SMARTPOP Documentation
Simulating **M**ating **A**lliances as a **R**eproductive **T**actic for **Pop**ulations

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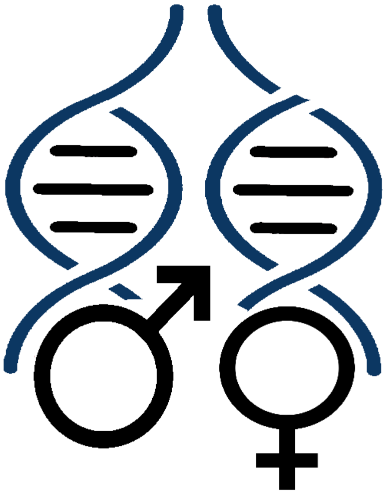
2013



Contents

1 Introduction to SMARTPOP

SMARTPOP is fast and flexible forward-in-time simulator for population genetics. Specially developed for speed efficiency, it is available in both serial or parallel versions. Developed for anthropological inferences on human populations, SMARTPOP simulates individuals with sequences of sex-linked DNA (mitochondrial, X and Y chromosomes) and autosomes. Studies of social dynamics are enabled using SMARTPOP's flexible demographic models and social rules of mating.

2 Requirements

SMARTPOP has been developed in C++ using the Boost C++ library. To build the software from source, you need a C++ compiler such as g++ or Visual Studio installed on your computer. To compile the parallel version of SMARTPOP, we recommend using mpic++ .

3 Installation

You can directly download a binary (executable) version of SMARTPOP compatible with your OS at `http://smartpop.sourceforge.net/download`
Alternatively you can build SMARTPOP from the source code following these instructions:

To build SMARTPOP from source on a UNIX machine:

- Download the source from `http://smartpop.sourceforge.net/download`
  ```
  wget http://smartpop.sourceforge.net/download/SMARTPOP.zip
  ```
- Move the archive to the folder where you want SMARTPOP to be installed
  ```
  mv SMARTPOP.zip /home/login/foo
  ```
- Uncompress the archives
  ```
  unzip SMARTPOP.zip
  ```
- Move to directory
  ```
  cd SMARTPOP/src-serial/
  ```
- Build SMARTPOP
  ```
  make
  ```
- Optional: Build the test package
  ```
  make test
  ```
- Optional: Run the test package
  ```
  ./test
  ```

SMARTPOP is then ready to launch via the command line:

```
./smartpop
```

- For builing the parallel version, go to the *src-parallel* directory:
  ```
  cd  /foo/SMARTPOP/src-parallel
  make
  ```
- Launch the parallel version (on UNIX system) on four cores:
  ```
  mpiexec -n 4 ./smartpopMPI
  ```

We have run tests on the main operating system available today, if you encounter any trouble please contact us.

4 SMARTPOP features

SMARTPOP must be called via the command line (`./smartpop`) from the directory where it is installed (or add the directory to your PATH). One call will launch a set of simulations having one set of parameters.

4.1 Inputs

A set of simulations rely on several parameters, all of which, but the population size and the random seed, have default values. You can either set these parameters using flags on the command line or via an input files.

4.1.1 Via the command line

You can define all the parameters to start a set of simulations using flags on the command line. All the parameters that are not called by flags will receive default values (see Table 3).
Note: you must always define the population size.
The order of parameters does not matter. If you give a wrong sequence of arguments on the command line, the program will raise an error and not start (in most cases).
To run a set of 1000 simulations with population size 200 evolving for 500 generations, enter:

```
./smartpop -p 200 -t 500 -nsimu 1000
```

4.1.2 Via input files

Instead of defining the parameters on the command line, you can also use an input file. For example, this is useful if you modify a lot of default value parameters.
You must respect the format of this file to make it work. Each line describes the value for one parameter. The order of lines does not matter. All the parameters that are not defined in this input file will take default values.

By default, each run of SMARTPOP creates a parameter file called SMARTPOP_parameters.txt. This has exactly the same format as the input parameter files such that running `./smartpop -i SMARTPOP_parameters.txt` will run the exact same set of simulations as you formerly ran. This is possible due to the fact that the random seed is one of the input parameters.

4.1.3 Windows executable

The available windows executable only handle input files. SMARTPOP will read the file *SMARTPOP_parameters.txt* which must be in the same directory. For each new launch of SMARTPOP you must set the parameters by modifying this file. If you want the seed to be picked randomly, remember to erase the line with the seed keyword from the parameter files.

Flag	Argument	Meaning
-v		Verbose
-i		Input file with parameters
-o	string	Name for the output files
-s	integer	Random seed
-p	integer	Population size
-sample	integer	Sample size
-nsimu	integer	Number of simulations
-t	integer	Number of generations between two sampling events
-nstep	integer	Number of sampling events through time for one simulation run
-mat	integer	Mating system
-noSib		Prevents siblings (sharing at least one parent) mating
-mu	double (x4)	Mutation rates (simple rates)
-muFull	double (x8)	Mutation rates (Kimura's two parameters model)
-mtdiv		Output diversity for mitochondrial DNA
-ydiv		Output diversity for Y chromosome
-xdiv		Output diversity for X chromosome
-adiv		Output diversity for autosomes
-nbLociA	integer	Number of unlinked autosomal loci
-sizeA	integer	Size, in number of sites, per autosomal locus
-nbLociX	integer	Number of unlinked loci on the X chromosome
-sizeX	integer	Size, in number of sites, per locus on the X chromosome
-sizeY	integer	Size, in number of sites, on the Y chromosome
-sizeMt	integer	Size, in number of sites, of the mitochondrial sequence
-burnin	double	Set the diversity threshold parameter for the burnin phase
-demog	double (x3) double	Set the demographic function
-fasta		Save each simulation in a fasta format file at the end of the run
-arl		Save each simulation in a arlequin format file at the end of the run
-save	string	Save all the simulations in a SMARTPOP format (.sim) in the directory given by the argument
-load	string	Load all the simulations in a SMARTPOP format (.sim) from the directory given by the argument
-header		Output the header at the beginning of diversity files

Table 1: Flags for command line call of SMARTPOP

Keyword	Argument	Meaning
verbose	boolean (0 or 1)	Verbose
fileOutput	string	Name of the output files
seed	integer	Random seed
populationSize	integer	Population size
sampleSize	integer	Sample size
nSimu	integer	Number of simulations
step	integer	Number of generations between two sampling events
nstep	integer	Number of sampling through time for one simulation run
matingSystem	integer (0 to 4)	Mating system
inbreeding	boolean (0 or 1)	1 prevents siblings (sharing at least one parent) mating; 0 allows sibling matings
muMtDnaTransition	double	Mutation rate (/site/generation) for mitochondrial transitions
muMtDnaTransversion	double	Mutation rate (/site/generation) for mitochondrial transversions
muXTransition	double	Mutation rate (/site/generation) for X chromosome transitions
muXTransversion	double	Mutation rate (/site/generation) for X chromosome transversions
muYTransition	double	Mutation rate (/site/generation) for Y chromosome transitions
muYTransversion	double	Mutation rate (/site/generation) for Y chromosome transversions
muAutosomeTransition	double	Mutation rate (/site/generation) for autosomal transitions
muAutosomeTransition	double	Mutation rate (/site/generation) for autosomal transversions
diversityToOutput	integer (0 to 4)	0 = output diversity for all the kind of DNA simulated 1 = output mitochondrial DNA 2 = output X chromosome 3 = output Y chromosome 4 = output autosomes
nbLociA	integer	Number of unlinked autosomal loci
sizeA	integer	Size, in number of sites, per autosomal locus
nbLociX	integer	Number of unlinked loci on the X chromosome
sizeX	integer	Size, in number of sites, per locus on the X chromosome
sizeY	integer	Size, in number of sites, of the Y chromosome
sizeMt	integer	Size, in number of sites, of the mitochondrial sequence
burninTheta	double	Set the diversity threshold parameter for the burn-in phase
demog	double double double	Set the demographic function
mito	integer	Mitochondrial simulation only
fastaOutput	boolean (0 or 1)	Save each simulation in a fasta format file at the end of the run
arlequinOutput	boolean (0 or 1)	Save each simulation in a Arlequin format file at the end of the run
save	boolean (0 or 1) (+ string)	If 1, save all the simulations in a SMARTPOP format (.sim) in the directory given by the argument If 0, no saving
load	boolean (0 or 1) (+string)	If 1, load all the simulations in a SMARTPOP format (.sim) from the directory given by the argument If 0, no saving.
headerOutput	boolean (0 or 1)	Output the header at the beginning of diversity files

Table 2: Parameter file definition

4.2 Simulation parameters

4.2.1 Verbose

It is recommended to begin using SMARTPOP with the verbose option on. This will make SMARTPOP return relevant information on the command line when the simulations are running. It is a good way to check that the parameters are set correctly, as well as to visualize the progress of the program.

4.2.2 Random seed

Simulations are highly reliant on random processes. Such processes are simulated via sequences of random numbers which are a large part of the program. Each time the program starts, it calls a random seed from which this sequence is produced uniquely. By default, the random seed is random, but it is possible to set it to repeat earlier runs.

4.2.3 Population size

The population size set in SMARTPOP corresponds to the census population size at the beginning of the simulation. If the population size is set to be non constant, this will change through time.

4.2.4 Sample size

Instead of analyzing the entire population, you can sample a certain number of individuals. This situation would match a “real life” situation where you do not have access to the DNA of your whole population. If you define a sample size, all the outputs (diversity, but also fasta and arlequin files) will be generated on a random sample in your population of the defined size.

4.2.5 Number of simulations

You can define the number of simulations that will be run with this set of parameters. If you are loading a set of simulations from a directory, this number must be smaller or equal to the number of saved simulations.

4.2.6 Number of generations to run

During each simulation, the population will evolve for a number of generations t between two samplingevents. By default, there is only one sampling event at the end of those t generations, where output files are produced and diversity is measured. If you define multiple sampling events ($N_{Sampling}$) through time, then t defines the number of generations to run between two sampling events:

$$G_{Total} = N_{Sampling} \times t$$

4.2.7 Mating system and number of offspring

Four mating systems are available designed by a number:

1. Monogamy
   Males and females are paired randomly to mate. No individuals can be paired with two different mates. The number of offspring per couple is set to follow a Poisson law.
2. Polygamy
   Males and females are paired randomly to mate. The number of offspring per female is set to follow a Poisson law.
3. Polygyny
   Males and females are paired randomly to mate. A female can only mate with one male. The number of offspring per female is set to follow a Poisson law.

4. Polyandry
   Males and females are paired randomly to mate. A male can only mate with one female. The number of offspring per male is set to follow a Poisson law.

5. Random mating
   Males and females are paired randomly to mate. There is no law on the number of offspring.

4.2.8 Sibling matings

For any mating system, you can forbid the mating between brothers and sisters (sharing at least one parent).

4.2.9 Mutation rates

Each type of DNA (mitochondrial, X, Y and autosomes) has two mutation rates: a transition and transversion rate. These rates must be set in mutations/site/generation. Overall eight mutation rates can be defined. If you do not know the ratio of transition over transversion, you can set transition rate equals to transversion rate equals to half the total mutation rate.
The rationale behind these eight mutation rates is that mutation rates measured for mtDNA, Y, X and autosomes can be different by more than an order of magnitude. Similarly, transition rates are usually an order of magnitude higher than transversion rates.

4.2.10 Burn-in phase

By default, simulations will start with the entire population having the same DNA. Alternatively, a burn-in phase allows you to start with an accelerated evolutionary process that will force your population to reach a given diversity θ_{burnin} from which your simulation will start. In this process, a higher mutation rate is applied to your population which quickly increases the diversity. The accelerated evolution stops when the threshold is reached or if it has been running for more than 100 generations.

4.2.11 DNA sequences

Each individual has a set of sex-linked DNA sequences:

- A mitochondrial sequence
- A sequence from the non-recombining Y chromosome
- A set of unlinked loci on the X chromosome
- A set of unlinked loci on the autosomes

It is possible to choose the length of each kind of sequencess. Note: all autosomal loci must share the same length; all X loci must share the same length. It is also possible to choose the number of loci on X and autosomes.
For computational reasons, the length of sequences must be a multiple of 32, or it will be automatically forced to the next higher multiple of 32. For instance, if you enter a length of 33, your simulated locus will have 64 sites. The size of the DNA considered unnecessary for a study can be set to zero, making the simulations faster.

4.2.12 Outputs

SMARTPOP can produce different outputs for each simulation:

- A file with the simulated DNA (at the end of the run) in fasta format
- A file with the simulated DNA (at the end of the run) in arlequin format [2]
- A file containing the whole population, included individual's DNA in a SMARTPOP format (.sim), that can be read by SMARTPOP.

SMARTPOP also produces output for the whole set of simulations:

- A diversity file for each kind of DNA
- A file containing the whole population, included individual's DNA in a SMARTPOP format (.sim), that can be read by SMARTPOP.

If the output name is set to 'foo' in the parameters, then the different files produced would be foo.fasta, foo.arl, foo_div_mt, foo_div_X, foo_div_Y and foo_div_A.

4.2.13 Save/Load

An entire set of simulations can be saved in a directory, and reloaded from the same directory. This allows the construction of complex scenarios with parameters changing through time. It can also be used if you were running very large and long simulations and your server only allows you limited time for each run. In such a case, you would run a succession of "short" simulations each being stopped and restarted to fit with the scheduler.

Using the *save* feature, each population will be written in a SMARTPOP special format (.sim). It is not necessary to understand this format to use the save/load option, but a small description is provided for more complex use of SMARTPOP.

A new file SMARTPOP_XX.sim with all the information needed to reload this population in to the software is written in the current directory when *save* is activated.
The header of this file is on two lines:
Population_size number_of_female generation size_Mito number_Loci_X size_Per_X size_Y number_Loci_A size_Per_Amating_
Thereafter each line represents an individual. The first number indicates the sex (1 for female, 0 for male) following by numbers representing its DNA.
The DNA sequence is written directly as a sequence of 64 bit number, so that the file is faster to save and load.

4.3 Outputs

4.3.1 Diversity tables

A file is created for each different type of DNA (mitochondrial, X, Y and autosome). If a name is provided, and the file already exists, the results will append to the end of the existing file.
This file contains different summary statistics for the population for each sample. Each line represent a sample. For each sample, for each DNA type, SMARTPOP will write in the file:

- Population size (not the sample size)
- Number of sites in the sequence evaluated
- Number of polymorphic sites
- Proportion of polymorphic sites
- Mean pairwise difference
- Number of haplotypes
- Allele heterozygosity

$$H_A = \frac{N}{N-1}\left(1 - \sum_{i=1}^{h} f_i^2\right)$$

- Nei's heterozygosity (i.e. heterozygosity averaged per site) [4]

$$H_N = \frac{1}{S}\frac{N}{N-1}\sum_{i=1}^{S}\left(1-\sum_{j=1}^{4} f_j^2\right)$$

- Theta Watterson θ_w

$$\theta_w = \frac{S}{\sum_{i=1}^{i=N-1}\frac{1}{i}}$$

- Theta homozygosity θ_H

$$\theta_H = \frac{1}{(1-H)} - 1$$

- Theta Pi θ_π

$$\theta_\pi = \frac{N}{N-1}\sum_{i=1}^{h}\sum_{j=1}^{h} dist\left(i,j\right)$$

- Tajima's D

$$D = \frac{\pi - \theta_w}{\sqrt{\left(b_1 - \frac{1}{a_1}\right)\frac{1}{a_1}S + \left(b_2 - \frac{n+2}{a_1 n} + \frac{a_2}{a_1^2}\frac{1}{a_1^2+a_2}\right)S\left(S-1\right)}}$$

$$a_1 = \sum_{i=1}^{n-1}\frac{1}{i}$$

$$a_2 = \sum_{i=1}^{n-1}\frac{1}{i^2}$$

$$b_1 = \frac{n+1}{3\left(n-1\right)}$$

$$b_2 = \frac{2\left(n^2+n+3\right)}{9n\left(n-1\right)}$$

4.3.2 Fasta

You can output the population, or a sample of it, in a fasta format file. Such a file can easily be piped through other population genetics software, such as COMPUTE from the libSequence package[5].

4.3.3 Arlequin

You can output the population, or a sample of it, in a file of the format of the Arlequin software. This allows you to make inferences on your simulations using ARLEQUIN [2].

4.4 Running SMARTPOP in parallel mode

It is possible to run SMARTPOP in parallel. You must build a specific version of SMARTPOP using a C++ compiler including Message Parsing Interface, such as mpic++.
When running in parallel, the simulations are distributed on several cores at the beginning at the simulations. Each process will write on different files to avoid conflict.
If you save and restart simulations for a complex scenario, be sure to use the same number of cores.

4.5 Setting up a complex scheme (change of parameters through time)

A set of simulations launched in one command line has a unique value for each parameter. It is possible to consider a complex scenario, where those parameters change through time, by successive use of SMARTPOP with different parameters.
After each parameter set, the simulations must all be saved. They are reloaded under the new set of parameters. This lets us link as many successive sets of parameters as desired. The saving / loading process is handled automatically under the flags *-save* and *-load*. The same process can be used to load a set of simulations and make it run longer without having to start again from the beginning.

4.6 Starting conditions: burn-in and pre-run

The starting conditions are a fundamental problem in forward-in-time simulations. How to determine the complete genetic set of the population from which the evolution starts? This is equivalent to asking what is the DNA state of an ancient population, which is totally unknown in most studies. In studies based on modern DNA, you have (at most) knowledge about past individuals who left descendants but nothing about the other past members of the population.
The question remains what to start the simulation with. A fully random DNA set is in no way meaningful. Instead the genetic patterns of real populations is the result of a long evolution process that creates haplotypes - individuals still sharing a large part of their DNA sequence.
The start must therefore be a shared sequence between individuals. From this null diversity, one must produce an artificial diversity, to correspond to a real population. There are three options:

- Assumed equilibrium
  It is possible that the population is in a state of 'equilibrium'. The definition of 'equilibrium' in population genetics is quite vague, but it is agreed that such equilibrium will be reached by running simulations for a very long time. How long is long enough? It must be at least the TMRCA, to be independent of starting conditions.
  As an indicator, the mean and variance of the time to the most recent common ancestor (TMRCA) assuming a constant population size [3, 1, 6] is:

$$E(T_{MRCA}) = 2n\left(1 - \frac{1}{n}\right)$$

$$var(T_{MRCA}) = n\left(8\sum_{i=2}^{i=n}\frac{1}{i^2} - 4\left(1 - \frac{1}{n}\right)^2\right)$$

- Burn-In
  Alternatively, we offer the user the possibility to start from a known diversity value, defined by its θ_π. For example one may want to study what happens to a population that had a θ_π of 0.2 one thousand generations ago.
  This starting point is produced by applying an accelerated mutation scheme on the population. It will assign a mutation rate one magnitude higher than the real rate, evolve the population and stop once the diversity threshold is reached. The *real* simulation can then start from this point.
  This approach is novel to SMARTPOP.

- Make your own recipe
  With the flexibility of SMARTPOP, you can choose of your own starting scheme. Controlling the mutation rate, you may reach higher diversity than equilibrium. You can also use the demography feature to create your own burn-in phase.

5 Examples

We present here three examples of analysis using SMARTPOP. The bash scripts and R code can be downloaded on `smartpop.sourceforge.net/download.html`.

- Equilibrium state of diversity depending on the population size
- Comparing the dynamics of diversity between monogamous and polygamous populations
- Dynamics of diversity in a population that grew before reaching a stable population size

Equilibrium state of diversity depending on the population size

In this example, we run 500 simulations (*-nsimu 500*) with a population of 100 individuals (*-p 100*) having a polygamous mating system (*-mat 2*). We measure diversity estimators for the population after a long run when the population has reached equilibrium (*-t 10000*). We check the diversity on a sample of 50 individuals (*-sample 20*). The output will be named *example1* (*-o example1*), and includes the header for the analysis (*-header*).

```
./smartpop -p 100 -mat 2 -t 10000 -sample 50 -header -o example1
```

To produce datasets for higher population sizes, we just repeat the same command with the desired population size. We will append the results to the same file. The header should not be added each time so we must remove the *-header* flag.

```
./smartpop -p 500 -mat 2 -t 10000 -sample 50 -o example1
```

```
./smartpop -p 1000 -mat 2 -t 10000 -sample 50 -o example1
```

Using an R script, we can look at the diversity at equilibrium depending on the population size.

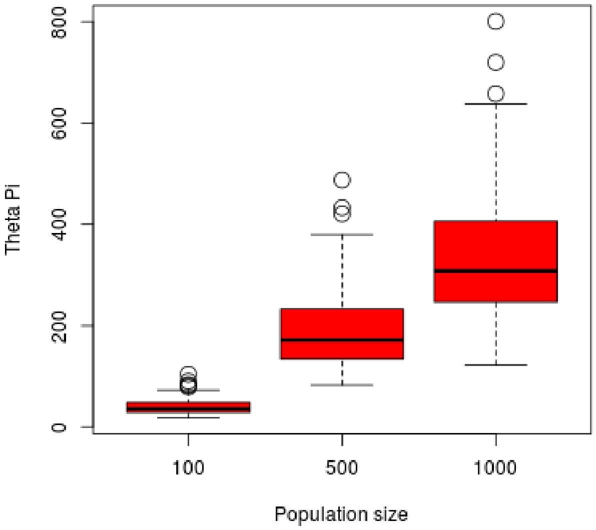


Figure 1: Simulated θ_{pi} depending on the population size.

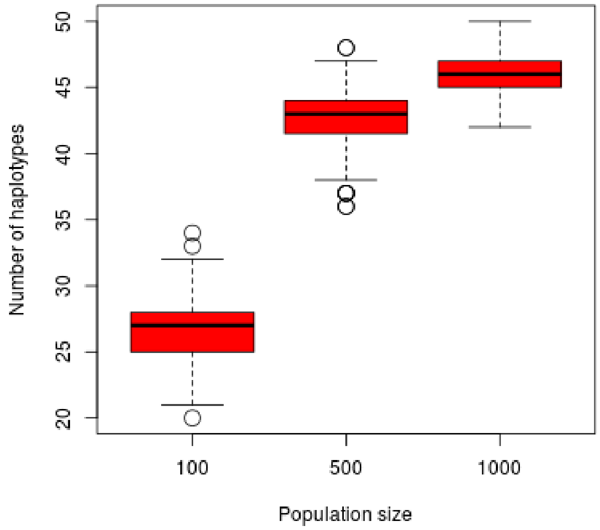


Figure 2: Simulated number of haplotypes depending on the population size

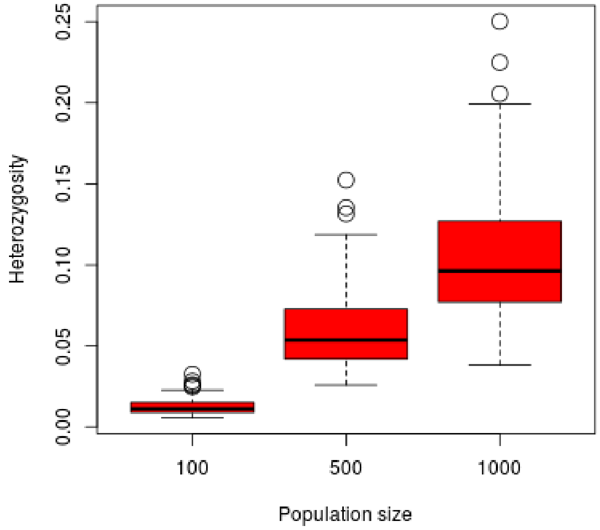


Figure 3: Simulated heterozygosity depending on the population size

Comparing the dynamics of diversity patterns between monogamy and polygamy

In this example, we run 500 simulations (*-nsimu 500*) with a population of 100 individuals (*-p 100*) having a monogamous system (*-mat 1*) with no sibling alliance (*-noSib*). This simulation uses a burn-in phase to first increase the population diversity until θ_{pi} reaches 25 (*-burnin 25*). We then follow different estimators in the population through time. The diversity is checked on a sample of 20 individuals (*-sample 20*) every 5 generations (*-t 5*), 50 successive times (*-nstep 50*). The output files will be named *example2_mono* (*-o example2_mono*) and include the header for the analysis (*-header*). The complete command line to produce the monogamous simulations is:

```
./smartpop -p 100 -nsimu 500 -mat 1 -sample 20 -noSib -t 5 -nstep 50 -o example2_mono -header
```

The complete command line to produce the polygamous simulations is:

```
./smartpop -p 100 -nsimu 500 -mat 2 -sample 20 -noSib -t 5 -nstep 50 -o example2_poly -header
```

This will create the following files:

- *example2_monoMt*: Estimators on simulated mtDNA through time under monogamy.
- *example2_monoX*: Estimators on simulated X chromosome through time under monogamy.
- *example2_monoY*: Estimators on simulated Y chromosome through time under monogamy.
- *example2_monoA*: Estimators on simulated autosomes through time under monogamy.
- *example2_polyMt*: Estimators on simulated mtDNA through time under polygamy.
- *example2_polyX*: Estimators on simulated X chromosome through time under polygamy.
- *example2_polyY*: Estimators on simulated Y chromosome through time under polygamy.
- *example2_polyA*: Estimators on simulated autosomes through time under polygamy.

Those outputs can be analyzed using R (cf. *example2.R*).

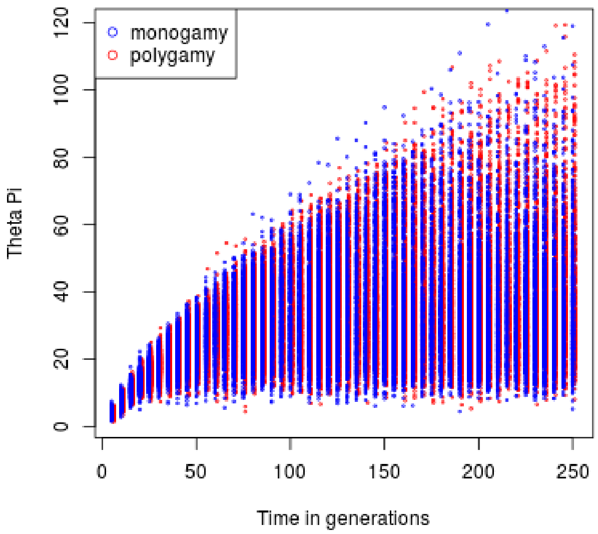


Figure 4: θ_π through time. Red points represent monogamous populations, blue points represent polygamous populations.

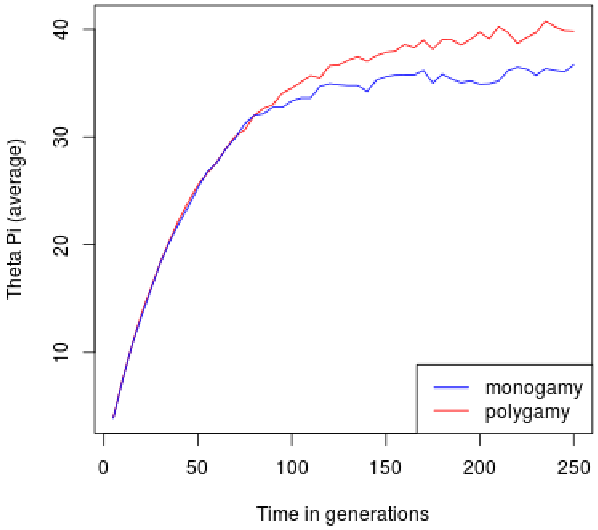


Figure 5: Average θ_π through time. The red line represents monogamous populations, the blue line represents polygamous populations

It is more readable to measure the mean of simulations having the same mating system at the same time point.

It is interesting to follow the number of haplotypes on the same simulation set.

With this example, looking at average values you can see that the mating system introduce a difference in the population genetic diversity using both estimators. This difference is however quite small. The scatter plot show a large variance between simulations which makes the difference between monogamy and polygamy non significant.

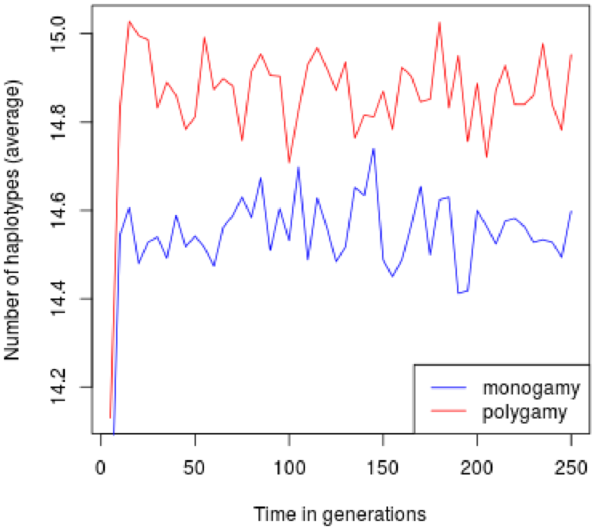


Figure 6: Average number of haplotypes through time. The red line represents monogamous populations, the blue line represents polygamous populations.

Dynamics of diversity in a population that grew before reaching a stable population size.

In this example, we run 500 simulations (*-nsimu 500*) with a population of 100 individuals (*-p 100*) at equilibrium, growing linearly to 200 individuals in 50 generations (thus gaining two individuals per generation for 50 generations), then staying constant for 5000 generations. To simulate such a complex scenario, we must divide the run in three phases, each phase having a unique set of parameters. In this case, we will first simulate the 100 individuals at equilibrium (i.e. evolving for a long time). The second phase will simulate the growth. The last phase will simulate the final 5000 generations with constant population size. The only trick to collate these scenarios is to save the populations and reload them using the flags *-save* and *-load*. We can also save the evolution of mtDNA from these simulation sampling 50 individuals every 20 years at the beginning, every 5 years during the growth, every 10 year in phase 3 the end. To look at mtDNA only, it is faster to use the flag *-mtdiv*. The output will be saved under the name *example3*.

```
./smartpop -p 100 -t 20 -nstep 50 -sample 50 -save phase1 -nbLociX 0 -sizeY 0 -nbLociA 0 -nsimu 100 -o example3 -header -nsimu 500
./smartpop -t 5 -nstep 10 -sample 50 -o example3 -demog 2 1 0 -load phase1 -save phase2 -mtdiv -nsimu 500
./smartpop -t 10 -nstep 100 -sample 50 -o example3 -load phase2 -mtdiv -nsimu 500
```

The output file *example3_mt_div.txt* can be analyzed with R to produce the following plots.

It can be interesting to follow the number of haplotypes on the same simulations set.

This example show the disequilibrium in diversity introduced by a very small growth (2 individuals / year). Although the number of haplotypes settle quite fast when the population size becomes stable, the mean pairwise distance, illustrated by θ_π takes hundreds of generation, i.e. thousands of years, before reaching its higher value.

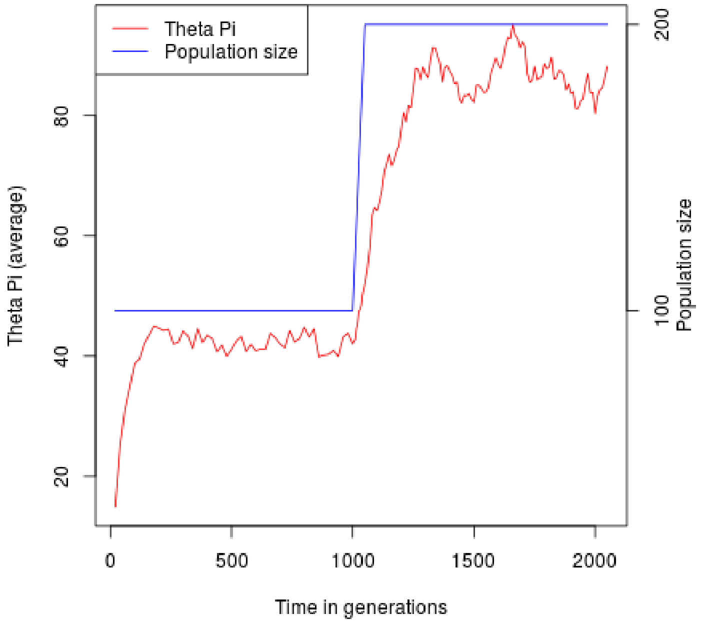


Figure 7: The red line represents the average θ_π through time (left axis). The blue line represents the population size through time (right axis).

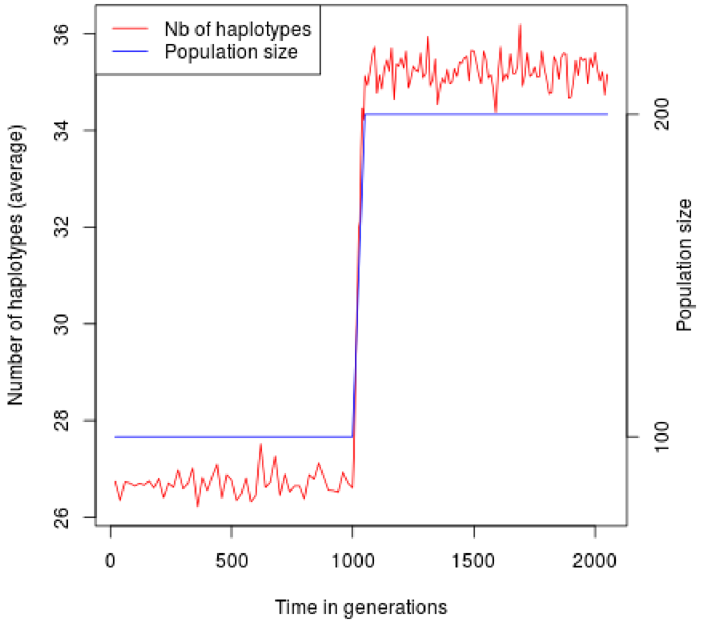


Figure 8: The red line represents the average number of haplotypes through time (left axis). The blue line represents the population size through time (right axis).

A Default parameters

Flag + Argument	Input File Keyword + Argument	Meaning	Example	Default Values
-v	verbose int	Verbose	Verbose 1	0
-i myfile.txt	NA	Input file with parameters	SMARTPOP_parameters.txt	NULL
-o filename	fileOutput filename	Name of the outputs	smartpop_13145105_2	fileOutput smartpop_seed_matingSystem
-s integer	seed integer	Random seed	seed 13145105	random
-p integer	populationSize integer	Census population size	populationSize 150	1000
-sample integer	sample integer	Sample size for estimation of diversity, and fasta/arlequin outputs	sample 100	100
-nsimu integer	nSimu integer	Number of simulations	nSimu 500	500
-t integer	step integer	Number of generations between two sampling events	step 100	100
-nstep integer	nstep integer	Number of sampling events through time for one simulation	nstep 10	1
-mat integer	matingSystem integer	1 monogamy, 2 polygamy, 3 polygyny, 4 polyandry, 5 random	matingSystem 4	2
-noSib	inbreeding integer	Prevents sibling matings	inbreeding 1	0
-mu double (x4)		Mutation rates (simple rates - respectively mtDNA, Y, X and autosome)	-mu 0.0001 0.0001 0.0001 0.0001	
-muFull double (x8)		Mutation rates (Kimura's model - respectively transition transversion for mtDNA, X, Y and autosomes)	-mu 0.0001 0.00001 0.0001 0.00001 0.0001 0.00001 0.0001 0.00001	
	muMtDnaTransition integer	Transition rate on mtDna	muMtDnaTransition 0.000001	0.000001
	muMtDnaTransversion integer	Transversion rate on mtDna	muMtDnaTransition 0.0000001	0
	muXTransition integer	Transition rate on X	muXTransition 0.0000001	1e-08
	muXTransversion integer	Transversion rate on X	muXTransversion 0.0000001	0
	muYTransition integer	Transition rate on Y	muYTransition 0.000001	1e-08
	muYTransversion integer	Transversion rate on Y	muYTransversion 0.0000001	0
	muAutosomeTransition integer	Transition rate on autosomes	muAutosomeTransition 0.000001	1e-08
	muAutosomeTransversion integer	Transversion rate on autosomes	muAutosomeTransversion 0.0000001	0
-mdiv	diversityToOutput 1	Output diversity for mitochondrial DNA		
-xdiv	diversityToOutput 2	Output diversity for X chromosome		
-ydiv	diversityToOutput 3	Output diversity for Y chromosome		
-adiv	diversityToOutput 4	Output diversity for autosomes		
	diversityToOutput X X X	XXX can be a list of the above numbers, for outputting diversity of the four types XXX = 0	diversityToOutput 1 2 3	0
-nbLociA integer	nbLociA integer	Number of unlinked autosomal loci	nbLociA 1	1
-sizeA integer	sizeA integer	Size, in number of sites, per autosomal locus	sizeA 3200	3200
-nbLociX integer	nbLociX integer	Number of unlinked loci on the X chromosome	nbLociX 1	1
-sizeX integer	sizeX integer	Size, in number of sites, per locus on the X chromosome	sizeX 3200	3200
-sizeY integer	sizeY integer	Size, in number of sites, of the Y chromosome	sizeY 3200	3200
-sizeMt integer	sizeMt integer	Size, in number of sites, of the mitochondrial sequence	sizeMt 3200	3200
-burnin double	burninTheta double	Set the diversity threshold parameter for the burn-in phase	burninTheta 0.5	0
-demog double(x3)	demog double (x3)	Set the demographic function $popsize(t+1) = a + b \times popsize(t) + c \times popsize(t)^2$	demog 0 1 0	0 1 0
-fasta	fastaOuput integer (0 or 1)	Save each simulation in a fasta format file at the end of the run	fastaOutput 1	0
-arl	arlequinOutput boolean (0 or 1)	Save each simulation in a arlequin format file at the end of the run	arlequinOuput 1	0
-save string	save boolean (0 or 1) (+string)	save all the simulations in the SMARTPOP format (.sim) in the directory given by the argument	save 1 mydirectory	0
-load string	load boolean (0 or 1) (+string)	load all the simulations in the SMARTPOP format (.sim) from the directory given by the argument	load 1 mydirectory	0
-header	headerOutput boolean (0 or 1)	Output the header at the beginning of	headerOutput 1	0

B References

[1] P Donnelly and S Tavaré. Coalescents and genealogical structure under neutrality. *Annual Review of Genetics*, 29(1):401–421, 1995.

[2] Laurent Excoffier and Heidi E L Lischer. Arlequin suite ver 3.5: A new series of programs to perform population genetics analyses under Linux and Windows. *Molecular Ecology Resources*, 10(3):564–567, May 2010.

[3] Richard R Hudson. Gene genealogies and the coalescent process. *Oxford Surveys in Evolutionary Biology*, 7(1):44, 1990.

[4] Masatoshi Nei. Estimation of average heterozygosity and genetic distance from a small number of individuals. *Genetics*, 89(3):583–590, 1978.

[5] K Thornton. LibSequence: A C++ class library for evolutionary genetic analysis. *Bioinformatics*, 19(17):2325–2327, 2003.

[6] John Wakeley. *Coalescent Theory: An Introduction*. Roberts & Company Publishers, first edition, 2009.