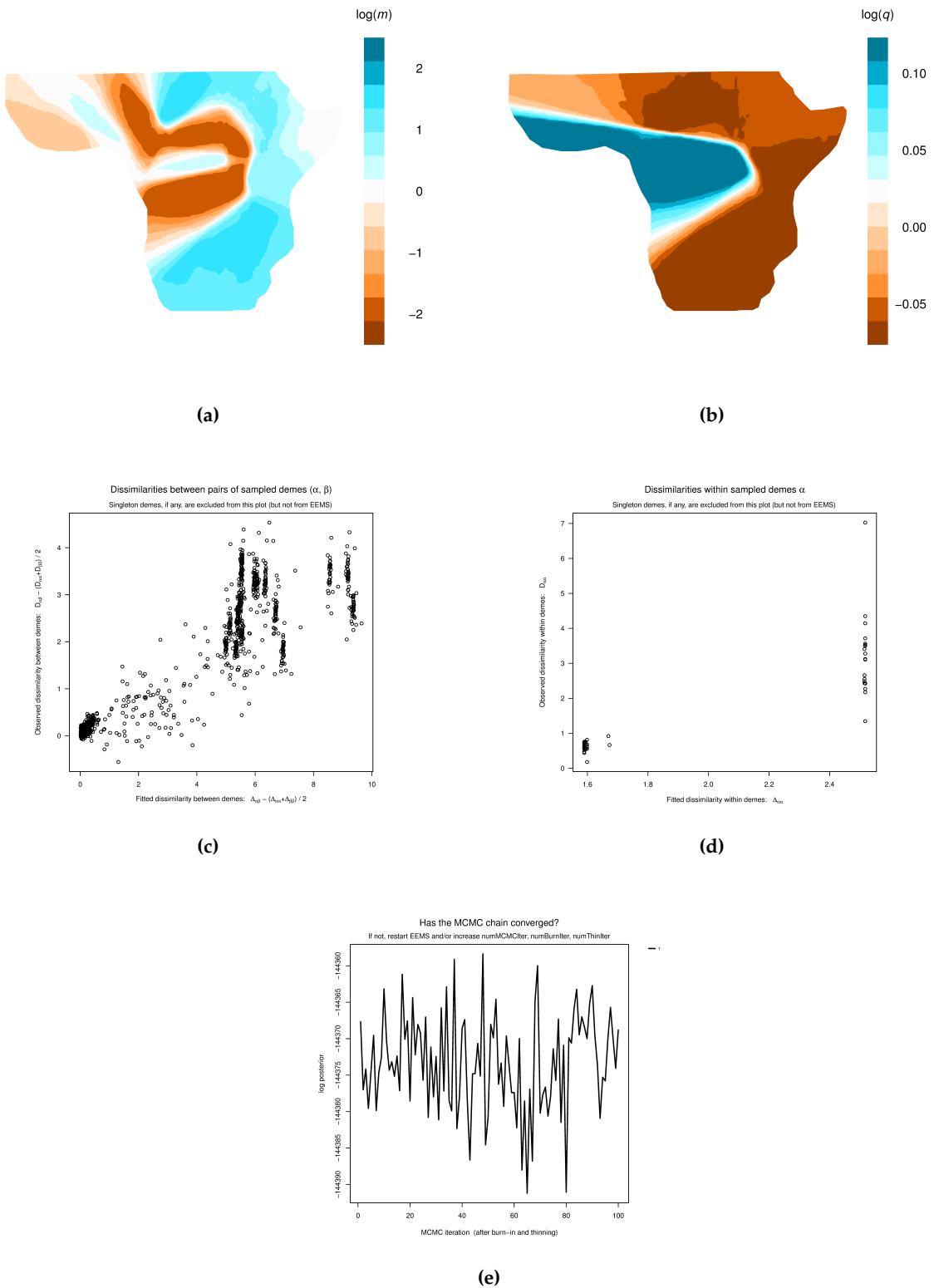
The between-demes component of the genetic dissimilarity is plotted in `plotpath-rdist01`, as a scatter plot of observed vs fitted values. The within-demes component of the genetic dissimilarity is plotted in `plotpath-rdist02`. See Figure 14 for an example. If the EEMS model fits the data well (after the MCMC chain has converged), we expect to see a strong linear relationship between the observed and fitted values in both scatter plots. Therefore, these scatter plots are useful for model-checking diagnostics.

However, once we are reasonably convinced that the EEMS model is appropriate for the data being analyzed, the parameters of the model are of greater interest than the expected dissimilarities, i.e.,  $m$  and  $q$  are more interesting than the deterministic functions  $f(m)$  and  $g(q)$ . Although the parametrized population grid is a discrete model (there are finite number of demes and edges), the estimated parameters are interpolated and plotted as smooth contour maps. The effective migration rates  $m$  are visualized in `plotpath-mrates01`, the effective diversity rates  $q$  are plotted in `plotpath-qrates01`, in both cases on the  $\log_{10}$  scale and after some normalization.

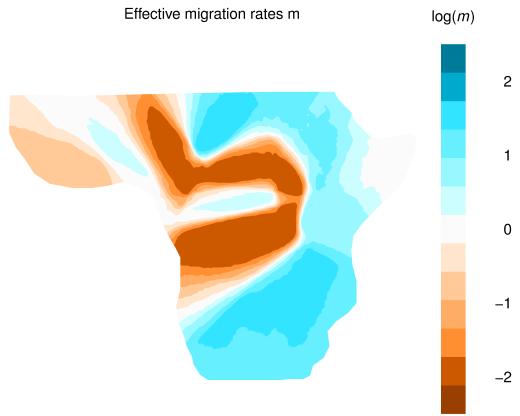
The scatter plot of the observed vs fitted pairwise genetic differences can also be usefully compared with the analogous plot for a “pure isolation by distance” model, as in Figure 14(c), where the observed dissimilarities between demes are plotted against the geographic distances between demes. Isolation by distance would correspond to a white contour plot, with no regional variation in effective migration rates. Colors in the estimated effective migration surface `plotpath-mrates01` correspond to local deviations from isolation by distance: in particular, effective migration is low in geographic regions where genetic similarity decays quickly.



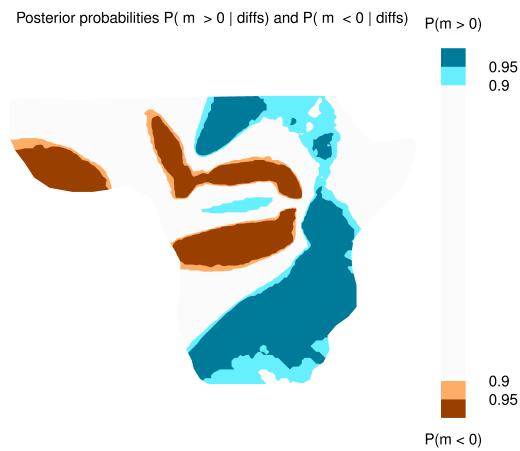
**Figure 4** A schematic overview of the EEMS method, using geo-referenced African elephant data [Wasser et al., 2015] for illustration. **(a)** There are two subspecies – forest and savanna, in green and orange, respectively – and they occupy roughly the east and the west regions. **(b)** First EEMS uses the available geographic information by assigning samples to vertices in a regular triangular grid. EEMS uses two spatial parameters to describe two different aspects of population structure in space. **(c)** Each vertex in the population grid has an effective diversity rate. These parameters quantify the genetic similarity of two individuals from the same location. **(d)** Each edges in the population edge has an effective migration rate. These parameters quantify how genetic similarity decays across space. **(e),(f)** EEMS uses Markov Chain Monte Carlo to estimate the diversity and migration parameters and produces smooth contour maps which represent the posterior mean of effective migration and effective diversity across space.



**Figure 5** The `eems.plots` function in the `rEEMSpplots` package produces several figures. **(a)** Estimated effective migration surface, on the  $\log_{10}$  scale and after mean centering. **(b)** Estimated effective diversity surface, on the  $\log_{10}$  scale and after mean centering. **(c)** Observed vs fitted dissimilarities: between-demes component. See Section 4 for more details. **(d)** Observed vs fitted dissimilarities: within-demes component. See Section 4 for more details. **(e)** Posterior probability trace.



(a)

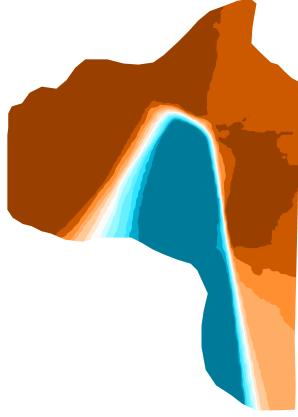


(b)

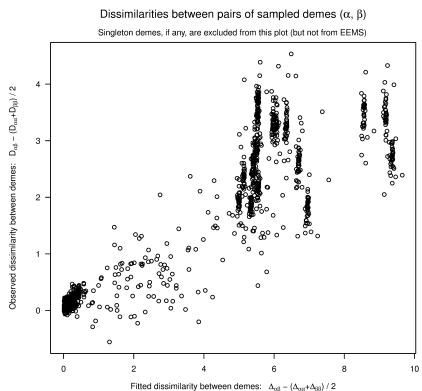
**Figure 6** The eems.plots function in the rEEMSplots package produces several figures (continued). **(a)** Estimated effective migration surface, on the  $\log_{10}$  scale and after mean centering. With this normalization, 0 corresponds to the overall mean migration rate. **(b)** Areas where the posterior probability  $\Pr\{m > 0 | D\}$  exceeds 90% are highlighted in blue, areas where the posterior probability  $\Pr\{m < 0 | D\}$  exceeds 90% are highlighted in orange. This plot emphasizes regions where the effective migration rates are significantly higher/lower than the overall average rate, i.e. “corridors” and “barriers”.



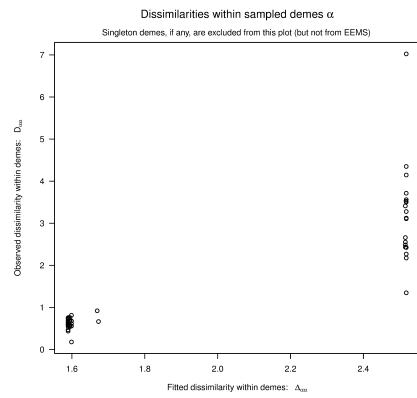
(a)



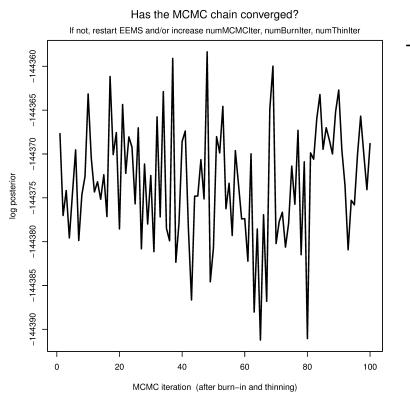
(b)



(c)

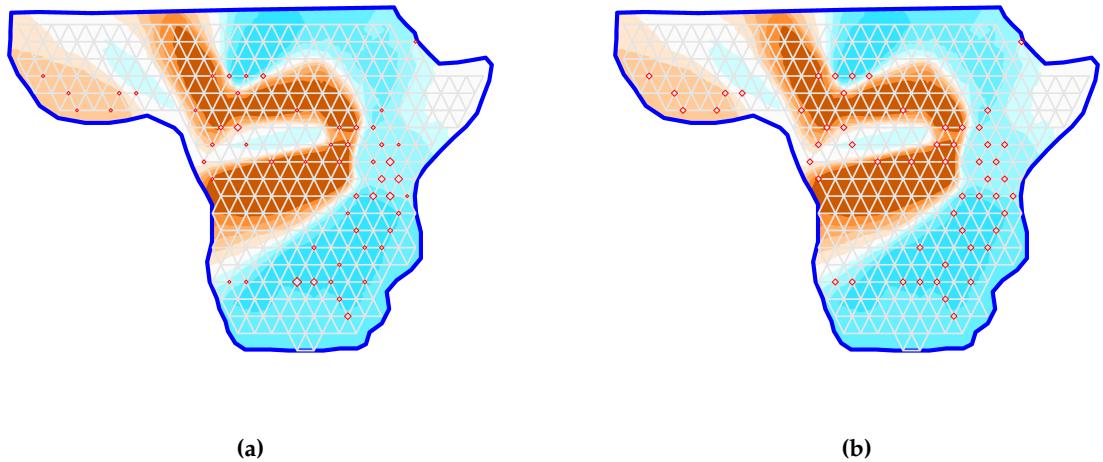


(d)

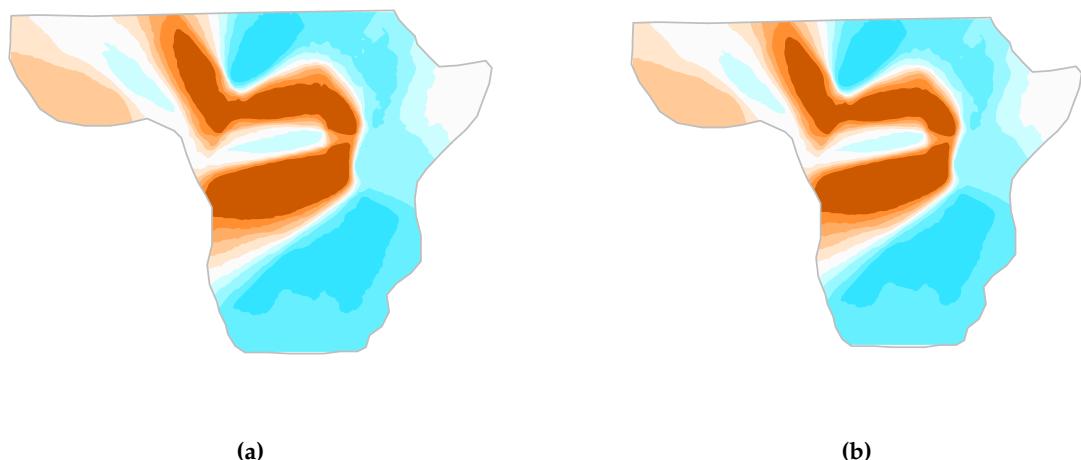


(e)

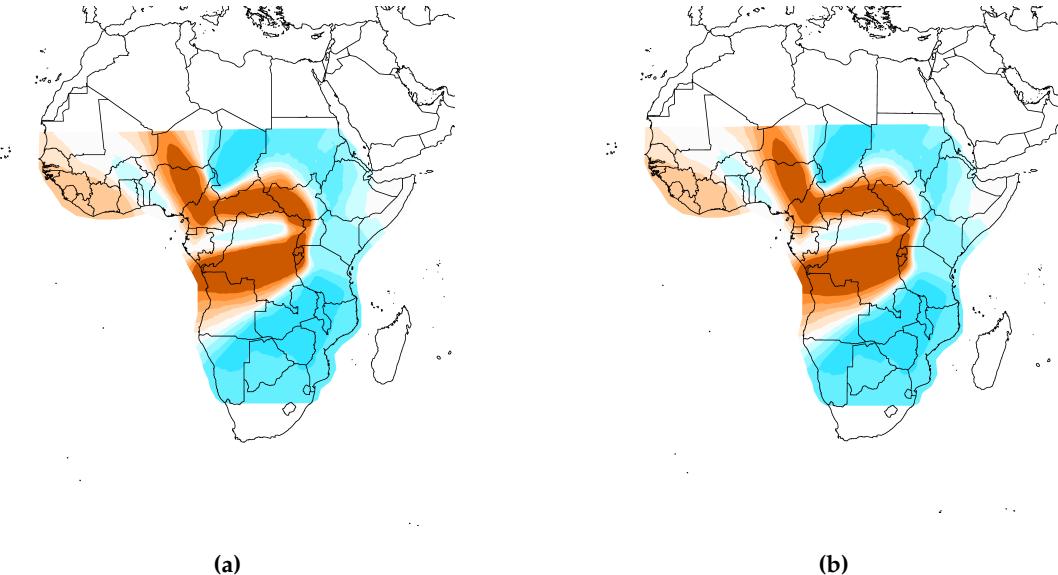
**Figure 7** In EEMS points in the habitat (e.g., the sampling locations, the demes, the tile seeds) are represented as ordered pairs  $(x, y)$ . The  $x$  and  $y$  axes can be flipped with the longlat argument to eems.plots: use longlat = TRUE for the original ordering of the two coordinates and longlat = FALSE to flip them. This changes the migration and the diversity figures, (a) and (b), but not the three diagnostic figures, (c), (d) and (e). In fact, all optional arguments to the plotting function modify only the migration and diversity contour plots.



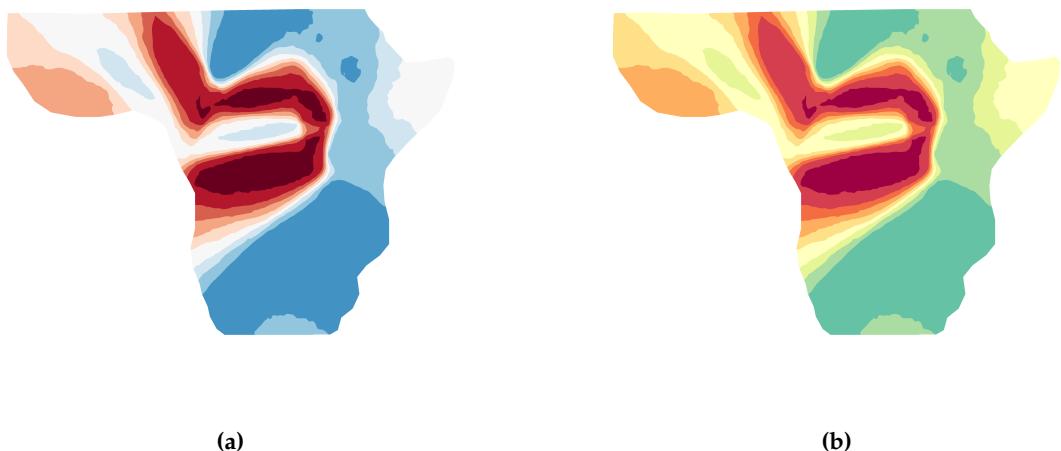
**Figure 8** Use the options `add.grid`, `add.demes`, `add.outline` to add the population grid, the sampled demes and/or the habitat outline. The colors, line width and the symbol/character can all be specified. Most importantly, the arguments `min.cex.demes` and `max.cex.demes` can be used to underline the sampling scheme, so that a deme with more samples is indicated with a larger symbol/character. **(a)** `min.cex.demes = 0.5, max.cex.demes = 1.5`  
**(b)** `min.cex.demes = max.cex.demes = 1`



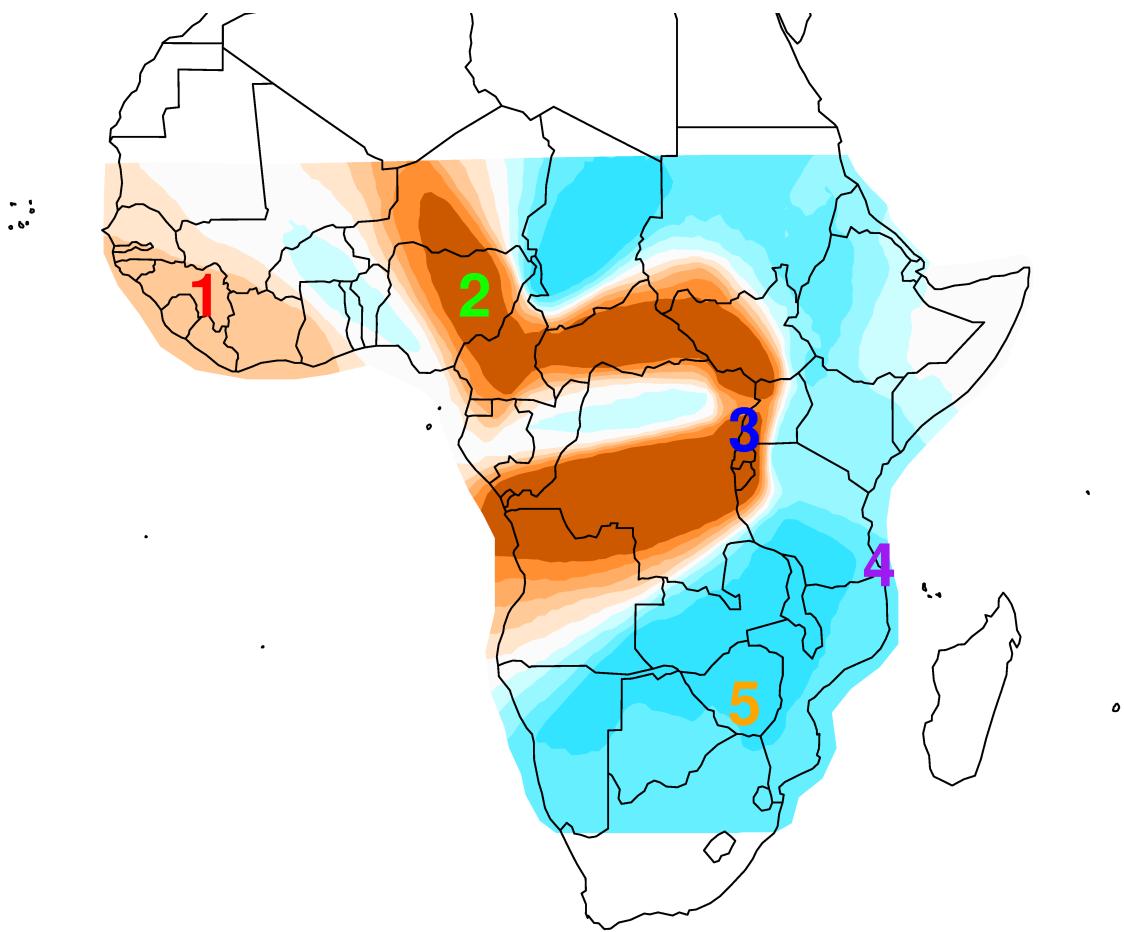
**Figure 9** Use the arguments `projection.in` and `projection.out` to specify the input and output projection, as valid PROJ.4 strings. This requires the `rgdal` package. **(a)** The effective migration surface with longitude and latitude untransformed: `projection.out = "+proj=longlat +datum=WGS84"`. **(b)** The same effective migration surface in the Mercator projection: `projection.out = "+proj=merc +datum=WGS84"`. There is more noticeable difference between the two projections at higher latitudes (away from the equator).



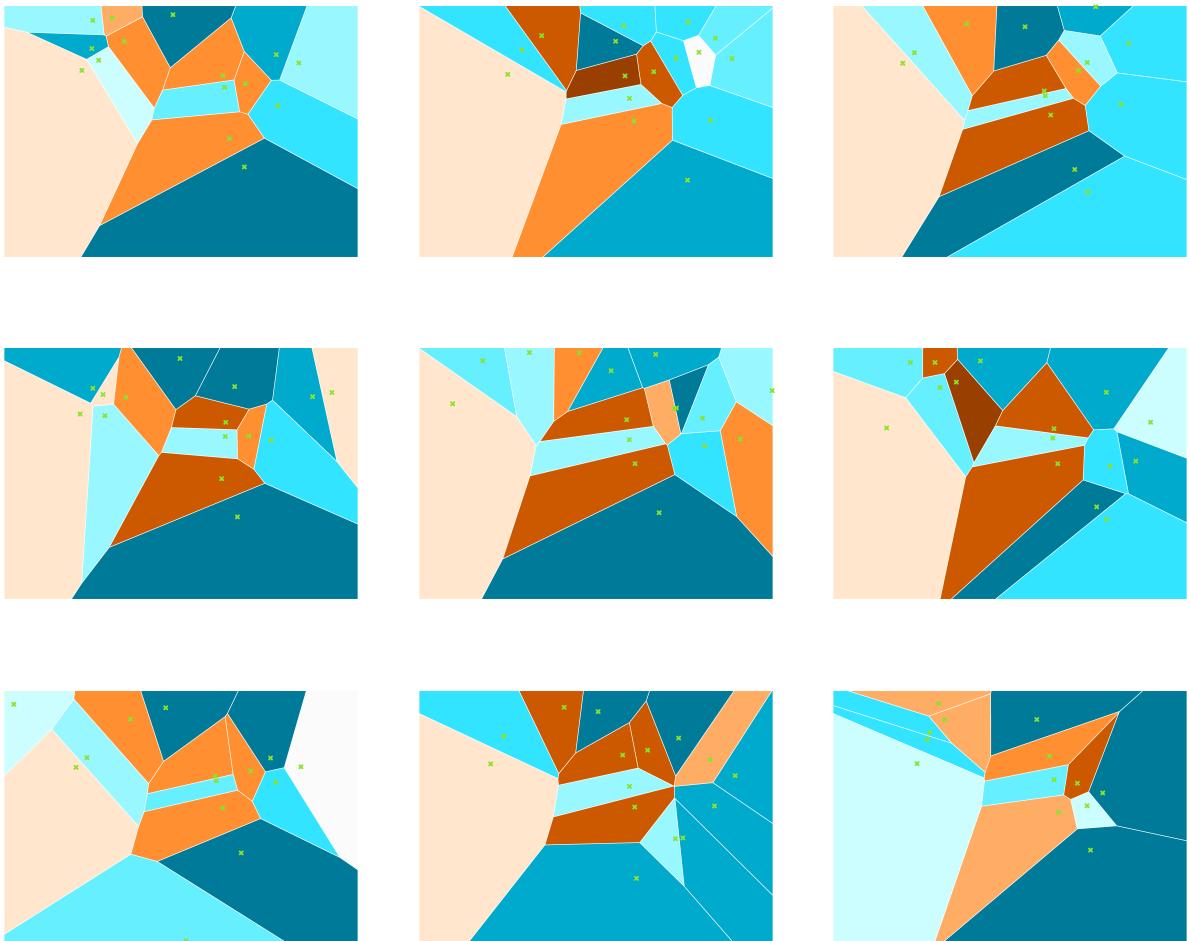
**Figure 10** If we know the input projection (e.g., if we know that the input coordinates are given in longitude/latitude), then we can add a geographic map to the migration and diversity contour plots. This requires the rworldmap package (for the getMap function which provides access a world map derived from Natural Earth data) and the rworldxtra package (for the high-resolution version of the map). **(a)** In the Mercator cylindrical projection. **(b)** In the Equidistant conic projection, with PROJ.4 string "`+proj=eqdc +lat_0=0 +lon_0=0 +lat_1=20 +lat_2=-23 +x_0=0 +y_0=0 +ellps=WGS84 +datum=WGS84 +units=m +no_defs`".



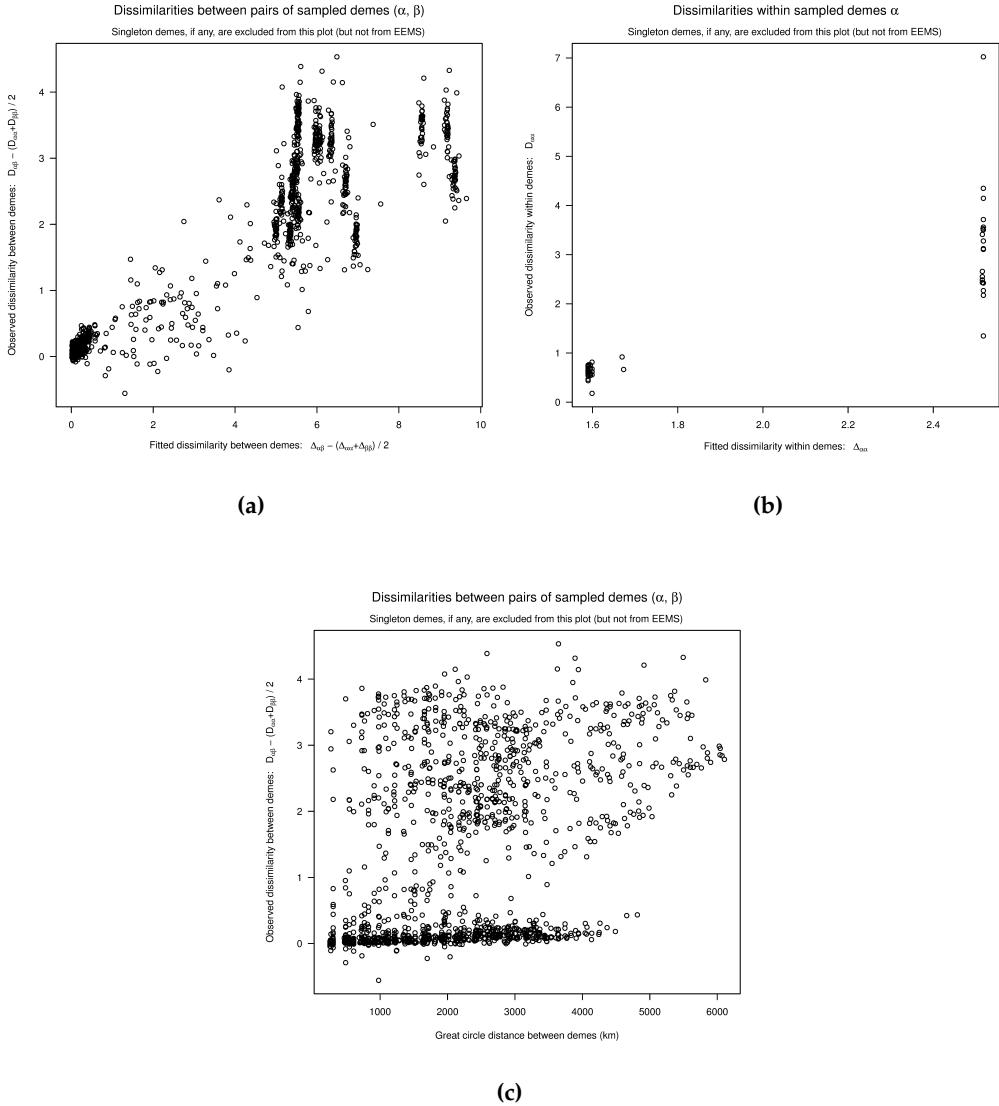
**Figure 11** By default, the plotting function `eems.plots` uses a DarkOrange to Blue color scheme, adapted from the dichromat package. [This scheme takes the dark oranges from the BluetoDarkOrange.12 theme and the blues the BrowntoBlue.12 theme.] To specify a different color scheme, we can supply a vector of colors with the `eems.colors` argument. These can be any colors but only a divergent scheme makes sense for a contour plot. **(a)** The effective migration surface in the RdBu palette from the RColorBrewer package. **(b)** The effective migration surface in the Spectral palette from the RColorBrewer package.



**Figure 12** We can add arbitrary graphical elements on top of the migration and diversity contour plots: points, lines, special geographic maps from a shape file, etc. In this example, we have added a set of file arbitrary “labels” as colored letters and a map of Africa from a shape file. The contour plots as well as the extra graphical elements are all shown in the Mercator projection.



**Figure 13** Voronoi diagrams drawn from the posterior distribution of the effective migration rates  $m$ , generated by `eems.voronoi.sample`.



**Figure 14** Observed vs fitted genetic dissimilarities, between and within demes, for the African elephant dataset. The observed genetic dissimilarities between individuals,  $D_{ij}$ , are averaged so that  $D_{\alpha\beta} = \frac{1}{n_{\alpha\beta}} \sum_{\delta(i)=\alpha, \delta(j)=\beta, i \neq j} D_{ij}$  where  $n_{\alpha\beta}$  is the number of pairs  $(i, j)$  such that  $\delta(i) = \alpha$ ,  $\delta(j) = \beta$ , i.e., sample  $i$  is assigned to deme  $\alpha$ , sample  $j$  is assigned to deme  $\beta$ , and  $i, j$  are distinct individuals. Singleton demes (those with a single sample) are excluded from both scatter plots. **(a)** Dissimilarities between demes: the fitted values  $B_{\alpha\beta} := \Delta_{\alpha\beta} - (\Delta_{\alpha\alpha} + \Delta_{\beta\beta})/2$  comprise the between-demes component of the genetic dissimilarity,  $B$ , which is modeled by the effective migration rates:  $B = f(m)$ . **(b)** Dissimilarities within demes: the fitted values  $W_\alpha := \Delta_{\alpha\alpha}$  comprise the within-demes component of the genetic dissimilarity,  $W$ , which is modeled by the effective diversity rates:  $W = g(q)$ . If the EEMS model fits the data well (after the MCMC chain has converged), we expect a strong linear relationship between the observed and fitted values in both scatter plots. See Section 4 for more details. **(c)** Dissimilarities between demes against geographic distances between demes. If isolation by distance (IBD) explains the spatial patterns in the data well, we expect a strong linear relationship between genetic dissimilarity and geographic distance. The African elephants violate exact IBD because forest and savanna elephants are strongly differentiated even though their habitats are side by side, particularly in the hybrid zone in Central Africa (the Democratic Republic of the Congo).

## References

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- [Wasser et al., 2008] Wasser, S. *et al.* (2008). Combating the illegal trade in African elephant ivory with DNA forensics. *Conserv. Biol.*, 22:1065–1071.
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