# simuPOP Reference Manual

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#### Abstract

simuPOP is a forward-time population genetics simulation environment. Unlike coalescent-based programs, simuPOP evolves populations forward in time, subject to arbitrary number of genetic and environmental forces such as mutation, recombination, migration and population/subpopulation size changes. Statistics of populations can be calculated and visualized dynamically which makes simuPOP an ideal tool to demonstrate population genetics models; generate datasets under various evolutionary settings, and more importantly, study complex evolutionary processes and evaluate gene mapping methods.

The core of simuPOP is a scripting language (Python) that provides a large number of building blocks (populations, mating schemes, various genetic forces in the form of operators, simulators and gene mapping methods) to construct a simulation. This provides a R/Splus or Matlab-like environment where users can interactively create, manipulate and evolve populations, monitor and visualize population statistics and apply gene mapping methods. The full power of simuPOP and Python (even R) can be utilized to simulate arbitrarily complex evolutionary scenarios.

simuPOP is written in C++ and is provided as Python modules. Besides a front-end providing an interactive shell and a scripting language, Python is used extensively to pass dynamic parameters, calculate complex statistics and write operators. Because of the openness of simuPOP and Python, users can make use of external programs, such as R, to perform statistical analysis, gene mapping and visualization. Depending on machine configuration, simuPOP can simulate large (think of millions) populations at reasonable speed.

This is a reference manual to all variables, functions, and objects of simuPOP. To learn different components of simuPOP and how to write simuPOP scripts, please refer to the *simuPOP User's Guide*.

#### How to cite simuPOP:

Bo Peng and Marek Kimmel (2005) simuPOP: a forward-time population genetics simulation environment. *bioinformatics*, **21**(18): 3686-3687

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**CHAPTER** 

ONE

# Introduction

This reference manual assumes that you have read the *simuPOP User's Guide* and know the basic concepts of simuPOP. It is also remcommended that you learn some basics of Python before you continue. I have listed a few Python resources at the end of this chapter, along with links to some simuPOP tutorials.

Almost all information contained in this manual can be accessed from command line, after you install and import the simuPOP module. For example, you can use help(population.addInfoField) to view the help information of member function addInfoField of class population.

```
Example 1.1: Getting help using the help() function

>>> help(population.addInfoField)

Help on method population_addInfoField:

population_addInfoField(...) unbound simuPOP_la.population method
    Description:

    add an information field to a population

Usage:

    x.addInfoField(field, init=0)

Arguments:

field:
    new information field. If it already exists, it will be re-initialized.
    init: initial value for the new field.

>>>
```

It is important that you understand that

• The constructor of a class is named \_\_init\_\_ in python. That is to say, you should use the following command to display the help information of the constructor of class population:

```
>>> help(population.__init___)
```

• Some classes are derived from other classes and have access to member functions of their base classes. For example, class population, individual and simulator are all derived from class GenoStruTrait. Therefore, you can use all GenoStruTrait member functions from these classes.

The constructor of a derived class also calls the constructor of its base class so you may have to refer to the base class for some parameter definitions. For example, parameters begin, end, step, at etc are shared by all operators, and are explained in details only in class baseOperator.

# 1.1 Loading simuPOP

simuPOP is composed of six modules: standard short, long and binary alleles, each of them have standard and optimized modules. A Message Passing Interface (MPI) version is under development but not yet available. The short modules use 1 byte to store each allele which limits the possible allele states to 256. This is enough most of the times but not so if you need to simulate models such as the infinite allele model. In those cases, you can use the long allele version of the modules, which use 2 bytes for each allele and can have  $2^{16}$  possible allele states. On the other hand, if you would like to simulate a large number of binary (SNP) markers, binary modules can save you a lot of RAM. Depending on applications, binary modules can be faster or slower than other modules.

Standard modules have detailed debug and run-time validation mechanism to make sure the simulations run correctly. Whenever something unusual is detected, simuPOP would terminate with a detailed error message. The cost of such run-time checking varies from application to application but can be very high under some extreme circumstances. Because of this, optimized versions for all modules are provided. They bypass all parameter checking and run-time validations and will simply crash if things go wrong. It is recommended that you use standard modules whenever possible and only use the optimized version when performance is needed and you are confident that your simulation is running as expected.

Example 1.2 and 1.3 demonstrate the differences between standard and optimized modules, by executing two invalid commands. The standard module returns proper error messages, while the optimized module returns erroneous results and even crashes.

Example 1.2: Use of standard simuPOP modules

```
>>> pop = population(10, loci=[2])
>>> pop.locusPos(10)
Traceback (most recent call last):
  File "refManual.py", line 1, in ?
    #
IndexError: src/genoStru.h:447 absolute locus index (10) out of range of 0 - 1
>>> pop.individual(20).setAllele(1, 0)
Traceback (most recent call last):
  File "refManual.py", line 1, in ?
IndexError: src/population.h:443 individual index (20) is out of range of 0 ~ 9
                    Example 1.3: Use of optimized simuPOP modules
% setenv SIMUOPTIMIZED
% python
>>> from simuPOP import *
simuPOP: Copyright (c) 2004-2006 Bo Peng
Developmental Version (May 21 2007) for Python 2.3.4
[GCC 3.4.6 20060404 (Red Hat 3.4.6-3)]
Random Number Generator is set to mt19937 with random seed 0x2f04b9dc5ca0fc00
This is the optimied short allele version with 256 maximum allelic states.
For more information, please visit http://simupop.sourceforge.net,
or email simupop-list@lists.sourceforge.net (subscription required).
>>> pop = population(10, loci=[2])
>>> pop.locusPos(10)
1.2731974748756028e-313
>>> pop.individual(20).setAllele(1, 0)
```

Segmentation fault

You can control the choice of modules in the following ways:

- Set environment variable SIMUALLELETYPE to 'short', 'long' or 'binary', and SIMUOPTIMIZED to use the optimized version. The default module is the standard short module.
- Before you load simuPOP, set options using simuOpt.setOptions(optimized, alleleType, quiet, debug). alleleType can be short, long or binary. quiet=True suppresses banner information when simuPOP is loaded, and debug is a comma-separated list of debug options specified by listDebugCode(). Debug information is only available for standard modules.
- If you are running a simuPOP script that conforms to simuPOP convention, you should be able to use optimized module using command line option --optimized.

After a simuPOP module is loaded, you can use the following functions to determine some module and platform dependent information.

- AlleleType(): return 'binary', 'short', or 'long'.
- Optimized(): return True or False.
- MaxAllele(): return 1 for binary modules, usually 255 for short modules and  $2^{16} 1$  for long modules.
- simuVer(): return the version string
- simuRev(): simuPOP revision number. If your script needs a recent version of simuPOP, it is a good idea to test simuRev() against the revision when the feature you need becomes available.
- Limits (): print the limits of this module on this platform, such as the maximum number of loci in a population.

Example 1.4: Use simuOpt to control which simuPOP module to load

```
>>> import simuOpt
>>> simuOpt.setOptions(optimized=False, alleleType='long', quiet=True)
>>> from simuPOP import *
>>> print alleleType()
Traceback (most recent call last):
   File "refManual.py", line 1, in ?
    #
NameError: name 'alleleType' is not defined
>>> print optimized()
Traceback (most recent call last):
   File "refManual.py", line 1, in ?
    #
NameError: name 'optimized' is not defined
```

After simuPOP is installed. It is recommended that you run the test scripts under the tests directory. This will make sure that your system is working correctly. To run all tests, run

```
sh run_tests.sh
```

Or, if you do not install RPy and R, run

```
sh run_tests.sh norpy
```

Windows users have to run

```
set SIMUALLELETYPE=short
python run_tests.py
```

repeatedly, with SIMUALLELETYPE set to short, long and binary.

# 1.2 References and the clone() member function

Assignment in Python only creates a new referrice to the exiting object. For example,

```
pop = population(...)
pop1 = pop
```

will create a reference pop1 to population pop. Modifying pop1 will modify pop as well. If you would like to have an independent copy, use

```
pop1 = pop.clone()
```

All simuPOP classes (objects) have a clone function that can be used to create an independent copy of the object. Because cloning a large population can be costly, a few methods are provided to access populations inside a simulator. Assuming that simu is a simulator with several populations,

1. simu.population(rep) returns a reference to the rep'th population. You can, although not recommended, modify simulator through this pop reference. Be cautious though, that the following seemingly innocent usage of this function will crash simuPOP, because the simulator simu will be destroyed after the call to func() is ended, leaving pop as a referece to an invalid population object.

Example 1.5: Reference to a population of a simulator

```
def func():
    simu = simulator(
        population(10),
        randomMating())
    # evolve simu ..., then return population
    return simu.population(0)

pop = func()
pop.popSize()
```

- 2. To get an independent copy of a population, you can use pop = simu.getPopulation(rep), which returns an independent copy of population rep of simu. simu is untouched.
- 3. If the simulator will be destroyed as in Example 1.5,

```
pop = simu.getPopulation(rep, destructive=True)
```

can be used. This function will *extract* population rep from the simulator instead of copying it, and bypassing a potentially very costly process.

# 1.3 Zero-based indexes, ranges, absolute and relative indexes

**All arrays in simuPOP start at index 0**. This conforms to Python and C++ indexes. To avoid confusion, I will refer the first locus as locus zero, the second locus as locus one; the first individual in a population as individual zero, and so on.

Ranges in simuPOP also conforms to Python ranges. That is to say, a range has the form of [a,b) where a belongs to the range, and b does not. For example, pop.chromBegin(1) refers to the index of the first locus on chromosome 1 (actually exists), and pop.chromEnd(1) is the index of the last locus on chromosome 1 plus 1, which might or might not be a valid index. In this way

```
for locus in range(pop.chromBegin(1), pop.chromEnd(1)):
    print locus
```

will iterate through all locus on chromosome 1.

Another two important concepts are the *absolute index* and the *relative index* of a locus. The former index ignores chromosome structure. For example, if there are 5 and 7 loci on the first two chromosomes, the absolute indexes of the two chromosomes are (0, 1, 2, 3, 4), (5, 6, 7, 8, 9, 10, 11) and the relative indexes are (0, 1, 2, 3, 4), (0, 1, 2, 3, 4, 5, 6). Absolute indexes are more frequently used because they avoid the trouble of having to use two numbers (chrom, index) to refer to a locus. Two functions <code>chromLocusPair(absIndex)</code> and <code>absLocusIndex(chrom,index)</code> are provided to convert between these two kinds of indexes. An individual can also be referred by its *absolute index* and *relative index* where *relative index* is the index in its subpopulation.

Example 1.6: Conversion between absolute and relative indexes

```
>>> pop = population(subPop=[20, 30], loci=[5, 6])
>>> print pop.chromLocusPair(7)
(1, 2)
>>> print pop.absLocusIndex(1,1)
6
>>> print pop.absIndIndex(10, 1)
30
>>> print pop.subPopIndPair(40)
(1, 20)
>>>
```

# 1.4 Function form of an operator

Operators are usually applied to populations through a simulator. They are created and passed as parameters to the evolve function of a simulator. During evolution, the evolve() function determines if an operator can be applied to a population and apply it when appropriate. More details about operators will be described in section 2.5.

You can ignore the specialties of an operator and call its apply() function directly. For example, you can initialize a population outside a simulator by

```
initByFreq([.3, .2, .5]).apply(pop)
```

or dump the content of a population by

```
dumper().apply(pop)
```

This usage is used so often that it deserves some simplification. Equivalent functions are defined for most of the operators. For example, function InitByFreq is defined for operator initByFreq as follows

```
Example 1.7: Function InitByFreq
```

```
>>> def InitByFreq(pop, *args, **kwargs):
... initByFreq(*args, **kwargs).apply(pop)
...
>>> InitByFreq(pop, [.2, .3, .4, .1])
>>>
```

The function form of an operator is listed after its class name in this reference manual.

# 1.5 The carray type

The return value of simuPOP functions with names starting with arr is of a special Python type carray. This object reflects the underlying C/C++ array which can be modified through this list-like interface, with the exception that you can not change the size of the array. Only count and index list functions can be used, but all comparison, assignment and slice operations are allowed.

Example 1.8: Usage of the carray type

```
>>> # obtain an object using one of the arrXXX functions
>>> pop = population(loci=[3,4], lociPos=[1,2,3,4,5,6,7])
>>> arr = pop.arrLociPos()
>>> # print and expression (just like list)
>>> print arr
[1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
>>> str(arr)
'[1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]'
>>> # count
>>> arr.count(2)
>>> # index
>>> arr.index(2)
>>> # can read write
>>> arr[0] = 0.5
>>> # the underlying locus position is also changed
>>> print pop.lociPos()
(0.5, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0)
>>> # convert to list
>>> arr.tolist()
[0.5, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
>>> # or simply
>>> list(arr)
[0.5, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
>>> # compare to list directly
>>> arr == [0.5, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
>>> # you can also convert and compare
>>>  list(arr) == [0.5, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0]
True
>>> # slice
>> arr[:] = [1,2,3,4,5,6,7]
>>> # assign from another part
>>> arr[1:3] = arr[3:5]
>>> # arr1 is 1,2,3
>>> arr1 = arr[:3]
>>> # assign slice from a number
>>> # arr will also be affected since arr1 point to a part of arr
>>> arr1[:] = 10
>>> # assign vector of the same length
>>> len(arr1)
>>> arr1[:] = [30,40, 50]
>>>
```

**Important note:** Objects returned from arrXXX functions should be considered temporary. There is no guarantee that the underlying array will still be valid after any population operation.

# 1.6 Random Number Generator

There are many random number generators (RNG) with different properties. Using a bad RNG can serious compromise the validity of simulation results. Although the default RNG mt19937 has good performance, simuPOP allows you to choose from a number of RNGs, all from GNU Scientific Library (GSL). Please refer to the documentation of GSL for more details about these RNGs.

If you need to use a RNG in your simuPOP script, you can either use Python random module (import random), use rng() function to get the RNG of simuPOP, or create a separate RNG using RNG(name, seed) function.

Example 1.9: Random number generator

#### 1.6.1 Random seed

When simuPOP is loaded, it creates a random number generator. This RNG gets its seed from:

- random number from /dev/urandom if it is available
- random number from /dev/random if it is available
- use Python random module and assign random seed with

```
(random.randint(0, sys.maxint) + int(time.time())) % sys.maxint
```

The last method is used mostly under windows, on which random devices are not available. It tries to avoid sole use of system time because simultaneously started jobs may get the same random seed.

Random seed can be retrieved using rnq().seed() function, which can be saved for future reference.

### 1.6.2 Class RNG

Random number generator

#### **Details**

This random number generator class wraps around a number of random number generators from GNU Scientific Library. You can obtain and change system random number generator through the rng() function. Or create a separate random number generator and use it in your script.

#### Initialization

Create a RNG object. You can also use rng() function to get the RNG used by simuPOP.

```
RNG(rng=None, seed=0)
```

#### **Member Functions**

- **x.max()** Maximum value of this RNG.
- x.maxSeed() Return the maximum allowed seed value
- x.name() Return RNG name
- x.pvalChiSq(chisq, df) Right hand side (single side) p-value for ChiSq value
- x.randBinomial(n, p) Binomial distribution B(n, p).
- x.randGeometric(p) Geometric distribution.
- **x.randGet()** Return a random number in the range of [0, 2, ... max()-1]
- **x.randInt(n)** Return a random number in the range of [0, 1, 2, ... n-1]
- x.randNormal(m, v) Normal distribution.
- x.randPoisson(p) Poisson distribution.
- **x.randUniform01()** Uniform distribution [0,1).
- x.seed() Return the seed of this RNG
- x.setRNG(rng=None, seed=0) Choose an random number generator, or set seed to the current RNG
  - **rng** name of the RNG. If rng is not given, environmental variable GSL\_RNG\_TYPE will be used if it is available. Otherwise, RNGmt19937 will be used.
  - **seed** random seed. If not given, /dev/urandom, /dev/random, system time will be used, depending on availability, in that order. Note that windows system does not have /dev so system time is used.
- x.setSeed(seed) Set random seed for this random number generator if seed is 0, method described in setRNG is used.

## 1.7 Name Conventions

simuPOP follows the following naming conventions.

• Classes (objects), member functions and parameter names start with small character and use capital character for the first character of each word afterward. For example

```
population, population::subPopSize(), individual::setInfo()
```

- Most standalone (global) functions start with capital character. This is how you can differ an operator from its function version. For example, initByFreq(vars) is an operator and InitByFreq(pop, vars) is its function version.
- Constants start with capital characters. For example

```
MigrByProportion, StatNumOfFemale
```

• The following words in function names are abbreviated:

```
pos (position), info (information), migr (migration), subPop (subpopulation),
(rep) replicate, gen (generation), grp (group(s)), ops (operators),
expr (expression), stmts (statements)
```

# 1.8 Online resources

There are several excellent Python books and tutorials. If you are new to Python, you can start with

- 1. The Python tutorial (http://docs.python.org/tut/tut.html)
- 2. Other online tutorials listed at http://www.python.org/doc/

The PDF version of this reference manual is distributed with simuPOP. You can also get the latest version of this file from the simuPOP subversion repository. To access it, go to http://simupop.sourceforge.net, click SF.net summary > Code > SVN Browse > trunk > doc > refManual.pdf and download the HEAD version. You can also find some tutorials that are not distributed with simuPOP from the subversion repository, such as

- 1. Forward-time simulations using simuPOP, a tutorial: a tutorial that was given in a simuPOP workshop held at University of Alabama at Birmingham.
- 2. Forward-time simulations using simuPOP, an in-depth course: a in-depth course about simuPOP components, with a lot of examples.

The filenames are tutorial.pdf and course.pdf, respectively. Note that these presentations will not be updated so their content can become out of date. This reference manual should be considered as the authoritative resource of simuPOP.

1.8. Online resources

# simuPOP Components

# 2.1 Genotypic structure

Genotypic structure refers to

- ploidy, the number of copies of basic number of chromosomes (c.f. ploidy(), ploidyName())
- the number of chromosomes (c.f. numChrom())
- the existence of sex chromosome (c.f. sexChrom())
- the number of loci on each chromosome (c.f. numLoci(ch), totNumLoci())
- the locus position on its chromosome (c.f. locusPos(loc), arrLociPos())
- allele name(s), default to allele number (c.f. alleleName(allele), alleleNames())
- ullet the maximum allele state (c.f. maxAllele())
- the names of the information fields (c.f. infoField(idx), infoFields())

Information fields refer to float numbers attached to each individual, such as fitness value, parent index, age. They are used to store auxiliary information of individuals, and are essential to the operations of some simuPOP components. For example, 'fitness' field is required by all selectors. Details please refer to section 2.8.

If sexChrom() is false, all chromosomes are assumed to be autosomes. You can also create populations with a sex chromosome. Currently, simuPOP only models the XY chromosomes in diploid population. This is to say,

- sex chromosome is always the last chromosome.
- sex chromosome can only be specified for diploid population (ploidy()=2).
- sex chromosomes (XY) may differ in length. You should specify the length of the longer one as the chromosome length. If there are more loci on X than Y, the rest of the Y chromosome is unused. Mutation may still occur at this unused part of chromosome to simplify implementation and usage.
- it is assumed that males have XY and females have XX chromosomes. The sex chromosomes of male individuals
  are in the order of XY.

Individuals in the same population share the same genotypic structure. Consequently, the genotypic information can be accessed from individual, population and simulator levels.

## 2.1.1 Class GenoStruTrait

Genotypic structure related functions, can be accessed from individuals, populations and simulator levels.

#### **Details**

Genotypic structure refers to the number of chromosomes, the number and position of loci on each chromosome, and allele and locus names etc. All individuals in a population share the same genotypic structure. Because class GenoStruTrait is inherited by class population, class individual, and class simulator, functions provided in this class can be accessed at the individual, population and simulator levels.

#### **Initialization**

This object can not be created directly. It is created by a population.

```
GenoStruTrait()
```

#### **Member Functions**

- **x.alleleName(allele)** Return the name of an allele (if previously specified). Default to allele index.
- x.alleleNames() Return an array of allele names
- x.arrLociPos() Return a carray of loci positions of all loci

**Note:** Modifying loci position directly using this function is strongly discouraged.

**x.arrLociPos(chrom)** Return a carray of loci positions on a given chromosome

**Note:** Modifying loci position directly using this function is strongly discouraged.

- x.chromBegin(chrom) Return the index of the first locus on a chromosome
- **x.chromEnd(chrom)** Return the index of the last locus on a chromosome plus 1
- x.chromLocusPair(locus) Return a (chrom, locus) pair of an absolute locus index, c.f.
  absLocusIndex
- x.genoSize() Return the total number of loci times ploidy
- x.hasInfoField(name) Determine if an information field exists
- x.infoField(idx) Obtain the name of information field idx
- x.infoFields() Return an array of all information fields
- x.infoIdx(name) Return the index of the field name, return -1 if not found
- x.infoSize() Obtain the number of information fields
- x.lociByNames(names) Return an array of locus indexes by locus names
- x.lociNames() Return names of all loci
- x.lociPos() Return loci positions
- x.locusByName(name) Return the index of a locus by its locus name
- x.locusName(loc) Return the name of a locus

- x.locusPos(locus) Return the position of a locus
- **x.maxAllele()** Return the maximum allele value for all loci. Default to maximum allowed allele state.

Maximum allele value has to be 1 for binary modules. maxAllele is the maximum possible allele value, which allows maxAllele+1 alleles 0, 1, ..., maxAllele.

- **x.numChrom()** Return the number of chromosomes
- x.numLoci(chrom) Return the number of loci on chromosome chrom, equivalent to numLoci()[chrom]
- **x.numLoci()** Return the number of loci on all chromosomes
- **x.ploidy()** Return ploidy, the number of homologous sets of chromosomes
- x.ploidyName() Return ploidy name, haploid, diploid, or triploid etc.
- **x.sexChrom()** Determine whether or not the last chromosome is sex chromosome
- x.totNumLoci() Return the total number of loci on all chromosomes

#### **Example**

### Example 2.1: Genotypic structure

```
>>> # create a population, most parameters have default values
>>> pop = population(size=5, ploidy=2, loci=[5,10],
        lociPos=[range(0,5), range(0,20,2)],
        alleleNames=['A','C','T','G'],
. . .
        subPop=[2,3], maxAllele=3)
>>> print pop.popSize()
>>> print pop.ploidy()
>>> print pop.ploidyName()
diploid
>>> print pop.numChrom()
>>> print pop.locusPos(2)
2.0
>>> print pop.alleleName(1)
>>> # get the fourth individual of the population
>>> ind = pop.individual(3)
>>> # access genotypic structure info
>>> print ind.ploidy()
>>> print ind.numChrom()
>>> print ind.numLoci(0)
>>> print ind.genoSize()
30
>>> # and from simulator level
>>> simu = simulator(pop, randomMating(), rep=3)
>>> print simu.numChrom()
2.
>>>
```

# 2.2 Population

population objects are essential to simuPOP. They are composed of subpopulations each with certain number of individuals having the same genotypic structure. Class population has a large number of member functions, ranging from reviewing simple properties to generating a new population from the current one. Fortunately, you do not have to know all the member functions to use a population unless you need to write pure Python functions/operators that involves complicated manipulation of populations.

simuPOP uses one-level population structure. That is to say, there is no sub-subpopulation or family in subpopulations. Mating is within subpopulations only. Exchanges of genetic information across subpopulations can only be done through migration. Population and subpopulation sizes can be changed, as a result of mating or migration. More specifically,

- migration can change subpopulation size; create or remove subpopulations. Since migration can not generate new individuals, the total population size will not be changed.
- mating can fill any population/subpopulation structure with offspring. Both population and subpopulation sizes can be changed. Since mating is within subpopulations, you can not create a new subpopulation through mating.
- a special operator pySubset can shrink the population size. It removes individuals according to their subPopID() status. (Will explain later.) This can be used to model a sudden population decrease due to some natural disaster.
- subpopulations can be split or merged.

Note that migration will most likely change the subpopulation sizes. To keep the subpopulation sizes constant, you can set the subpopulation sizes during mating so that the next generation will have desired subpopulation sizes.

# 2.2.1 Class population

A collection of individuals with the same genotypic structure.

#### **Details**

A simuPOP population consists of individuals of the same genotypic structure, which refers to the number of chromosomes, number and position of loci on each chromosome etc. The most important components of a population are:

- subpopulation. A population is divided into subpopulations (unstructured population has a single subpopulation, which is the whole population itself). Subpopulation structure limits the usually random exchange of genotypes between individuals by disallowing mating between individuals from different subpopulations. In the presence of subpopulation structure, exchange of genetic information across subpopulations can only be done through migration. Note that in simuPOP there is no sub-subpopulation or family in subpopulations.
- variables. Every population has its own variable space, or *local namespace* in simuPOP term. This namespace is a Python dictionary that is attached to each population and can be exposed to the users through vars() or dvars() function. Many functions and operators work and store their results in this namespace. For example, function Stat sets variables such as alleleFreq[loc], and you can access it via pop.dvars().alleleFreq[loc][allele].
- ancestral generations. A population can save arbitrary number of ancestral generations. During evolution, the latest several (or all) ancestral generations are saved. Functions to switch between ancestral generations are provided so that one can examine and modify ancestral generations.

Other concepts like *information fields* are explained in class individual.

#### Note

Although a large number of member functions are provided, most of the operations are performed by *operators*. These functions will only be useful when you need to manipulate a population explicitly.

#### Initialization

Create a population object with given size and genotypic structure.

```
population(size=0, ploidy=2, loci=[], sexChrom=False, lociPos=[],
subPop=[], ancestralDepth=0, alleleNames=[], lociNames=[],
maxAllele=ModuleMaxAllele, infoFields=[], chromMap=[])
```

This is techniquely the \_\_init\_\_ function of the population object.

- alleleNames An array of allele names. For example, for a locus with alleles A,C,T,G, you can specify alleleNames as ('A','C','T','G').
- ancestralDepth Number of most recent ancestral generations to keep during evolution. Default to 0, which means only the current generation will be available. You can set it to a positive number m to keep the latest m generations in the population, or -1 to keep all ancestral populations. Note that keeping track of all ancestral generations may quickly exhaust your computer RAM. If you really need to do that, use savePopulation operator to save each generation to a file is a much better choice.
- chromMap For MPI modules, currently unused.
- infoFields Name of information fields that will be attached to each individual. For example, if you need to record the parents of each individual using operator c parentTagger(), you will need two fields father\_idx and mother\_idx.
- **loci** An array of numbers of loci on each chromosome. The length of parameter loci determines the number of chromosomes. Default to [1], meaning one chromosome with a single locus.
  - The last chromosome can be sex chromosome. In this case, the maximum number of loci on X and Y should be provided. I.e., if there are 3 loci on Y chromosme and 5 on X chromosome, use 5.
- **lociNames** An array or a matrix (separated by chromosomes) of names for each locus. Default to "locX-Y" where X is chromosome index and Y is locus number, both starting from 1.
- lociPos A 1-d or 2-d array specifying positions of loci on each chromosome. You can use a nested array to specify loci position for each chromosome. For example, you can use lociPos=[1,2,3] when loci=[3] or lociPos=[[1,2],[1.5,3,5]] for loci=[2,3]. simuPOP does not assume a unit for these positions, although they are usually interpreted as centiMorgans. The default values are 1, 2, etc. on each chromosome.
- maxAllele Maximum allele number. Default to the maximum allowed allele state of the current library. This will set a cap for all loci. For individual locus, you can specify maxAllele in mutation models, which can be smaller than global maxAllele but not larger. Note that this number is the number of allele states minus 1 since allele number starts from 0.
- **ploidy** Number of sets of homologous copies of chromosomes. Default to 2 (diploid).
- **sexChrom** TRUE or false. Diploid population only. If true, the last homologous chromosome will be treated as sex chromosome. (XY for male and XX for female.) If X and Y have different number of loci, number of loci of the longer one of the last (sex) chromosome should be specified in loci.
- size Population size. Can be ignored if subPop is specified. In that case, size is the sum of subPop. Default to 0.

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**subPop** An array of subpopulation sizes. Default value is [size] which means a single subpopulation of the whole population. If both size and subPop are provided, subPop should add up to size.

#### **Member Functions**

x.absIndIndex(ind, subPop) Return the absolute index of an individual in a subpopulation

index index of an individual in a subpopulation subPop
subPop subpopulation index (start from 0)

x.addInfoField(field, init=0) Add an information field to a population

**field** new information field. If it already exists, it will be re-initialized.

init initial value for the new field.

x.addInfoFields(fields, init=0) Add one or more information fields to a population

**fields** an array of new information fields. If one or more of the fields alreay exist, they will be re-initialized. **init** initial value for the new fields.

x.ancestralDepth() Ancestral depth of the current population

**Note:** The returned value is the number of ancestral generations exist in the population, not necessarily equals to the number set by setAncestralDepth().

**x.ancestralGen()** Currently used ancestral population (0 for the latest generation)

Current ancestral population activated by useAncestralPop(). There can be several ancestral generations in a population. 0 (current), 1 (parental) etc. When useAncestralPop(gen) is used, current generation is set to one of the parental generations, which is the information returned by this function. useAncestralPop(0) should always be used to set a population to its usual ancestral order after operations to the ancestral generation are done.

x.arrGenotype(order) Get the whole genotypes

Return an editable array of all genotypes of the population. You need to know how these genotypes are organized to safely read/write genotype directly.

```
order if order is true, individuals will be ordered such that pop.individual(x). arrGenotype()
== pop.arrGenotype()[x*pop. genoSize():(x+1)*pop. genoSize()].
```

**x.arrGenotype(subPop, order)** Get the whole genotypes of individuals in a subpopulation

Return an editable array of all genotype in a subpopulation.

order if order is true, individuals will be ordered.
subPop index of subpopulation (start from 0)

x.arrIndInfo(order) Get an editable array (Python list) of all information fields

The length of the array is infoSize()\*popSize().

**order** whether or not the list has the same order as individuals

x.arrIndInfo(subPop, order) Get an editable array (Python list) of all information fields

**order** whether or not the list has the same order as individuals

**x.clone(keepAncestralPops=-1)** Deep copy of a population. (In python, pop1 = pop will only create a reference to pop.)

This function by default copies all ancestral generations, but you can copy only one (current, keepAncestralPops=0), or specified number of ancestral generations.

x.evaluate(expr="", stmts="") Evaluate a python statment/expression in the population's local namespace

This function evaluates a Python statment( stmts )/expression( expr ) and return its result as a string. Optionally run statement( stmts ) first.

- x.execute(stmts="") Execute a statement (can be a multi-line string) in the population's local namespace
- x.gen() Current generation during evolution
- **x.grp()** Current group ID in a simulator which is not meaningful for a stand-alone population.
- x.indInfo(idx, order) Get information field idx of all individuals

idx index of the information field

order if true, sort returned vector in individual order

x.indInfo(name, order) Get information field name of all individuals

name name of the information field

order if true, sort returned vector in individual order

x.indInfo(idx, subPop, order) Get information field idx of all individuals in a subpopulation subPop

idx index of the information field

order if true, sort returned vector in individual order

subPop subpopulation index

x.indInfo(name, subPop, order) Get information field name of all individuals in a subpopulation
subPop

name name of the information field

order if true, sort returned vector in individual order

subPop subpopulation index

x.individual(ind, subPop=0) Reference to individualind in subpopulation subPop

This function is named individual in the Python interface.

ind individual index within subPop

**subPop** subpopulation index

**x.individuals()** Return an iterator that can be used to iterate through all individuals

Typical usage is

for ind in pop.individuals():

- **x.individuals(subPop)** Return an iterator that can be used to iterate through all individuals in subpopulation subPop
- x.insertAfterLoci(idx, pos, names=[]) Append loci at given locations

Append loci at some given locations. Alleles at inserted loci are initialized with zero allele.

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idx an array of locus index. The loci will be added *after* each index. If you need to append to the first locus of a chromosome, use insertBeforeLoci instead. If your index is the last locus of a chromosome, the appended locus will become the last locus of that chromosome. If you need to append multiple loci after a locus, repeat that locus number.

**names** an array of locus names. If this parameter is not given, some unique names such as "insX\_Y" will be given.

**pos** an array of locus positions. The positions of the appended loci have to be between adjacent markers.

## x.insertAfterLocus(idx, pos, name=string) Append an locus at a given location

insertAfterLocus(idx, pos, name) is a shortcut to insertAfterLoci([idx], [pos],
[name]).

## x.insertBeforeLoci(idx, pos, names=[]) Insert loci at given locations

Insert loci at some given locations. Alleles at inserted loci are initialized with zero allele.

idx an array of locus index. The loci will be inserted *before* each index. If you need to append to the last locus, use insertAfterLoci instead. If your index is the first locus of a chromosome, the inserted locus will become the first locus of that chromosome. If you need to insert multiple loci before a locus, repeat that locus number.

**names** an array of locus names. If this parameter is not given, some unique names such as "insX\_Y" will be given.

**pos** an array of locus positions. The positions of the appended loci have to be between adjacent markers.

#### x.insertBeforeLocus(idx, pos, name=string) Insert an locus at given location.

insertBeforeLocus(idx, pos, name) is a shortcut to insertBeforeLoci([idx], [pos],
[name])

# x.mergePopulation(pop, newSubPopSizes=[], keepAncestralPops=-1) Merge populations by individuals

Merge individuals from pop to the current population. Two populations should have the same genotypic structures. By default, subpopulations of the merged populations are kept. I.e., if you merge two populations with one subpopulation, the resulting population will have two subpopulations. All ancestral generations are also merged by default.

**keepAncestralPops** ancestral populations to merge, default to all (-1)

**newSubPopSizes** subpopulation sizes can be specified. The overall size should be the combined size of the two populations. Because this parameter will be used for all ancestral generations, it may fail if ancestral generations have different sizes. To avoid this problem, you can run mergePopulation without this parameter, and then adjust subpopulation sizes generation by generation.

**Note:** Population variables are not copied to pop.

## 

Two populations should have the same number of individuals. This also holds for any ancestral generations. By default, chromosomes of pop are appended to the current population. You can change this arrangement in two ways

- specify new chromosome structure using parameter newLoci and newLociPos. Loci from new and old populations are still in their original order, but chromosome number and positions can be changed in this way.
- specify by Chromosome = true so that chromosomes will be merged one by one. In this case, loci position of two populations are important because loci will be arranged in the order of loci position; and identical loci position of two loci in two populations will lead to error.

by Chromosome merge chromosome by chromosome, loci are ordered by loci position Default to False.

**newLociPos** the new loci position if number of loci on each chromosomes are changed with newNumLoci. New loci positions should be in order on the new chromosomes.

**newNumLoci** the new number of loci for the combined genotypic structure.

#### Note:

- Information fields are not merged.
- All ancestral generations are merged because all individuals in a population have to have the same genotypic structure.
- x.mergeSubPops(subPops=[], removeEmptySubPops=False) Merge given subpopulations

Merge subpopulations, the first subpopulation ID (the first one in array subPops) will be used as the ID of the new subpopulation. That is to say, all merged subpopulations will take the ID of the first one. The subpopulation ID of the empty subpopulations will be kept (so that other subpopulations are unaffected, unless they are removed by removeEmptySubPops = True).

- x.newPopByIndID(keepAncestralPops=-1, id=[], removeEmptySubPops=False) Form a new population according to individual subpopulation ID. Individuals with negative subpopulation ID will be removed.
- x.newPopWithPartialLoci(remove=[], keep=[]) Obtain a new population with selected loci

Copy current population to a new one with selected loci keep or remove specified loci remove (no change on the current population), equivalent to

```
y=x.clone
y.removeLoci(remove, keep)
```

- x.numSubPop() Number of subpopulations in a population
- x.popSize() Total population size
- **x.pushAndDiscard(rhs, force=False)** Absorb rhs population as the current generation of a population This function is used by a simulator to push offspring generation rhs to the current population, while the current population is pushed back as an ancestral population (if ancestralDepath() != 0). Because rhs population is swapped in, rhs will be empty after this operation.
- x.removeEmptySubPops() Remove empty subpopulations by adjusting subpopulation IDs
- x.removeIndividuals(inds=[], subPop=-1, removeEmptySubPops=False) Remove individuals. If a valid subPop is given, remove individuals from this subpopulation. Indexes in inds will be treated
  as relative indexes.
- **x.removeLoci(remove=[], keep=[])** Remove some loci from the current population. Only one of the two parameters can be specified.
- x.removeSubPops(subPops=[], shiftSubPopID=True, removeEmptySubPops=False)
  Remove subpopulations and adjust subpopulation IDs so that there will be no 'empty' subpopulation left
  Remove specified subpopulations (and all individuals within). If shiftSubPopID is false, subPopID will be kept intactly.
- x.reorderSubPops(order=[], rank=[], removeEmptySubPops=False) Reorder subpopulations
  by order or by rank
  - **order** new order of the subpopulations. For examples, 3 2 0 1 means subpop3, subpop2, subpop0, subpop1 will be the new layout.

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- rank you may also specify a new rank for each subpopulation. For example, 3,2,0,1 means the original subpopulations will have new IDs 3,2,0,1, respectively. To achive order 3,2,0,1, the rank should be 1 0 2
- x.rep() Current replicate in a simulator which is not meaningful for a stand-alone population
- x.resize(newSubPopSizes, propagate=False) Resize population

Resize population by giving new subpopulation sizes.

**newSubPopSizes** an array of new subpopulation sizes. If there is only one subpopulation, use [newPopSize].

**propagate** if propagate is true, copy individuals to new comers. I.e., 1, 2, 3 ==> 1, 2, 3, 1, 2, 3, 1

Note: This function only resizes the current generation.

x.savePopulation(filename, format="auto", compress=True) Save population to a file

filename save to filename

**format** format to save. Can be one of the following: 'txt', 'bin', or 'xml', or 'auto' which is determined by the extension of filename.

x.setAncestralDepth(depth) Set ancestral depth.

**depth** 0 for none, -1 for unlimited, a positive number sets the number of ancestral generations to save.

x.setIndInfo(values, idx, order=True) Set individual information for the given information field (index),

idx index to the information field.

order if true, info will be in the order of individuals

values an array that has the same length as population size.

x.setIndInfo(values, name) is equivalent to the idx version x.setIndInfo(values, x.infoIdx(name)).

x.setIndSubPopID(id) Set subpopulation ID with given ID

Set subpopulation ID of each individual with given ID. Individuals can be rearranged afterwards using setSubPopByIndID.

id an array of the same length of population size, resprenting subpopulation ID of each individual.

- x.setIndSubPopIDWithID() Set subpopulation ID of each individual with their current subpopulation ID
- x.setInfoFields(fields, init=0) Set information fields for an existing population. The existing fields
  will be removed.

fields an array of fields

**init** initial value for the new fields.

x.setSubPopByIndID(id=[]) Adjust subpopulation according to individual subpopulation ID.

Rearrange individuals to their new subpopulations according to their subpopulation ID (or the new given ID). Order within each subpopulation is not respected.

id new subpopulation ID, if given, current individual subpopulation ID will be ignored.

**Note:** Individual with negative info will be removed!

x.setSubPopStru(newSubPopSizes, allowPopSizeChange=False) Set population/subpopulation
structure given subpopulation sizes

allowPopSizeChange if this parameter is true, population will be resized.

**subPopSize** an array of subpopulation sizes. The population may or may not change according to parameter allowPopSizeChange if the sum of subPopSize does not match popSize.

x.splitSubPop(which, sizes, subPopID=[]) Split a subpopulation into subpopulations of given sizes

The sum of given sizes should be equal to the size of the split subpopulation. Subpopulation IDs can be specified. The subpopulation IDs of non-split subpopulations will be kept. For example, if subpopulation 1 of 0 1 2 3 is split into three parts, the new subpop id will be 0 (1 4 5) 2 3.

**Note:** subpop with negative ID will be removed. So, you can shrink one subpop by splitting and setting one of the new subpop with negative ID.

**x.splitSubPopByProportion(which, proportions, subPopID=[])** Split a subpopulation into subpopulations of given proportions

The sum of given proportions should add up to one. Subpopulation IDs can be specified.

**Note:** subpop with negative ID will be removed. So, you can shrink one subpop by splitting and setting one of the new subpop with negative ID.

- x.subPopBegin(subPop) Index of the first individual of a subpopulation subPop
- x.subPopEnd(subPop) Return the value of the index of the last individual of a subpopulation subPop plus 1
- x.subPopIndPair(ind) Return the (sp, idx) pair from an absolute index of an individual
- x.subPopSize(subPop) Return size of a subpopulation subPop

**subPop** index of subpopulation (start from 0)

- **x.subPopSizes()** Return an array of all subpopulation sizes
- x.swap(rhs) Swap the content of two populations
- x.turnOffSelection() Turn off selection for all subpopulations

This is only used when you would like to apply two selectors. Maybe using two different information fields.

- **x.useAncestralPop(idx)** Use an ancestral generation. 0 for the latest generation.
  - idx Index of the ancestral generation. 0 for current, 1 for parental, etc. idx can not exceed ancestral depth (see setAncestralDepth).
- **x.vars(subPop=-1)** Return variables of a population. If subPop is given, return a dictionary for specified subpopulation.

## **Example**

Example 2.2: Population initialization and member functions

```
>>> # use of population function
>>> # a Wright-Fisher population
>>> WF = population(size=100, ploidy=1, loci=[1])
>>>
>>> # a diploid population of size 10
>>> # there are two chromosomes with 5 and 7 loci respectively
>>> pop = population(size=10, ploidy=2, loci=[5, 7], subPop=[2, 8])
```

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```
>>>
>>> # a population with SNP markers (with names A,C,T,G)
>>> # range() are python functions
>>> pop = population(size=5, ploidy=2, loci=[5,10],
        lociPos=[range(0,5), range(0,20,2)],
       alleleNames=['A','C','T','G'],
        subPop=[2,3], maxAllele=3)
>>>
>>> #
>>> # population structure functions
>>> print pop.popSize()
>>> print pop.numSubPop()
>>> print pop.subPopSize(0)
>>> print pop.subPopSizes()
(2, 3)
>>> print pop.subPopBegin(1)
>>> print pop.subPopEnd(1)
>>> print pop.subPopIndPair(3)
(1, 1)
>>> print pop.absIndIndex(1,1)
3
>>>
>>> #
>>> # functions of setting population structure
>>> pop.setIndSubPopID([1,2,2,3,1])
>>> pop.setSubPopByIndID()
>>> pop.removeLoci(keep=range(2,7))
>>> Dump(pop)
Ploidy:
                        2
Number of chrom:
                        2
Number of loci:
                        3 2
Maximum allele state:
Loci positions:
                2 3 4
                0 2
Loci names:
                loc1-3 loc1-4 loc1-5
                loc2-1 loc2-2
population size:
                        5
                        4
Number of subPop:
                        0 2 2 1
Subpop sizes:
Number of ancestral populations:
individual info:
sub population 1:
   0: MU AAA AA | AAA AA
   1: MU AAA AA | AAA AA
sub population 2:
   2: MU AAA AA | AAA AA
   3: MU AAA AA | AAA AA
```

```
sub population 3:
   4: MU AAA AA | AAA AA
End of individual info.
No ancenstral population recorded.
>>>
>>> #
>>> # save and load population
>>> # save it in various formats, default format is "txt"
>>> pop = population(1000, loci=[2, 5, 10])
>>> pop.savePopulation("pop.txt")
>>> pop.savePopulation("pop.txt", compress=False)
>>> pop.savePopulation("pop.xml", format="xml")
>>> pop.savePopulation("pop.bin", format="bin")
>>>
>>> # load it in another population
>>> pop1 = LoadPopulation("pop.xml", format="xml")
>>>
```

## 2.2.2 Ancestral populations

By default, a population object only holds the current generation. All ancestral populations (generations) will be discarded. You can, however, keep as many ancestral generations as you wish, provided that you have enough RAM to store all these extra information.

Parameter ancestralDepth is used to specify the number of generations to keep. This parameter is default to 0, meaning keeping no ancestral population. You can specify a positive number n to store most recent n generations; or -1 to store all populations.

Several important usage of ancestral generations:

- dumper() operator and Dump() function has a parameter ancestralPops. If set to True, they will dump all ancestral generations.
- function population::setAncestralDepth() and operator setAncestralDepth() set the number of ancestral generations to keep for a population. A typical use of setAncestralDepth() is

```
simu.evolve(...
  setAncestralDepth(3, at=[-3])
)
```

which saves the last three generations in populations so that pedigree based sampling schemes can be used.

• pop.useAncestralPop(idx) set the current generation of population pop to idx generation. idx = 1 for the first ancestral generation, 2 for second ancestral ..., and 0 for the current generation. After this function, all functions, operators will be applied to this ancestral generation. You should always call setAncestralPop(0) after you examined the ancestral generations.

A typical use of this function is demonstrated in example 2.3. In this example, a population with two loci is created and with initial genotype 0. Two kamMutator with different mutation rates are applied to these two loci. Five most recent populations are kept. The allele frequencies at these generations are calculated afterward. (Note that this is not the best way to exam the changes of allele frequencies, a stat operator should be used.)

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## Example 2.3: Ancestral populations

```
>>> simu = simulator(population(10000, loci=[2]), randomMating())
>>> simu.evolve(
        ops = [
            setAncestralDepth(5, at=[-5]),
            kamMutator(rate=0.01, loci=[0], maxAllele=1),
            kamMutator(rate=0.001, loci=[1], maxAllele=1)
        ],
. . .
        end = 20
. . .
True
>>> pop = simu.population(0)
>>> # start from current generation
>>> for i in range(pop.ancestralDepth()+1):
        pop.useAncestralPop(i)
        Stat(pop, alleleFreq=[0,1])
. . .
        print '%d
                       %5f
                               %5f' % \
            (i, pop.dvars().alleleFreq[0][1], pop.dvars().alleleFreq[1][1])
. . .
. . .
      0.171450
                    0.018200
0
1
      0.162400
                    0.017250
      0.155750
                    0.017350
3
      0.149950
                    0.015800
4
      0.142700
                    0.015150
5
      0.138000
                    0.015150
>>> # restore to the current generation
>>> pop.useAncestralPop(0)
>>>
```

# 2.2.3 Save and Load a Population

Internally, population can be saved/loaded in "txt", "xml" or "bin" formats using savePopulation(file, format, compress=True) member function, global SavePopulation(pop, file, format) and LoadPopulation. (Yes, it is Load.. not load.. since savePopulation is a member function and LoadPopulation is a global function.) These formats have their own advantages and disadvantages:

- xml: most readable, easy transformation to other formats, largest file size
- bin: not readable, small file size. May not be portable.
- txt: human readable with no structure, portable, median file size.
- auto: the format is determined by the filename extension specified.

Populations are by default compressed in gzip format. If you are interested in viewing the content of the file, you can use compress=False when saving a population, or decompress the saved files using gzip -d command.

Populations can also be saved in other formats such as FSTAT so that they can be directly analyzed by other programs. These formats are not supported internally. They are handled in Python in the form of Python function or pure-Python operator. If you would like to save/load simuPOP population in your own format, you can do it by mimicking these functions in simuUtil.py.

Shared variables (c.f section 2.7) are also saved (except for big objects like samples). Since the number of shared variables can be very large, it maybe a good idea to clear these variables before you save a population. On the other

hand, you may want to save key parameters used to generate this population in the local namespace so that you will know these parameters after the population is loaded. For example, you can do

Example 2.4: Save population variables

```
pop.vars().clear()
pop.dvars().migrationRate = 0.002
pop.dvars().diseaseLoci = [4, 30]
SavePopulation(pop, 'pop.bin')
```

# 2.2.4 View a population (GUI, wxPython required)

Introduced in version 0.6.9, simuViewPop.py can be used to view a population. It can be used as a standalone application, or in an interactive session. First, you can use this script as a standalone application, simply run

```
simuViewPop.py mypop.bin
```

will fire a GUI and allow you to exam population property, genotype and calculate statistics.

In a Python session, import this module will provide a function viewPop, apply it on a in-memory population or a filename will have the same effect. For example,

Example 2.5: Use simuViewPop to view a population

```
import simuViewPop
simuViewPop.viewPop(myPop)
simuViewPop.viewPop(filename='mypop.bin')
```

## 2.3 Individuals

Individuals of a population can be accessed through individual(), or its iteration form individuals() function:

- individual (ind) returns the ind'th individual (absolute index) of the whole population.
- individual(ind, subPop) returns the ind'th (relative index) individual in the subPop'th subpopulation.
- individuals () return an iterator that can be used to iterate through all individuals in a population.
- individuals(subPop) return an iterator that can be used to iterate through all individuals in the subPop'th subpopulations.

For example, example 2.6 iterates through all individuals in subpopulation 2 using population::individual() function, while 2.7 uses population::individuals(). The latter is usually easier to use.

Example 2.6: Function population::individual()

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## 2.3.1 Class individual

Individuals with genotype, affection status, sex etc.

#### **Details**

Individuals are the building blocks of populations, each having the following individual information:

- shared genotypic structure information
- genotype
- sex, affection status, subpopulation ID
- optional information fields

Individual genotypes are arranged by locus, chromosome, ploidy, in that order, and can be accessed from a single index. For example, for a diploid individual with two loci on the first chromosome, one locus on the second, its genotype is arranged as 1-1-1 1-1-2 1-2-1 2-1-1 2-1-2 2-2-1 where x-y-z represents ploidy x chromosome y and locus z. An allele 2-1-2 can be accessed by allele(4) (by absolute index), allele(1, 1) (by index and ploidy) or allele(1, 1, 0) (by index, ploidy and chromosome).

#### Initialization

Individuals are created by populations automatically. Do not call this function directly.

```
individual()
```

#### **Member Functions**

- x.affected() Whether or not an individual is affected
- x.affectedChar() Return A or U for affection status
- x.allele(index) Return the allele at locus index

index absolute index from the beginning of the genotype, ranging from 0 to totNumLoci()\*ploidy()

x.allele(index, p) Return the allele at locus index of the p-th copy of the chromosomes

index index from the begining of the p-th set of the chromosomes, ranging from 0 to totNumLoci()
p index of the ploidy

- x.allele(index, p, ch) Return the allele at locus index of the ch-th chromosome of the p-th chromosome set
  - ch index of the chromosome in the p-th chromosome set

index index from the beginning of chromosome ch of ploidy p, ranging from 0 to numLoci (ch)

- **p** index of the polidy
- x.alleleChar(index) Return the name of allele(index)
- x.alleleChar(index, p) Return the name of allele(index, p)
- x.alleleChar(index, p, ch) Return the name of allele(idx, p, ch)
- x.arrGenotype() Return an editable array (a carray of length totNumLoci()\*ploidy()) of genotypes of an individual

This function returns the whole genotype. Although this function is not as easy to use as other functions that access alleles, it is the fastest one since you can read/write genotype directly.

```
x.arrGenotype(p, ch) Return a carray with the genotype of the ch-th chromosome of the p-th copy
x.arrInfo() Return a carray of all information fields (of size infosSize()) of this individual
x.info(idx) Get information field idx
     idx index of the information field
x.info(name) Get information field name
     Equivalent to info(infoIdx(name)).
     name name of the information field
x.setAffected(affected) Set affection status
x.setAllele(allele, index) Set the allele at locus index
     allele allele to be set
     index index from the begining of genotype, ranging from 0 to totNumLoci()*ploidy()
x.setAllele(allele, index, p) Set the allele at locus index of the p-th copy of the chromosomes
     allele allele to be set
     index index from the begining of the poloidy p, ranging from 0 to totNumLoci(p)
     p index of the poloidy
x.setAllele(allele, index, p, ch) Set the allele at locus index of the ch-th chromosome in the
     p-th chromosome set
     allele allele to be set
     ch index of the chromosome in ploidy p
     index index from the begining of the chromosome, ranging from 0 to numLoci(ch)
     p index of the ploidy
x.setInfo(value, idx) Set information field by idx
x.setInfo(value, name) Set information field by name
x.setSex(sex) Set sex. sex can be Male of Female.
x.setSubPopID(id) Set new subpopulation ID, pop.rearrangeByIndID will move this individual to that
     population
x.sex() Return the sex of an individual, 1 for males and 2 for females.
x.sexChar() Return the sex of an individual, M or F
x.subPopID() Return the ID of the subpopulation to which this individual blongs
     Note: subPopID is not set by default. It only corresponds to the subpopulation in which this individual resides
     after pop::setIndSubPopID is called.
x.unaffected() Equals to not affected()
```

**x.arrGenotype(p)** Return a carray with the genotype of the p-th copy of the chromosomes

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**Example** 

### Example 2.8: Individual member functions

```
>>> pop = population(500, loci=[2, 5, 10])
>>> # get an individual
>>> ind = pop.individual(9)
>>> # oops, wrong index
>>> ind = pop.individual(3)
>>> # you can access genotypic structure info
>>> print ind.ploidy()
>>> print ind.numChrom()
>>> # ...
>>> # as well as genotype
>>> print ind.allele(1)
>>> ind.setAllele(1,5)
>>> print ind.allele(1)
>>> # you can also use an overloaded function
>>> # with a second parameter being the ploidy index
>>> print ind.allele(1,1) # second locus at the second copy of chromosome
>>> # other information
>>> print ind.affected()
False
>>> print ind.affectedChar()
>>> ind.setAffected(1)
>>> print ind.affectedChar()
>>> print ind.sexChar()
M
>>>
```

# 2.4 Mating Scheme

### 2.4.1 Class mating

The base class of all mating schemes - a required parameter of simulator

### **Details**

Mating schemes specify how to generate offspring from the current population. It must be provided when a simulator is created. Mating can perform the following tasks:

- change population/subpopulation sizes;
- randomly select parent(s) to generate offspring to populate the offspring generation;
- apply during-mating operators;
- apply selection if applicable.

#### Initialization

Create a mating scheme (do not use this base mating scheme, use one of its derived classes instead)

```
mating(numOffspring=1.0, numOffspringFunc=None, maxNumOffspring=0,
mode=MATE_NumOffspring, newSubPopSize=[], newSubPopSizeExpr="",
newSubPopSizeFunc=None)
```

By default, a mating scheme keeps a constant population size, generates one offspring per mating event. These can be changed using certain parameters. newSubPopSize, newSubPopSizeExpr and newSubPopSizeFunc can be used to specify subpopulation sizes of the offspring generation. mode, numOffspring, maxNumOffspring can be used to specify how many offspring will be produced at each mating event. This mode parameter can be one of

- MATE\_NumOffspring: a fixed number of offspring at all mating events at this generation. If numOffspring is given, all generations use this fixed number. If numOffspringFunc is given, the number of offspring at each generation is determined by the value returned from this function.
- MATE\_NumOffspringEachFamily: each family can have its own number of offspring. Usually, numOffspringFunc is used to determine the number of offspring of each family. If numOffspring is used, MATE\_NumOffspringEachFamily is equivalent to MATE\_NumOffspring.
- MATE\_GeometricDistribution: a Geometric distribution with parameter numOffspring is used to determine the number of offspring of each family.
- MATE\_PoissonDistribution: a Poisson distribution with parameter numOffspring is used to determine the number of offspring of each family.
- MATE\_BinomialDistribution: a Binomial distribution with parameter numOffspring is used to determine the number of offspring of each family.
- MATE\_UniformDistribution: a Uniform distribution [a, b] with parameter numOffspring (a) and maxNumOffspring (b) is used to determine the number of offspring of each family.

maxNumOffspring Used when numOffspring is generated from a binomial distribution

newSubPopSize An array of subpopulaitons sizes

**newSubPopSizeExpr** An expression that will return the new subpopulation size

**newSubPopSizeFunc** A function that accepts an int parameter(generation), an array of current population size and return an array of subpopulation sizes. This is usually easier to use than its expression version of this parameter.

**numOffspring** The number of offspring or p for a random distribution. Default to 1. This parameter determines the number of offspring that a mating event will produce. Therefore, it determines the family size.

**numOffspringFunc** A Python function that returns the number of offspring or p

### **Member Functions**

x.clone() Deep copy of a mating scheme

### **Example**

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Example 2.9: Demographic models and control of number of offspring per mating event

```
>>> # arbitrary demographic model
>>> def lin inc(gen, oldsize=[]):
        return [10+gen]*5
>>> simu = simulator(
        population(subPop=[5]*5, loci=[1]),
        randomMating(newSubPopSizeFunc=lin_inc)
...)
>>> simu.evolve(
        ops = [
            stat(popSize=True),
. . .
            pyEval(r'"%d %d\n"%(gen, subPop[0]["popSize"])'),
        ],
. . .
        end=5
. . .
...)
0 10
1 11
2 12
3 13
4 14
5 15
True
>>>
>>> #
>>> # control the number of offspring per mating event
>>> # famSizes is only defined when DBG_MATING is defined
>>> TurnOnDebug(DBG_MATING)
>>> simu = simulator(population(50, loci=[1]),
        randomMating(numOffspring=2,
            maxNumOffspring=5,
            mode=MATE UniformDistribution))
>>> simu.step(ops=[])
>>> print simu.population(0).dvars().famSizes
[5, 2, 4, 2, 4, 3, 4, 3, 3, 2, 3, 5, 5, 2, 3]
>>> TurnOffDebug(DBG MATING)
Debug code DBG_MATING is turned off. cf. ListDebugCode(), TurnOnDebug().
>>>
```

### 2.4.2 Class noMating

A mating scheme that does nothing

#### **Details**

In this scheme, there is

- no mating. Parent generation will be considered as offspring generation.
- no subpopulation change. *During-mating* operators will be applied, but the return values are not checked. I.e., subpopsizes will be ignored although some during-mating operators may be applied.

### Initialization

Creat a scheme with no mating

```
noMating(numOffspring=1.0, numOffspringFunc=None, maxNumOffspring=0,
mode=MATE_NumOffspring, newSubPopSize=[], newSubPopSizeExpr="",
newSubPopSizeFunc=None)
```

#### Note

All parameters are ignored!

#### **Member Functions**

x.clone() Deep copy of a scheme with no mating

### 2.4.3 Class binomial Selection

A mating scheme that uses binomial selection, regardless of sex

#### **Details**

No sex information is involved (binomial random selection). Offspring is chosen from parental generation by random or according to the fitness values. In this mating scheme,

- numOffspring protocol is honored;
- population size changes are allowed;
- selection is possible;
- haploid populaton is allowed.

#### Initialization

Create a binomial selection mating scheme

```
binomialSelection(numOffspring=1., numOffspringFunc=None,
maxNumOffspring=0, mode=MATE_NumOffspring, newSubPopSize=[],
newSubPopSizeExpr="", newSubPopSizeFunc=None)
```

Please refer to class mating for parameter descriptions.

#### **Member Functions**

**x.clone()** Deep copy of a binomial selection mating scheme

# 2.4.4 Class randomMating

A mating scheme of basic sexually random mating

### **Details**

In this scheme, sex information is considered for each individual, and ploidy is always 2. Within each subpopulation, males and females are randomly chosen. Then randomly get one copy of chromosomes from father and mother. When only one sex exists in a subpopulation, a parameter (contWhenUniSex) can be set to determine the behavior. Default to continuing without warning.

### Initialization

Create a random mating scheme

```
randomMating(numOffspring=1., numOffspringFunc=None,
maxNumOffspring=0, mode=MATE_NumOffspring, newSubPopSize=[],
newSubPopSizeFunc=None, newSubPopSizeExpr="", contWhenUniSex=True)
```

contWhenUniSex Continue when there is only one sex in the population, default to true

Please refer to class mating for descriptions of other parameters.

maxNumOffspring Used when numOffspring is generated from a binomial distribution

**newSubPopSize** An array of subpopulation sizes, should have the same number of subpopulations as the current population

newSubPopSizeExpr An expression that will be evaluated as an array of subpopulation sizes

**newSubPopSizeFunc** An function that have parameter gen and oldSize (current subpopulation size)

**numOffspring** Number of offspring or p in some modes

**numOffspringFunc** A python function that determines the number of offspring or p

#### Member Functions

x.clone() Deep copy of a random mating scheme

# 2.4.5 Class pyMating

A Python mating scheme

#### **Details**

Hybird mating scheme. This mating scheme takes a Python function that accepts both the parental and offspring populations and this function is responsible for setting genotype, sex of the offspring generation. During-mating operators, if needed, have to be applied from this function as well. Note that the subpopulation size parameters are honored and the passed offspring generation has the desired (sub) population sizes. Parameters that control the number of offspring of each family are ignored.

This is likely an extremely slow mating scheme and should be used for experimental uses only. When a mating scheme is tested, it is recommended to implement it at the C++ level.

### Initialization

Create a Python mating scheme

```
pyMating(func=None, newSubPopSize=[], newSubPopSizeExpr="",
newSubPopSizeFunc=None)
```

**func** A Python function that accepts two parameters: the parental and the offspring populations. The offspring population is empty, and this function is responsible for setting genotype, sex etc. of individuals in the offspring generation.

### **Member Functions**

x.clone() Deep copy of a Python mating scheme

# 2.4.6 Determine the number of offspring during mating

The default value of numOffspring parameter makes a mating scheme produce one offspring per mating. This is the real random mating and should be used whenever possible. However, various situations require a larger family size or even changing the family size. simuPOP provides a comprehensive way to deal with this problem.

As described in the class reference, the method to determine the number of offspring is to set the mode parameter:

- MATE\_NumOffspring: if numOffspringFunc is not given, the number of offspring will be the constant numOffspring all the time. Otherwise, numOffspringFunc(gen) will be called **once** for each generation to get the number of offspring for the matings happen in this generation.
- MATE\_NumOffspringEachFamily: numOffspringFunc has to be given and will be called whenever a mating happens. Since numOffspringFunc can be **any** Python function, this mode allows arbitrary model of assigning the number of offspring during mating. The mode can be slow though.
- MATE\_GeometricDistribution: numOffspring or the result of numOffspringFunc (evaluated at each generation) will be considered as p for a geometric distribution. The number of offspring for each mating is determined by

$$P(k) = p(1-p)^{k-1}$$
 for  $k \ge 1$ 

• MATE\_PoissonDistribution: numOffspring or result of numOffspringFunc (evaluated at each generation) will be considered as p for a Poission distribution. The number of offspring for each mating is determined by

$$P(k) = \frac{p^{k-1}}{(k-1)!}e^{-p} \text{ for } k \ge 1$$

Since the mean of this shifted Poisson distribution is p + 1, you need to specify, for example, 2, if you want a mean family size 3.

• MATE\_BinomialDistribution: numOffspring or the result of numOffspringFunc (evaluated at each generation) will be considered as p for a Binomial distribution. Let  $N=\max$ NumOffspring, the number of offspring for each mating is determined by

$$P(k) = \frac{(n-1)!}{(k-1)!(n-k)!} p^{k-1} (1-p)^{n-k} \text{ for } N \ge k \ge 1$$

• MATE\_UniformDistribution: numOffspring or the result of numOffspringFunc (evaluated at each generation), and maxNumOffspring will be considered as *a*, *b* for a Uniform distribution, respectively. The number of offspring for each mating is determined by

$$P(k) = \frac{1}{b-a}$$
 for  $b \ge k \ge a$ 

Note that all these distributions are adjusted to produce at least one offspring.

### 2.4.7 Determine subpopulation sizes of the next generation

The default behavior of simuPOP is to use the same population/subpopulation sizes as those of the parent generation. You can change this behavior by setting one of newSubPopSize, newSubPopSizeExpr, and newSubPopSizeFunc parameters:

• If you would like to have fixed subpopulation sizes, use newSubPopSize=some\_fixed\_values. This is useful when subpopulation sizes are changed by migration and you do want to keep constant subpopulation sizes.

- If subpopulation sizes can be easily calculated through an expression, you can use newSubPopSizeExpr to determine the new subpopulation sizes. For example, newSubPopSizeExpr='[gen+10]' uses the generation number + 10 as the new population size. More complicated expressions can be used, maybe along with pyExec operators, but in these cases, a specialized function and newSubPopSizeFunc are recommended.
- A more organized (and thus recommended) way to set new population/subpopulation sizes is through parameter newSubPopSizeFunc. To use this parameter, you need to define a Python function that takes two parameters: the generation number and the current subpopulation sizes, and return an array of new subpopulation sizes (return [newsize] instead of newsize when you do not have any subpopulation structure). The example of class Mating demonstrates the use of this parameter.

# 2.4.8 Demographic change functions

newSubPopSizeFunc can take a function with parameters gen and oldSize. A few functions are defined in simuUtil.py that will return such a function with given parameters. All these functions support a burnin stage and then split to equal sized subpopulations. For all these functions, you can test them by

```
func = oneOfTheDemographicFunc(parameters)
gen = range(0, yourEndGen)
r.plot(gen, [func(x)[0] for x in gen])
```

numSubPop is default to 1. split is default to 0 or given burnin value. Population size change happens after burnin (start at burnin+1) and split happens at split.

```
ConstSize(size, split, numSubPop, bottleneckGen, bottleneckSize)
```

The population size is constant, but will split into numSubPop subpopulations at generation split. If bottleneckGen is specified, population size will be bottleneckSize at that generation.

```
LinearExpansion(initSize, endSize, end, burnin, split, numSubPop,
    bottleneckGen, bottleneckSize)
```

Linearly expand the population size from intiSize to endSize after burnin, split the population at generation split. If bottleneckGen is specified, population size will be bottleneckSize at that generation.

Exponentially expand the population size from intiSize to endSize after burnin, split the population at generation split. If bottleneckGen is specified, population size will be bottleneckSize at that generation.

```
InstantExpansion(initSize, endSize, end, burnin, split,
    numSubPop, bottleneckGen, bottleneckSize)
```

Instaneously expand the population size from intiSize to endSize after burnin, split the population at generation split. If bottleneckGen is specified, population size will be bottleneckSize at that generation.

#### 2.4.9 Sex chromosomes

Currently, only randomMating() in diploid population supports sex chromosomes. When sexChrom() is False, the sex of an offspring is determined randomly with probability 1/2. Otherwise, it is determined by the existence of Y chromosome, I.e., what kind of sex chromosome an offspring get from his father.

Recombinations on sex chromosomes of females (XX) are just like those on autosomes. However, this is not true in males. Currently, recombinations between male sex chromosomes (XY) are *not* allowed (a bug/feature of recombinators). This may change later if exchanges of genes between pseudoautosomal regions of XY need to be modeled.

# 2.5 Operators

### 2.5.1 Class baseOperator

Base class of all classes that manipulate populations

#### **Details**

Operators are objects that act on populations. They can be applied to populations directly using their function forms, but they are usually managed and applied by a simulator.

There are three kinds of operators:

- built-in: written in C++, the fastest. They do not interact with Python shell except that some of them set variables that are accessible from Python.
- hybrid: written in C++ but calls a Python function during simulation. Less efficient. For example, a hybrid mutator pyMutator determines if an allele will be mutated and call a user-defined Python function to mutate it.
- pure Python: written in Python. The same speed as Python. For example, a varPlotter can plot Python variables that are set by other operators.

Operators can be applied at different stages of the life cycle of a generation. It is possible for an operator to apply multiple times in a life cycle. For example, a savePopulation operator might be applied before and after mating to trace parental information. More specifically, operators can be applied at *pre-*, *during-*, *post-mating*, or a combination of these stages. Applicable stages are usually set by default but you can change it by setting stage=(PreMating|PostMating|DuringMating|PrePostMating) parameter. Some operators ignore stage parameter because they only work at one stage.

Operators do not have to be applied at all generations. You can specify starting/ending generation (parameter start, end), gaps between applicable generations (parameter step), or specific generations (parameter at). For example, you might want to start applying migrations after certain burn-in generations, or calculate certain statistics only sparsely. Generation numbers can count from the last generation, using negative generation numbers.

Most operators are applied to every replicate of a simulator during evolution. However, you can apply operators to one (parameter rep) or a group of replicates only (parameter grp). For example, you can initialize different replicates with different initial values and then start evolution. c.f. simulator::setGroup .Operators can have outputs, which can be standard (terminal) or a file. Output can vary with replicates and/or generations, and outputs from different operators can be accumulated to the same file to form table-like outputs.

Filenames can have the following format:

- 'filename' this file will be overwritten each time. If two operators output to the same file, only the last one will succeed;
- '>filename' the same as 'filename';
- '>>filename' the file will be created at the beginning of evolution (simulator::evolve) and closed at the end. Outputs from several operators are appended;
- '>>>filename' the same as '>>filename' except that the file will not be cleared at the beginning of evolution if it is not empty;
- '>' standard output (terminal);

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• " supress output.

The output filename does not have to be fixed. If parameter outputExpr is used (parameter output will be ignored), it will be evaluated when a filename is needed. This is useful when you need to write different files for different replicates/generations.

#### **Initialization**

Common interface for all operators (this base operator does nothing by itself.)

```
baseOperator(output, outputExpr, stage, begin, end, step, at, rep,
qrp, infoFields)
```

at An array of active generations. If given, stage, begin, end, and step will be ignored.

**begin** The starting generation. Default to 0. A negative number is allowed.

end Stop applying after this generation. A negative numbers is allowed.

```
grp Applicable group. Default to GRP_ALL. A group number for each replicate is set by simulator.__init__ or simulator::setGroup().
```

**output** A string of the output filename. Different operators will have different default output (most commonly '>' or ").

outputExpr An expression that determines the output filename dynamically. This expression will be evaluated against a population's local namespace each time when an output filename is required. For example, "'>>out%s\_%s.xml' % (gen, rep)" will output to >>>out1\_1.xml for replicate 1 at generation 1.

**rep** Applicable replicates. It can be a valid replicate number, REP\_ALL (all replicates, default), or REP\_LAST (only the last replicate). REP\_LAST is useful in adding newlines to a table output.

**step** The number of generations between active generations. Default to 1.

### Note

- Negative generation numbers are allowed for parameter begin, end and at. They are interpreted as endGen + gen + 1. For example, begin = -2 in simu.evolve(..., end=20) starts at generation 19.
- REP\_ALL, REP\_LAST, GRP\_ALL are special constant that can only be used in the constructor of an operator. That is to say, explicit test of rep() == REP\_LAST will not work.

#### **Member Functions**

- **x.apply(pop)** Apply to one population. It does not check if the operator is activated.
- x.clone() Deep copy of an operator
- **x.diploidOnly()** Determine if the operator can be applied only for diploid population
- **x.haploidOnly()** Determine if the operator can be applied only for haploid population
- x.infoField(idx) Get the information field specified by user (or by default)
- x.infoSize() Get the length of information fields for this operator

### Example

### Example 2.10: Common features of all operators

```
>>> simu = simulator(population(1), binomialSelection(), rep=2)
>>> op1 = pyOutput("a", begin=5, end=20, step=3)
>>> op2 = pyOutput("a", begin=-5, end=-1, step=2)
>>> op3 = pyOutput("a", at=[2,5,10])
>>> op4 = pyOutput("a", at=[-10,-5,-1])
>>> simu.evolve([pyEval(r"str(gen)+'\n'", begin=5, end=-1, step=2)],
                                   end=10)
5
5
7
7
9
9
True
>>> #
>>> #
>>> # operator group
>>> from simuUtil import *
>>> simu = simulator(population(1), binomialSelection(), rep=4,
        qrp=[1,2,1,2]
>>> simu.step(
       ops = [
. . .
            pyEval(r"grp+3", grp=1),
            pyEval(r"grp+6", grp=2),
. . .
            pyOutput('\n', rep=REP_LAST)
. . .
        ]
. . .
...)
4848
True
>>>
>>> #
>>> # parameter output
>>> simu = simulator(population(100), randomMating(), rep=2)
>>> simu.step(
        preOps=[
            initByFreq([0.2, 0.8], rep=0),
. . .
            initByFreq([0.5, 0.5], rep=1)],
. . .
        ops = [
            stat(alleleFreq=[0]),
            pyEval('alleleFreq[0][0]', output='a.txt')
. . .
        ]
. . .
...)
True
>>> # only from rep 1
>>> print open('a.txt').read()
0.465
>>>
>>> simu.step(
        ops = [
. . .
            stat(alleleFreq=[0]),
. . .
            pyEval('alleleFreq[0][0]', output='>>a.txt')
. . .
        ])
. . .
True
```

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```
>>> # from both rep0 and rep1
>>> print open("a.txt").read()
0.220.45
>>>
>>> outfile='>>>a.txt'
>>> simu.step(
        ops = [
            stat(alleleFreq=[0]),
            pyEval('alleleFreq[0][0]', output=outfile),
            pyOutput("\t", output=outfile),
. . .
            pyOutput("\n", output=outfile, rep=0)
        ],
. . .
True
>>> print open("a.txt").read()
0.220.450.245
0.45
>>> #
>>> # Output expression
>>> outfile="'>>a'+str(rep)+'.txt'"
>>> simu.step(
        ops = [
. . .
            stat(alleleFreq=[0]),
            pyEval('alleleFreq[0][0]', outputExpr=outfile)
        1
...)
True
>>> print open("a0.txt").read()
0.26
>>> print open("a1.txt").read()
0.475
>>>
```

### 2.6 Simulator

### 2.6.1 Class simulator

Simulator manages several replicates of a population, evolve them using given mating scheme and operators

#### **Details**

Simulators combine three important components of simuPOP: population, mating scheme and operator together. A simulator is created with an instance of population, a replicate number rep and a mating scheme. It makes rep number of replicates of this population and control the evolutionary process of them.

The most important function of a simulator is evolve(). It accepts an array of operators as its parameters, among which, preOps and postOps will be applied to the populations at the beginning and the end of evolution, respectively, whereas ops will be applied at every generation.

A simulators separates operators into *pre-*, *during-*, and *post-mating* operators. During evolution, a simulator first apply all pre-mating operators and then call the mate() function of the given mating scheme, which will call during-mating operators during the birth of each offspring. After mating is completed, post-mating operators are applied to the offspring in the order at which they appear in the operator list.

Simulators can evolve a given number of generations (the end parameter of evolve), or evolve indefinitely until a certain type of operators called terminator terminates it. In this case, one or more terminators will check the status of evolution and determine if the simulation should be stopped. An obvious example of such a terminator is a fixation-checker.

A simulator can be saved to a file in the format of 'txt', 'bin', or 'xml'. This allows youm to stop a simulator and resume it at another time or on another machine.

#### **Initialization**

Create a simulator

```
simulator(pop, matingScheme, stopIfOneRepStops=False,
applyOpToStoppedReps=False, rep=1, grp=[])
```

**applyOpToStoppedReps** If set, the simulator will continue to apply operators to all stopped replicates until all replicates are marked 'stopped'.

grp Group number for each replicate. Operators can be applied to a group of replicates using its grp parameter.

matingScheme A mating scheme

**population** A population created by population() function. This population will be copied rep times to the simulator. Its content will not be changed.

rep Number of replicates. Default to 1.

**stopIfOneRepStops** If set, the simulator will stop evolution if one replicate stops.

#### **Member Functions**

x.addInfoField(field, init=0) Add an information field to all replicates

Add an information field to all replicate, and to the simulator itself. This is important because all populations must have the same genotypic information as the simulator. Adding an information field to one or more of the replicates will compromise the integrity of the simulator.

**field** information field to be added

x.addInfoFields(fields, init=0) Add information fields to all replicates

Add given information fields to all replicate, and to the simulator itself.

- x.clone() Deep copy of a simulator
- x.evolve(ops, preOps=[], postOps=[], end=-1, dryrun=False) Evolve all replicates of the
  population, subject to operators

Evolve to the end generation unless end=-1. An operator (terminator) may stop the evolution earlier. ops will be applied to each replicate of the population in the order of:

- all pre-mating opertors
- during-mating operators called by the mating scheme at the birth of each offspring
- all post-mating operators If any pre- or post-mating operator fails to apply, that replicate will be stopped. The behavior of the simulator will be determined by flags applyOpToStoppedReps and stopIfOneRepStopss.

dryrun dryrun mode. Default to False.

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- end ending generation. Default to -1. In this case, there is no ending generation and a simulator will only be ended by a terminator. Otherwise, it should be a number greater than current generation number.
- **ops** operators that will be applied at each generation, if they are active at that generation. (Determined by the begin, end, step and at parameters of the operator.)

**postOps** operators that will be applied after evolution. evolve() function will *not* check if they are active.

**preOps** operators that will be applied before evolution. evolve() function will *not* check if they are active.

**Note:** When end = -1, you can not specify negative generation parameters to operators. How would an operator know which generation is the -1 generation if no ending generation is given?

- x.gen() Return the current generation number
- x.getPopulation(rep, destructive=False) Return a copy of populationrep

By default return a cloned copy of populationrep of the simulator. If destructive==True, the population is extracted from the simulator, leaving a defunct simulator.

**destructive** if true, destroy the copy of population within this simulator. Default to false. getPopulation(rep, true) is a more efficient way to get hold of a population when the simulator will no longer be used.

rep the index number of the replicate which will be obtained

- x.group() Return group indexes
- **x.numRep()** Return the number of replicates
- **x.population(rep)** Return a reference to the rep replicate of this simulator.
  - rep the index number of replicate which will be accessed

**Note:** The returned reference is temporary in the sense that the refered population will be invalid after another round of evolution. If you would like to get a persistent population, please use getPopulation(rep).

x.saveSimulator(filename, format="auto", compress=True) Save simulator in 'txt',
 'bin' or 'xml' format

compress whether or not compress the file in 'gzip' format

filename filename to save the simulator. Default to simu.

format format to save. Default to auto. I.e., determine the format by file extensions.

- x.setAncestralDepth(depth) Set ancestral depth of all replicates
- **x.setGen(gen)** Set the current generation. Usually used to reset a simulator.

gen new generation index number

- **x.setGroup(grp)** Set groups for replicates
- x.setMatingScheme(matingScheme) Set a new mating scheme
- x.step(ops=[], preOps=[], postOps=[], steps=1, dryrun=False) Evolve steps generation
- x.vars(rep, subPop=-1) Return the local namespace of populationrep, equivalent to x.population(rep).vars(subPop).

### 2.6.2 Generation number

Several aspects of the generation number may cause confusion:

- · generation starts from zero
- a generation number presents a 'to-be-evolved' generation
- the ending generation specified in evolve() will be executed

That is to say, a new simulator will have generation 0 (at the beginning of generation 0). If you do evolve(..., end=0), evolve will evolve one generation and stop at the beginning of generation 1.

It may sound strange that

```
evolve(end=2)
```

evolve the population 3 generations. Generation 0, generation 1, and generation 2. When you use start=0, step=5, end=10 for your operator, it will be applied at generations 0,5,10 etc. At the end of the simulation, current generation number is 3! (If you are familiar with C, this is like a for loop index). This is why you should test if a simulation is finished correctly by

```
if(simu.gen() == endGen+1)
```

instead of simu.gen() == endGen. (endGen is the value for parameter end).

# 2.6.3 Operator calling sequence

In a simulation, operators are applied at different stages, pre-, during-, and post-mating (controlled by stage parameter), at specified generations (controlled by begin, end, step, at parameters), and to specified replicates (controlled by rep, grp parameters). The order of applying operators usually does not matter but errors may occur if you are not careful. For example, stat(...) calculates the statistics of the current population. It is a pre-mating operator so you should set stage=PostMating and put it after all operators if you would like to measure a post-mating population. It also should be put before any operator (such as an terminator) that uses the shared variable set by stat(...).

If you are not sure about the calling sequence of operators, you can set the dryrun parameter of evolve() function to True. evolve will then print out the order of operators to apply. Consider that operators can be PreMating, PostMating, PrePostMating, DuringMating and the default value (parameter stage) may not be what you expect. Having a look at the calling sequence before the real evolution is always a good idea.

### 2.6.4 Save and Load

Using function saveSimulator, we can save a simulator to a file in the format of 'txt', 'bin', or 'xml'. However, a mating scheme can not be saved and has to be re-specified in LoadSimulator().

Example 2.11: Save and load a simulator

```
>>> simu.saveSimulator("s.txt")
>>> simu.saveSimulator("s.xml", format="xml")
>>> simu.saveSimulator("s.bin", format="bin")
>>> simu1 = LoadSimulator("s.txt", randomMating())
>>> simu2 = LoadSimulator("s.xml", randomMating(), format="xml")
>>> simu3 = LoadSimulator("s.bin", randomMating(), format="bin")
>>>
```

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# 2.7 Population variables

Populations are associated with Python variables. These variables are usually set by various operators but you can also set them manually. For example, stat operator calculates many population statistics and store the results in a population's local namespace.

### 2.7.1 vars() and dvars() functions

Conceptually, population variables are organized as follows (looking from a simulator's point of view):

```
simu.vars(0)
                    simu.vars(1) ...
                                         // replicate
  popSize
                      popSize
                                         // local namespace
  alleleFreq[0]
                      alleleFreq[0]
                                        // allele frequency at locus 1
  alleleFreq[1]
                      alleleFreq[1]
                                         // at locus 2
                      . . . .
  subPop[0]
                      subPop[0]
                                         // subpop namespace
                                         // subpopulation 1 size
   popSize
                        popSize
                        allaleFreq[0]
    allaleFreq[0]
                                         // allele frequency at locus 1
                                         // variables for subpop 2
  subPop[1]
                      subPop[1]
```

You can refer to these variables using population::vars() or population::dvars() function. The returned values of vars() and dvars() reflect the same dictionary, but dvars() uses a little Python magic so that you can use attribute syntax to access dictionary keys. Because a.allaleFreq[0] is easier to read than a ['alleleFreq'][0], dvars() is more frequently used.

There are several ways to use these two functions

- pop.vars(), pop.dvars() return the variables of population pop
- pop.vars(subPop), pop.dvars(subPop) returns dictionary pop.vars()['subPop'][subPop]
- simu.vars(rep), simu.dvars(rep) return the variables of the rep'th population of simulator simu, i.e. simu.population(rep).vars().
- simu.vars(rep, subPop), simu.dvars(rep, subPop) returns dictionary simu.vars(rep)['subPop'][subPop]

Direct access to variables pop.vars()['subPop'][subPop] is provided because statistics calculator stat, by default, calculates the same set of statistics for all subpopulations (and the whole population).

To have a look at all variables defined in this dictionary, you can use function ListVars defined in simuUtil.py. With wxPython installed, this function opens a nice window with a tree representing the variables. Without wxPython (or use parameter useWxPython=False), variables are displayed in an indented form. Several parameters can be used to limit your display. They are

- level: the level of the tree, further nested variables will not be displayed
- name: the name of the variable to display
- subPop: whether or not display variables for each subpopulation.

### Example 2.12: Population variables

```
>>> from simuUtil import ListVars
>>> pop = population(subPop=[1000, 2000], loci=[1])
>>> InitByFreq(pop, [0.2, 0.8])
>>> ListVars(pop.vars(), useWxPython=False)
 rep : -1
 grp : -1
>>> Stat(pop, popSize=1, alleleFreq=[0])
>>> # subPop is True by default, use name to limit the variables to display
>>> ListVars(pop.vars(), useWxPython=False, subPop=False, name='alleleFreq')
 alleleFreq :
   [0]
     [0]
                0.1973333333333
     [1]
                0.802666666667
>>> # print number of allele 1 at locus 0
>>> print pop.vars()['alleleNum'][0][1]
>>> print pop.dvars().alleleNum[0][1]
4816
>>> print pop.dvars().alleleFreq[0]
[0.19733333333333333, 0.80266666666666664]
>>> print pop.dvars(1).alleleNum[0][1]
3223
>>>
```

# 2.7.2 Local namespace, pyEval and pyExec operators

Population variables is a Python dictionary, and furthermore a *Local namespace*, which means that you can use dictionary items as variables during evaluation. To evaluate in a population's local namespace, you can use function population::evalulate() or population::execute(). For example:

Example 2.13: Local namespaces of populations

```
>>> pop = population(subPop=[1000, 2000], loci=[1])
>>> InitByFreq(pop, [0.2, 0.8])
>>> Stat(pop, popSize=1, alleleFreq=[0])
>>> print pop.evaluate('alleleNum[0][0] + alleleNum[0][1]')
>>> pop.execute('newPopSize=int(popSize*1.5)')
>>> ListVars(pop.vars(), level=1, useWxPython=False)
newPopSize :
                4500
grp : -1
rep: -1
                3000
popSize :
numSubPop :
alleleNum :
   list of length 1
 subPopSize :
   list of length 2
alleleFreq :
   list of length 1
 subPop
   list of length 2
>>> # this variable is 'local' to the population and is
```

```
>>> # not available in the main namespace
  >>> newPopSize
  Traceback (most recent call last):
    File "refManual.py", line 1, in ?
  NameError: name 'newPopSize' is not defined
  >>> simu = simulator(population(10),noMating(), rep=2)
  >>> # evaluate an expression in different areas
  >>> print simu.vars(1)
  {'rep': 1, 'gen': 0, 'grp': 1}
  >>> print simu.population(0).evaluate("grp*2")
  >>> print simu.population(1).evaluate("grp*2")
  >>> # a statement (no return value)
  >>> simu.population(0).execute("myRep=2+rep*rep")
  >>> simu.population(1).execute("myRep=2*rep")
  >>> print simu.vars(0)
  {'rep': 0, 'myRep': 2, 'gen': 0, 'grp': 0}
  >>>
These two functions are rarely used, because
  pop.evaluate('alleleNum[0][1] + 1')
is equivalent to
  pop.dvar().alleleNum[0][1] + 1
```

Operators pyEval/pyExec are more useful in that they can be applied to different populations during evolution, and report statistics calculated by operator stat dynamically. The difference between these two operators are that pyEval evaluates a Python expression and returns its value, while pyExec executes a list of statements in the form of a multi-line string, and does not return any value.

Example 2.14: Use of operators pyEval and pyExec

```
>>> simu = simulator(population(100, loci=[1]),
        randomMating(), rep=2)
>>> simu.evolve(
        preOps = [initByFreq([0.2, 0.8])],
        ops = [ stat(alleleFreq=[0]),
. . .
            pyExec('myNum = alleleNum[0][0] * 2'),
            pyEval(r'"gen %d, rep %d, num %d, myNum %d\n"' \
                 ' % (gen, rep, alleleNum[0][0], myNum)')
. . .
        end=2
. . . )
gen 0, rep 0, num 26, myNum 52
gen 0, rep 1, num 34, myNum 68
gen 1, rep 0, num 24, myNum 48
gen 1, rep 1, num 27, myNum 54
gen 2, rep 0, num 18, myNum 36
gen 2, rep 1, num 18, myNum 36
True
>>>
```

# 2.8 Information fields

An individuals have genotype, sex and affection status information, but other information may be needed. For example, one or more trait values may be needed to calculate quantitative traits, and one may want to keep track of all offspring of a parent. Because the need for information fields varies from simulation to simulation, simuPOP does not fix the amount of information fields, and allow users to specify these fields during the construction of populations, or add them when you need them.

Operators may require certain information fields to work properly. For example, all selectors require field fitness to store evaluated fitness values for each individual. parentTagger needs father\_idx and mother\_idx to store indices of the parents of each individual in the parental generation. These information fields can be added by the infoFields parameter of the population constructor or be added later using relevant function. If a required information field is unavailable, an error message will appear and tell you which field is needed. Some operators allow you to specify which information field(s) to use. For example, quantitative trait operator can work on specified fields so an individual can have several quantitative traits.

The information fields is usually set during population creation, using the infoFields option of population constructor. It can also be set or added by functions

- pop.setInfoFields(fields, init) set information fields of a population, removing all previous ones
- pop.addInfoField(field, init) add an information field to a population
- pop.addInfoFields(fields, init) add information fields to a population
- simu.addInfoField(field, init) add an information field to all populations in a simulator
- simu.addInfoFields(fields, init) add information fields to all populations in a simulator

When adding information fields to a simulator, information fields are added to all populations of the simulator. Note that it is illegal to add information field (or in a broader sense changing genotypic structure) to part of the populations of a simulator, because all populations in a simulator should have the same genotypic structure.

One can read/write information fields at individual level:

- ind.info(idx), ind.info(name) return individual information field by index or name
- ind.setInfo(value, idx), ind.setInfo(value, name) set individual information field by index or name
- ind.arrInfo() returns a carray of all information fields of an individual

or at the population level

- pop.indInfo(idx, order), pop.indInfo(name, order) return an information field (referred by index or name) of all individuals
- pop.indInfo(idx, subPop, order), pop.indInfo(name, subPop, order) return an information field (referred by index or name) of all individuals in a subpopulation subPop.
- pop.setIndInfo(values, idx, order), pop.setInfIndo(values, name, order) set information fields of all individuals with values in an array.
- pop.arrIndInfo(order) return an carray of all information fields
- pop.arrIndInfo(subPop, order) return an carray of all information fields of subpopulation subPop.

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Both idx or name can be used in these functions. name is easier to use but idx, which can be obtained by idx=pop.infoIdx(name), is faster. Although population information fields are kept in a population object linearly, there is no guarantee that they are ordered. If you would like to access info individual by individual, passing order=True to these functions will ensure that the returned information fields are ordered by individual order. If you only need to get a summary of some information fields, passing order=False will speed up the process.

ind.arrInfo() returns an carray f1, f2, f3 (assuming infoSize()==3) of individual ind. At a population level, pop.arrIndInfo([subPop], order) returns a carray of f1, f2, f3, f1, f2, f3, ... of individual information fields, which are not necessarily in the order of individuals unless order = True is set. indInfo is more convenient but it is less efficient than arrIndInfo. For example, the following two examples both assign an information field from the value of another one, but 2.16 is more efficient.

Example 2.15: Use regular information field function

```
>>> pop = population(10, infoFields=['a', 'b'])
>>> aIdx = pop.infoIdx('a')
>>> bIdx = pop.infoIdx('b')
>>> for ind in pop.individuals():
       a = ind.info(aIdx)
       ind.setInfo(a+1, bIdx)
. . .
. . .
>>> print pop.indInfo(bIdx, False)
>>>
                Example 2.16: Use carray information fields function
>>> pop = population(10, infoFields=['a', 'b'])
>>> aldx = pop.infoldx('a')
>>> bIdx = pop.infoIdx('b')
>>> info = pop.arrIndInfo(False)
>>> sz = pop.infoSize()
>>> for idx in range(pop.popSize()):
       info[sz*idx + bIdx] = info[sz*idx + aIdx] + 1
>>> print pop.indInfo(bIdx, False)
```

**CHAPTER** 

THREE

# Operator References

This chapter will list all functions, types and operators by category. The reference for class baseOperator is in section 2.5.

# 3.1 Python operators

A Python operator that works directly on simuPOP population or individuals.

# 3.1.1 Class pyOperator

A python operator that directly operate a population.

#### **Details**

This operator accepts a function that can take the form of

- func(pop) when stage=PreMating or PostMating, without setting param;
- func(pop, param) when stage=PreMating or PostMating, with param;
- func(pop, off, dad, mom) when stage=DuringMating and passOffspringOnly=False, without setting param;
- func(off) when stage=DuringMating and passOffspringOnly=True, and without setting param;
- func(pop, off, dad, mom, param) when stage=DuringMating and passOffspringOnly=False, with param;
- func(off, param) when stage=DuringMating and passOffspringOnly=True, with param.

For Pre- and PostMating usages, a population and an optional parameter is passed to the given function. For DuringMating usages, population, offspring, its parents and an optional parameter are passed to the given function. Arbitrary operations can be applied to the population and offspring (if stage=DuringMating).

### Initialization

Python operator, using a function that accepts a population object.

```
pyOperator(func, param=None, stage=PostMating, formOffGenotype=False,
passOffspringOnly=False, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

formOffGenotype This option tells the mating scheme this operator will set the genotype of offspring (valid only for stage=DuringMating). By default (formOffGenotype=False), a mating scheme will set the genotype of offspring before it is passed to the given Python function. Otherwise, a 'blank' offspring will be passed.

**func** A Python function. Its form is determined by other parameters.

**param** Any Python object that will be passed to func after pop parameter. Multiple parameters can be passed as a tuple.

passOffspringOnly If True, pyOperator will expect a function of form func(off [,param]), instead of func(pop, off, dad, mom [, param]) which is used when passOffspringOnly is False. Because many during-mating pyOperator only need access to offspring, this will improve efficiency. Default to False.

#### Note

- Output to output or outputExpr is not supported. That is to say, you have to open/close/append to files explicitly in the Python function.
- This operator can be applied Pre-, During- or Post- mating and is applied PostMating by default. For example, if you would like to examine the fitness values set by a selector, a PreMating Python operator should be used.

### **Member Functions**

**x.apply(pop)** Apply the pyOperator operator to one population

```
x.clone() Deep copy of a pyOperator operator
```

A Python operator accepts a function and an optional parameter. When pyOperator is called, it will simply pass the accepted population (or parents and offspring in the case of stage=DuringMating) to the function. To use this operator, in case of stage=PostMating, you will need to

• define a function that handle a population as you wish.

```
def myOperator(pop, para):
    'do whatever you want'
    return True
```

If you return False, this operator will work like a terminator.

• use pyOperator in the form of

```
pyOperator(mfunc=pyOperator, param=para)
```

all parameters of an operator are supported except for output and outputExpr which are ignored for now.

This operator allows implementation of arbitrarily complicated operators,. To use this operator, you will have to know how to use population-related functions. The following example shows how to implement a dynamic mutator which mutate loci according to their allele frequencies.

```
Example 3.1: Define a python operator
```

```
>>> def dynaMutator(pop, param):
...
''' this mutator mutate common loci with low mutation rate
and rare loci with high mutation rate, as an attempt to
```

```
bring allele frequency of these loci at an equal level.''
           # unpack parameter
           (cutoff, mu1, mu2) = param;
  . . .
           Stat(pop, alleleFreq=range( pop.totNumLoci() ) )
           for i in range( pop.totNumLoci() ):
  . . .
               # 1-freq of wild type = total disease allele frequency
               if 1-pop.dvars().alleleFreq[i][1] < cutoff:</pre>
                    KamMutate(pop, maxAllele=2, rate=mu1, loci=[i])
               else:
                    KamMutate(pop, maxAllele=2, rate=mu2, loci=[i])
           return True
  ... #end
  . . .
                            Example 3.2: Use of python operator
  >>> pop = population(size=10000, ploidy=2, loci=[2, 3])
  >>> simu = simulator(pop, randomMating())
  >>>
  >>> simu.evolve(
           preOps = [
               initByFreq( [.6, .4], loci=[0,2,4]),
  . . .
               initByFreq([.8, .2], loci=[1,3])],
  . . .
           ops = [
               pyOperator( func=dynaMutator, param=(.5, .1, 0) ),
               stat(alleleFreq=range(5)),
               pyEval(r'"%f\t%f\n"%(alleleFreq[0][1],alleleFreq[1][1])', step=10)
  . . .
               ],
           end = 30
  ...)
  0.398250
                    0.202200
                    0.208100
  0.396300
  0.391300
                    0.192250
  0.393250
                    0.182500
  True
  >>>
pyOperator can also be a during-mating operator. You will need to define a function
  def Func(pop, off, dad, mom, para)
  def shortFunc(off, para)
where para can be ignored. To use this operator, you can do
  pyOperator(stage=DuringMating, func=Func, param=someparam, formOffGenotype=True)
  pyOperator(stage=DuringMating, func=shortFunc, param=someparam,
  formOffGenotype=False, passOffspringOnly=True)
```

If your during-mating pyOpeartor returns False, the individual will be discarded. Therefore, you can write a filter in this way. However, since the Python function will be called for each mating event, the cost of using such an operator is high, especially when population size is large.

or

or

An example of during-mating pyOperator can be found in scripts/demoPyOperator.py.

### 3.1.2 Class pyIndOperator

Individual operator

#### **Details**

This operator is similar to a pyOperator but works at the individual level. It expects a function that accepts an individual, optional genotype at certain loci, and an optional parameter. When it is applied, it passes each individual to this function. When infoFields is given, this function should return an array to fill these infoFields. Otherwise, True/False is expected. More specifically, func can be

- func (ind) when neither loci nor param is given.
- func(ind, genotype) when loci is given
- func(ind, param) when param is given
- func(ind, genotype, param) when both loci and param are given.

#### Initialization

A Pre- or PostMating Python operator that apply a function to each individual

```
pyIndOperator(func, loci=[], param=None, stage=PostMating,
formOffGenotype=False, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

func A Python function that accepts an individual and optional genotype and parameters.

infoFields If given, func is expected to return an array of the same length and fill these infoFields of an individual.

**param** Any Python object that will be passed to func after pop parameter. Multiple parameters can be passed as a tuple.

### **Member Functions**

- **x.apply(pop)** Apply the pyIndOperator operator to one population
- x.clone() Deep copy of a pyIndOperator operator

### **Example**

### Example 3.3: Applying a pyIndOperator

```
>>> def indFunc(ind, param):
...     ind.setInfo(ind.info('info2')+param[1], 'info2')
...     print ind.info('info2')
...     return True
...
>>> simu = simulator(
...     population(5, loci=[2,5], infoFields=['info1', 'info2']),
...     randomMating(), rep=1)
>>> simu.step(
```

# 3.2 Initialization

### 3.2.1 Class initializer

Initialize alleles at the start of a generation

#### **Details**

Initializers are used to initialize populations before evolution. They are set to be PreMating operators by default. simuPOP provides three initializers. One assigns alleles by random, one assigns a fixed set of genotypes, and the last one calls a user-defined function.

#### Initialization

Create an initializer. default to be always active

```
initializer(subPop=[], indRange=[], loci=[], atPloidy=-1,
maleFreq=0.5, sex=[], stage=PreMating, begin=0, end=-1, step=1,
at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

atPloidy Initialize which copy of chromosomes. Default to all.

indRange A [begin, end] pair of the range of absolute indexes of individuals, for example, ([1,2]); or an array of [begin, end] pairs, such as ([[1,4],[5,6]]). This is how you can initialize individuals differently within subpopulations. Note that ranges are in the form of [a,b). I.e., range [4,6] will intialize individual 4, 5, but not 6. As a shortcut for [4,5], you can use [4] to specify one individual.

loci A vector of locus indexes at which initialization will be done. If empty, apply to all loci.

locus A shortcut to loci

maleFreq Male frequency. Default to 0.5. Sex will be initialized with this parameter.

**subPop** An array specifies applicable subpopulations

### **Member Functions**

```
x.clone() Deep copy of an initializer
```

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### 3.2.2 Class initByFreq (Function form: InitByFreq)

Initialize genotypes by given allele frequencies, and sex by male frequency

#### **Details**

This operator assigns alleles at loci with given allele frequencies. By default, all individuals will be assigned with random alleles. If identicalInds=True, an individual is assigned with random alleles and is then copied to all others. If subPop or indRange is given, multiple arrays of alleleFreq can be given to given different frequencies for different subpopulation or individual ranges.

#### **Initialization**

Randomly assign alleles according to given allele frequencies

```
initByFreq(alleleFreq=[], identicalInds=False, subPop=[],
indRange=[], loci=[], atPloidy=-1, maleFreq=0.5, sex=[],
stage=PreMating, begin=0, end=1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

**alleleFreq** An array of allele frequencies. The sum of all the frequencies must be 1; or for a matrix of allele frequencies, each row corresponses to a subpopulation or range.

**identicalInds** Whether or not make individual genotypies identical in all subpopulation. If True, this operator will randomly generate genotype for an individual and spread it to the whole subpopulation in the given range.

**sex** An array of sex [Male, Female, Male...] for individuals. The length of sex will not be checked. If it is shorter than the number of individuals, sex will be reused from the beginning.

stage Default to PreMating

### **Member Functions**

```
x.apply(pop) Apply this operator to populationpop
```

```
x.clone() Deep copy of the operator initByFreq
```

### **Example**

### Example 3.4: Operator initByFreq

```
End of individual info.

No ancenstral population recorded.
True
>>>
```

# 3.2.3 Class initByValue (Function form: InitByValue)

Initialize genotype by value and then copy to all individuals

#### **Details**

Operator initByValue gets one copy of chromosomes or the whole genotype (or of those corresponds to loci) of an individual and copy them to all or a subset of individuals. This operator assign given alleles to specified individuals. Every individual will have the same genotype. The parameter combinations should be

- value subPop/indRange: individual in subPop or in range(s) will be assigned genotype 'value';
- subPop/indRange: subPop or indRange should have the same length as values. Each item of values will be assigned to each subPop or indRange.

#### **Initialization**

Initialize populations by given alleles

```
initByValue(value=[], loci=[], atPloidy=-1, subPop=[], indRange=[],
proportions=[], maleFreq=0.5, sex=[], stage=PreMating, begin=0,
end=1, step=1, at=[], rep=REP ALL, grp=GRP ALL, infoFields=[])
```

maleFreq Male frequency

proportions An array of percentages for each item in values. If given, assign given genotypes randomly.

**sex** An array of sex [Male, Female, Male...] for individuals. The length of sex will not be checked. If length of sex is shorter than the number of individuals, sex will be reused from the beginning.

stages Default to PreMating

value An array of genotypes of one individual, having the same length as the length of loci() or loci()\*ploidy() or pop.genoSize() (whole genotype) or totNumLoci() (one copy of chromosome). This parameter can also be an array of arrays of genotypes of one individual. Should have length one or equal to subpop or ranges or proportion. If value is an array of values, it should have the same length as subpop, indRange or proportions.

### **Member Functions**

```
x.apply(pop) Apply this operator to populationpop
```

**x.clone()** Deep copy of the operator initByValue

#### **Example**

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#### Example 3.5: Operator initByValue

```
>>> simu = simulator(
        population(subPop=[2,3], loci=[5,7], maxAllele=9),
        randomMating(), rep=1)
>>> simu.step([
        initByValue([1]*5 + [2]*7 + [3]*5 + [4]*7),
        dumper(alleleOnly=True)])
individual info:
sub population 0:
   0: FU 33333 2222222 | 33333 2222222
   1: MU 11111 4444444 | 11111 4444444
sub population 1:
   2: FU 33333 4444444 | 33333 2222222
   3: FU 11111 4444444 | 11111 2222222
   4: FU 11111 2222222 | 33333 2222222
End of individual info.
No ancenstral population recorded.
>>>
```

# 3.2.4 Class spread (Function form: Spread)

Copy the genotype of an individual to all individuals

#### **Details**

Function Spread(ind, subPop) spreads the genotype of ind to all individuals in an array of subpopulations. The default value of subPop is the subpopulation where ind resides.

### Initialization

Copy genotypes of ind to all individuals in subPop

```
spread(ind, subPop=[], stage=PreMating, begin=0, end=1, step=1,
at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

### **Member Functions**

**x.apply(pop)** Apply this operator to populationpop

x.clone() Deep copy of the operator spread

### **Example**

### Example 3.6: Operator spread

```
>>> pop = population(ploidy=2, loci=[2], subPop=[4, 4])
>>> InitByFreq(pop, [.5, .5])
>>> Spread(pop, 2, subPop=[1]),
(None,)
>>> Dump(pop)
Ploidy: 2
Number of chrom: 1
```

```
Number of loci:
Maximum allele state:
                         255
Loci positions:
                 1 2
Loci names:
                 loc1-1 loc1-2
population size:
                         8
                         2
Number of subPop:
Subpop sizes:
                         4 4
                                          0
Number of ancestral populations:
individual info:
sub population 0:
   0: FU
           1 0 |
                        1
                     1
           1
   1: MU
              1 |
                     1
                        1
              1 |
                        0
   2: MU
           1
                     1
   3: MU
           1
              1 |
sub population 1:
   4: FU
           1 1
                     1
   5: MU
                       0
           1
              1 |
                     1
   6: MU
           1
              1
                     1
                        0
   7: FU
           1
              1 |
                     1
End of individual info.
No ancenstral population recorded.
>>>
```

# 3.2.5 Class pyInit (Function form: PyInit)

A python operator that uses a user-defined function to initialize individuals.

#### **Details**

PYINIT is a hybrid initializer. User should define a function with parameters allele, ploidy and subpopulation indexes, and return an allele value. Users of this operator must supply a Python function with parameter (index, ploidy, subpop). This operator will loop through all individual in each subpopulation and call this function to initialize populations. The arrange of parameters allows different initialization scheme for each subpop.

#### Initialization

Initialize populations using given user function

```
pyInit(func, subPop=[], loci=[], atPloidy=-1, indRange=[],
maleFreq=0.5, sex=[], stage=PreMating, begin=0, end=1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

atPloidy Initialize which copy of chromosomes. Default to all.

**func** A Python function with parameter (index, ploidy, subpop), where

- index is the allele index ranging from 0 to totNumLoci(-1),
- ploidy is the index of the copy of chromosomes)
- subpop is the subpopulation index.

The return value of this function should be an integer.

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```
loci A vector of loci indexes. If empty, apply to all loci.
```

```
locus A shortcut to loci
```

```
stage Default to PreMating
```

#### **Member Functions**

- **x.apply(pop)** Apply this operator to populationpop
- x.clone() Deep copy of the operator pyInit

### **Example**

Example 3.7: Operator pyInit

```
>>> def initAllele(ind, p, sp):
     return sp + ind + p
>>> simu = simulator(
       population(subPop=[2,3], loci=[5,7]),
       randomMating(), rep=1)
>>> simu.step([
       pyInit(func=initAllele),
       dumper(alleleOnly=True, dispWidth=2)])
individual info:
sub population 0:
                            7 8 9 10 11 12 |
   0: MU
          0 1 2
                                                 1 2 3 4
  8 9 10 11
   1: MU
          0 1 2 3
                               7
                                  8 9 10 11 |
7 8 9 10 11
sub population 1:
                               8
                                 9 10 11 12 |
                                                    2
   2: MU
          1 2 3
                                                 1
                                                                   8
9 10 11 12 13
  3: FU
             2
                     5
                            7 8 9 10 11 12
                                                   2
                                                      3
          1
                3
                   4
                          6
                                                 1
                                                                  8
9 10 11 12 13
   4: MU
                               8 9 10 11 12 |
          2 3 4 5 6
                          6 7
                                                 2
                                                   3
                                                         5
                                                                7
9 10 11 12 13
End of individual info.
No ancenstral population recorded.
True
>>>
```

# 3.3 Migration

### 3.3.1 Class migrator

Migrate individuals from a (sub) population to another (sub) population

#### **Details**

Migrator is the only way to mix genotypes of several subpopulations because mating is strictly within subpopulations in simuPOP. Migrators are quite flexible in simuPOP in the sense that

- Migration can happen from and to a subset of subpopulations.
- Migration can be done by probability, proportion or by counts. In the case of probability, if the migration rate from subpopulation a to b is r, then everyone in subpopulation a will have this probability to migrate to b. In the case of proportion, exactly r\*size\_of\_subPop\_a individuals (chosen by random) will migrate to subpopulation b. In the last case, a given number of individuals will migrate.
- New subpopulation can be generated through migration. You simply need to migrate to a new subpopulation number.

#### **Initialization**

Create a migrator

```
migrator(rate, mode=MigrByProbability, fromSubPop=[], toSubPop=[],
stage=PreMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

**fromSubPop** An array of 'from' subpopulations. Default to all. If a single subpop is specified, [] can be ignored. I.e., [a] is equivalent to a.

```
mode One of MigrByProbability (default), MigrByProportion or MigrByCounts
```

rate Migration rate, can be a proportion or counted number. Determined by parameter mode. rate should be an m by n matrix. If a number is given, the migration rate will be a m by n matrix of value r

```
stage Default to PreMating
```

**toSubPop** An array of 'to' subpopulations. Default to all subpopulations. If a single subpop is specified, [] can be ignored.

#### Note

- The overall population size will not be changed. (Mating schemes can do that). If you would like to keep the subpopulation size after migration, you can use the newSubPopSize or newSubPopSizeExpr parameter of a mating scheme.
- rate is a matrix with dimensions determined by fromSubPop and toSubPop. By default, rate is a matrix with element r(i,j), where r(i, j) is the migration rate, probability or count from subpopulation i to j. If fromSubPop and/or toSubPop are given, migration will only happen between these subpopulations. An extreme case is 'point migration', rate=[[r]], fromSubPop=a, toSubPop=b which migrate from subpopulation a to b with given rate r.

### **Member Functions**

```
x.apply(pop) Apply the migrator
```

x.clone() Deep copy of a migrator

**x.rate()** Return migration rate

x.setRates(rate, mode) Set migration rate

Format should be 0-0 0-1 0-2, 1-0 1-1 1-2, 2-0, 2-1, 2-2. For mode MigrByProbability or MigrByProportion, 0-0,1-1,2-2 will be set automatically regardless of input.

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# 3.3.2 Functions (Python) MigrIslandRates, MigrStepstoneRates (simuUtil.py)

Migrator is very flexible. It can accept arbitrary migration matrix, from any subset of subpopulations to any (even new) other subset of subpopulations. To facilitate the use of common theoretical migration models, several functions are defined in simuUtil.py.

• MigrIslandRates(r, n) returns a migration matrix

$$\begin{pmatrix} 1-r & \frac{r}{n-1} & \dots & \dots & \frac{r}{n-1} \\ \frac{r}{n-1} & 1-r & \dots & \dots & \frac{r}{n-1} \\ & & & & & \\ \frac{r}{n-1} & \dots & \dots & 1-r & \frac{r}{n-1} \\ \frac{r}{n-1} & \dots & \dots & \frac{r}{n-1} & 1-r \end{pmatrix}$$

• MigrStepstoneRates(r, n, circular=False) returns a migration matrix

$$\begin{pmatrix}
1-r & r \\
r/2 & 1-r & r/2 \\
& & \dots \\
& & r/2 & 1-r & r/2 \\
& & & r & 1-r
\end{pmatrix}$$

and if circular=True, returns

$$\begin{pmatrix} 1-r & r/2 & & r/2 \\ r/2 & 1-r & r/2 & & & \\ & & \dots & & & \\ & & r/2 & 1-r & r/2 \\ r/2 & & & r/2 & 1-r \end{pmatrix}$$

# 3.3.3 Class pyMigrator

A more flexible Python migrator

#### **Details**

This migrator can be used in two ways

- define a function that accepts a generation number and returns a migration rate matrix. This can be used in the varying migration rate cases.
- define a function that accepts individuals etc, and returns the new subpopulation ID.

More specifically, func can be

- func(ind) when neither loci nor param is given.
- func(ind, genotype) when loci is given.
- func(ind, param) when param is given.
- func(ind, genotype, param) when both loci and param are given.

### Initialization

Create a hybrid migrator

```
pyMigrator(rateFunc=None, mode=MigrByProbability, fromSubPop=[],
toSubPop=[], indFunc=None, loci=[], param=None, stage=PreMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

**indFunc** A Python function that accepts an individual, optional genotype and parameter, then returns a subpopulation id. This method can be used to separate a population according to individual genotype.

**rateFunc** A Python function that accepts a generation number, current subpopulation sizes, and returns a migration rate matrix. The migrator then migrate like a usual migrator.

stage Default to PreMating

#### **Member Functions**

```
x.apply(pop) Apply a pyMigrator
x.clone() Deep copy of a pyMigrator
```

# 3.3.4 Class splitSubPop (Function form: SplitSubPop)

Split a subpopulation

#### Initialization

Split a subpopulation or the whole population as subpopulation 0

```
splitSubPop(which=0, sizes=[], proportions=[], subPopID=[],
randomize=True, stage=PreMating, begin=0, end=-1, step=1, at=[],
rep=REP ALL, grp=GRP ALL, infoFields=[])
```

**proportions** Proportions of new subpopulations. Should be added up to 1.

**sizes** New subpopulation sizes. The sizes should be added up to the original subpopulation (subpopulation which) size.

**subPopID** New subpopulation IDs. Otherwise, the operator will automatically set new subpopulation IDs to new subpopulations.

which Which subpopulation to split. If there is no subpopulation structure, use 0 as the first (and only) subpopulation.

#### **Member Functions**

```
x.apply(pop) Apply a splitSubPop operator
x.clone() Deep copy of a splitSubPop operator
```

### **Example**

### Example 3.8: Operator splitSubPop

```
>>> pop = population(size=10, loci=[2,6])
>>> InitByFreq(pop, [.2,.4,.4])
>>> SplitSubPop(pop, which=0, sizes=[2,8], randomize=False)
>>> print pop.subPopSizes()
(2, 8)
>>>
```

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### 3.3.5 Class mergeSubPops (Function form: MergeSubPops)

Merge subpopulations

### **Details**

This operator merges subpopulations subPops to a single subpopulation. If subPops is ignored, all subpopulations will be merged.

#### Initialization

Merge subpopulations

```
mergeSubPops(subPops=[], removeEmptySubPops=False, stage=PreMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

subPops Subpopulatinos to be merged. Default to all.

#### **Member Functions**

```
x.apply(pop) Apply a mergeSubPops operator
x.clone() Deep copy of a mergeSubPops operator
```

### 3.4 Mutation

### 3.4.1 Class mutator

Base class of all mutators.

#### **Details**

The base class of all functional mutators. It is not supposed to be called directly. Every mutator can specify rate (equal rate or different rates for different loci) and a vector of applicable loci (default to all but should have the same length as rate if rate has length greater than one). Maximum allele can be specified as well but more parameter, if needed, should be implemented by individual mutator classes. There are number of possible allelic states. Most theoretical studies assume an infinite number of allelic states to avoid any homoplasy. If it facilitates any analysis, this is however extremely unrealistic.

### Initialization

Create a mutator

```
mutator(rate=[], loci=[], maxAllele=0, output=">", outputExpr="",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

All mutators have the following common parameters. However, the actual meaning of these parameters may vary according to different model. The only differences between the following mutators are they way they actually mutate an allele, and corresponding input parameters. The number of mutation events at each locus is recorded and can be accessed from the mutationCount or mutationCounts functions.

**loci** A vector of loci indexes. Will be ignored only when single rate is specified. Default to all loci.

maxAllele Maximum allowable allele. Interpreted by each sub mutaor class. Default to pop.maxAllele().

rate Can be a number (uniform rate) or an array of mutation rates (the same length as loci)

#### **Member Functions**

```
x.apply(pop) Apply a mutator
x.clone() Deep copy of a mutator
x.maxAllele() Return maximum allowable allele number
x.mutate(allele) Describe how to mutate a single allele
x.mutationCount(locus) Return mutation count at locus
x.mutationCounts() Return mutation counts
x.rate() Return the mutation rate
x.setMaxAllele(maxAllele) Set maximum allowable allele
x.setRate(rate, loci=[]) Set an array of mutation rates
```

### 3.4.2 Class kamMutator (Function form: KamMutate)

K-Allele Model mutator.

#### **Details**

This mutator mutate an allele to another allelic state with equal probability. The specified mutation rate is actually the 'probability to mutate'. So the mutation rate to any other allelic state is actually  $\frac{rate}{K-1}$ , where K is specified by parameter maxAllele.

#### Initialization

Create a K-Allele Model mutator

```
kamMutator(rate=[], loci=[], maxAllele=0, output=">", outputExpr="",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

loci A vector of loci indexes. Will be ignored only when single rate is specified. Default to all loci.

**maxAllele** Maximum allele that can be mutated to. For binary libraries allelic states will be [0, maxAllele]. Otherwise, they are [1, maxAllele].

rate Mutation rate. It is the 'probability to mutate'. The actual mutation rate to any of the other K-1 allelic states are rates/(K-1).

### **Member Functions**

```
x.clone() Deep copy of a kamMutator
```

x.mutate(allele) Mutate to a state other than current state with equal probability

### Example

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### Example 3.9: Operator kamMutator

```
>>> simu = simulator(population(size=5, loci=[3,5]), noMating())
>>> simu.step([
       kamMutator( rate=[.2,.6,.5], loci=[0,2,6], maxAllele=9),
       dumper(alleleOnly=True)])
individual info:
sub population 0:
  0: MU
         0 0 5
                   0 0 0 0 0
                                    0 0 9
                                                        0
  1: MU
          2 0 5
                   0 0 0 2
                              0 |
                                    0 0 0
          0 0
                   0 0 0 4
                              0 |
                                    0 0 2
                                             0 0
  2: MU
               3
                                                        0
                   0 0 0 0 0 1
                                    6 0 7
  3: MU
          0 0 8
                                             0 0 0 0 0
  4: MU
          0 0 0
                   0 0
                         0 0
                              0 |
                                    0 0 5
End of individual info.
No ancenstral population recorded.
True
>>>
```

# 3.4.3 Class smmMutator (Function form: SmmMutate)

The stepwise mutation model.

#### **Details**

The *Stepwise Mutation Model* (SMM) assumes that alleles are represented by integer values and that a mutation either increases or decreases the allele value by one. For variable number tandem repeats loci (VNTR), the allele value is generally taken as the number of tandem repeats in the DNA sequence.

### Initialization

Create a SMM mutator

```
smmMutator(rate=[], loci=[], maxAllele=0, incProb=0.5, output=">",
outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

The stepwise mutation model (SMM) is developed for allozymes. It provides better description for these kinds of evolutionary processes. Please see mutator for the description of other parameters.

**incProb** Probability to increase allele state. Default to 0.5.

#### **Member Functions**

```
x.clone() Deep copy of a smmMutator
```

### Example

### Example 3.10: Operator smmMutator

```
>>> simu = simulator(population(size=3, loci=[3,5]), noMating())
>>> simu.step([
... initByFreq([.2,.3,.5]),
... smmMutator(rate=1, incProb=.8),
```

```
dumper(alleleOnly=True, stage=PrePostMating)])
individual info:
sub population 0:
   0: FU
           0 1
                     2
                        2
                              0
                                 1 |
                                                             1
                                                    0
                              2
                                 1
   1: MU
           1
                                                    2
                     2 1 0
                              2
                                 2 |
   2: MU
End of individual info.
No ancenstral population recorded.
individual info:
sub population 0:
   0: FU
           1 2 1
                     3
                        3
                             1
                                 2 |
                                       2
                                          1
                                                             2
                           1
                                 2 |
                     0 1 1
                              3
                                       1
                                          1
                                             3
                                                 3 1
                                                             2
   1: MU
           3 3 2
                     3 2 1 1
                                 3 |
                                       3
   2: MU
End of individual info.
No ancenstral population recorded.
True
>>>
```

## 3.4.4 Class gsmMutator (Function form: GsmMutate)

Generalized stepwise mutation model

#### **Details**

The Generalized Stepwise Mutation model (GSM) is an extension to stepwise mutation model. This model assumes that alleles are represented by integer values and that a mutation either increases or decreases the allele value by a random value. In other words, in this model the change in the allelic state is drawn from a random distribution. A geometric generalized stepwise model uses a geometric distribution with parameter p, which has mean  $\frac{p}{1-p}$  and variance  $\frac{p}{(1-p)^2}$ .

gsmMutator implements both models. If you specify a Python function without a parameter, this mutator will use its return value each time a mutation occur; otherwise, a parameter p should be provided and the mutator will act as a geometric generalized stepwise model.

#### Initialization

Create a gsmMutator

```
gsmMutator(rate=[], loci=[], maxAllele=0, incProb=0.5, p=0,
func=None, output=">", outputExpr="", stage=PostMating, begin=0,
end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

The generalized stepwise mutation model (GMM) is developed for allozymes. It provides better description for these kinds of evolutionary processes. Please see mutator for the description of other parameters.

func A function that returns the number of steps. This function does not accept any parameter.

**incProb** Probability to increase allele state. Default to 0.5.

## **Member Functions**

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### x.mutate(allele) Mutate according to the GSM model

### **Example**

```
Example 3.11: Operator gsmMutator
>>> simu = simulator(population(size=3, loci=[3,5]), noMating())
>>> simu.step([
       initByFreq([.2,.3,.5]),
. . .
       gsmMutator(rate=1, p=.8, incProb=.8),
       dumper(alleleOnly=True, stage=PrePostMating)])
individual info:
sub population 0:
  0: FU
          2 1 1
                   2 0 2 1
                               2 |
                                     0
                                       0 2
                                              1 0
                                                   2 2 0
                           2 0 |
  1: FU
          2 2 0
                   1 2 2
                                     2
                                       2 1
                                              2 0 0 2 0
                   2 2 0 2 2 |
  2: MU
          1 2 2
                                    1 2 2
                                              0 0 2 1 0
End of individual info.
No ancenstral population recorded.
individual info:
sub population 0:
  0: FU
          4 2 2
                   3 1 3 0 3 |
                                    3 0 3
                                              2 1
                   2 3 3 3 1 |
                                     4 3 0
                                              3 1 1 4 2
          3
             3 1
  1: FU
  2: MU
          2 3 3
                    3 1 1 3 3 |
                                              1 1
End of individual info.
No ancenstral population recorded.
True
>>>
>>> import random
>>> def rndInt():
     return random.randrange(3,6)
>>> simu.step([
       initByFreq([.2,.3,.5]),
       gsmMutator(rate=1, func=rndInt, incProb=.8),
. . .
       dumper(alleleOnly=True, stage=PrePostMating)
. . .
...)
individual info:
sub population 0:
  0: MU
          2 2 2
                   2 1 0 2 1 |
                                     0 2 2
  1: MU
          0 2 1
                   2 2 2 0 1 |
                                     2 2 1
                                              2 1 1 2 1
   2: FU
          2 1 2
                   0 2 1 0 2 |
End of individual info.
No ancenstral population recorded.
individual info:
sub population 0:
  0: MU 0 7 0 0 6 4 0 6
                                   4 6 7 7 7 4 5 0
```

```
1: MU 5 7 6 6 0 6 4 5 | 0 7 4 5 4 0 5 6 2: FU 5 4 7 3 7 5 5 0 | 5 4 6 6 5 6 4 0 End of individual info.

No ancenstral population recorded.

True
```

## 3.4.5 Class pyMutator (Function form: PyMutate)

A hybrid mutator.

#### **Details**

Parameters such as mutation rate of this operator are set just like others and you are supposed to provide a Python function to return a new allele state given an old state. pyMutator will choose an allele as usual and call your function to mutate it to another allele.

#### Initialization

Create a pyMutator

```
pyMutator(rate=[], loci=[], maxAllele=0, func=None, output=">",
outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

#### **Member Functions**

x.clone() Deep copy of a pyMutator

x.mutate(allele) Mutate according to the mixed model

### **Example**

Example 3.12: Operator pyMutator

```
>>> def mut(x):
      return 8
>>> simu = simulator(population(size=3, loci=[3,5]), noMating())
>>> simu.step([
      pyMutator(rate=.5, loci=[3,4,5], func=mut),
      dumper(alleleOnly=True)])
individual info:
sub population 0:
   0: MU
           0 0 0
                     0 8
                           8
                              0
                                 0 |
           0 0 0
                           8
                             0
                                 0 |
                                       0
                                          0
                                                 0 8 8 0
   1: MU
                     8 0
                                            0
           0 0 0
                           8
                              0
                                 0 |
                                       0
                                          0
End of individual info.
No ancenstral population recorded.
True
>>>
```

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## 3.4.6 Class pointMutator (Function form: PointMutate)

Point mutator

### **Details**

Mutate specified individuals at a specified loci to a specified allele. I.e., this is a non-random mutator used to introduce diseases etc. pointMutator, as its name suggest, does point mutation. This mutator will turn alleles at loci on the first chromosome copy to toAllele for individualinds. You can specify atPloidy to mutate other, or all ploidy copies.

### Initialization

Create a pointMutator

```
pointMutator(loci, toAllele, atPloidy=[], inds=[], output=">",
outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

Please see mutator for the description of other parameters.

```
inds Individuals who will mutatetoAllele Allele that will be mutate to
```

#### **Member Functions**

```
x.apply(pop) Apply a pointMutator
x.clone() Deep copy of a pointMutator
x.mutationCount(locus) Return mutation count at locus
x.mutationCounts() Return mutation counts
```

## 3.5 Recombination

## 3.5.1 Class recombinator

### Recombination

### **Details**

In simuPOP, only one recombinator is provided. Recombination events between loci a/b and b/c are independent, otherwise there will be some linkage between loci, users need to specify physical recombination rate between adjacent loci. In addition, for the recombinator

- it only works for diploid (and for females in haplodiploid) populations.
- the recombination rate must be comprised between 0.0 and 0.5. A recombination rate of 0.0 means that the loci are completely linked, and thus behave together as a single linked locus. A recombination rate of 0.5 is equivalent to free recombination. All other values between 0.0 and 0.5 will represent various linkage intensities between adjacent pairs of loci. The recombination rate is equivalent to 1-linkage and represents the probability that the allele at the next locus is randomly drawn.

#### Initialization

Recombine chromosomes from parents

```
recombinator(intensity=-1, rate=[], afterLoci=[], maleIntensity=-1,
maleRate=[], maleAfterLoci=[], begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

**afterLoci** An array of locus indexes. Recombination will occur after these loci. If rate is also specified, they should have the same length. Default to all loci (but meaningless for those loci located at the end of a chromosome). If this parameter is given, it should be ordered, and can not include loci at the end of a chromosome.

**intensity** Intensity of recombination. The actually recombination rate between two loci is determined by intensity\*locus distance between them.

maleAfterLoci If given, males will recombine at different locations.

**maleIntensity** Recombination intensity for male individuals. If given, parameter intensity will be considered as female intensity.

maleRate Recombination rate for male individuals. If given, parameter rate will be considered as female recombination rate.

rate Recombination rate regardless of locus distance after all afterLoci. It can also be an array of recombination rates. Should have the same length as afterLoci or totNumOfLoci(). The recombination rates are independent of locus distance.

### Note

There is no recombination between sex chromosomes of male individuals if sexChrom() = True. This may change later if the exchanges of genes between pseudoautosomal regions of XY need to be modeled.

#### **Member Functions**

- x.clone() Deep copy of a recombinator
- x.recCount(locus) Return recombination count
- **x.recCounts()** Return recombination counts

## **Example**

Example 3.13: Operator recombinator

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```
1: MU 1032 13121 232001 | 1103 32333 223232
   2: MU 0002 23111 223220 |
                             2222 22133 011010
   3: FU 3122 20122 301231 | 1231 20223 213032
End of individual info.
No ancenstral population recorded.
individual info:
sub population 0:
   0: FU 0002 22133 011010 |
                             3122 20223 213032
   1: FU 2200 03300 020102
                             1231 20223 213032
                             1231 20122 213032
   2: MU 1223 21120 020102
   3: FU 1223 03300 020102 | 1231 20122 301231
End of individual info.
No ancenstral population recorded.
True
>>> simu.step([
      parentsTagger(),
      recombinator(rate=[1,1,1], afterLoci=[2,6,10])
      postOps = [ dumper(alleleOnly=True)]
...)
individual info:
sub population 0:
   0: FU 3122 20233 211010 |
                             1221 21122 210102
   1: MU 2201 03323 023032
                             1233 21122 023032
   2: FU 1233 03322 300102 | 1221 20120 023032
   3: MU 2201 20200 023032 | 1233 20120 023032
End of individual info.
No ancenstral population recorded.
True
```

## 3.6 Selection

>>>

## 3.6.1 Mechanism

It is not very clear that our method agrees with the traditional 'average number of offspring' definition of fitness. (Note that this concept is very difficult to simulate because we do not know who will determine the number of offspring if two parents are involved.) We can, instead, look at the consequence of selection in a simple case (as derived in any population genetics textbook):

At generation t, genotype  $P_{11}, P_{12}, P_{22}$  has fitness values  $w_{11}, w_{12}, w_{22}$  respectively. In the next generation the proportion of genotype  $P_{11}$  etc., should be

$$\frac{P_{11}w_{11}}{P_{11}w_{11} + P_{12}w_{12} + P_{22}w_{22}}$$

Now, using the 'ability-to-mate' approach, for the sexless case, the proportion of genotype 11 will be the number of 11 individuals times its probability to be chosen:

$$n_{11} \frac{w_{11}}{\sum_{n=1}^{N} w_n}$$

This is, however, exactly

$$n_{11} \frac{w_{11}}{\sum_{n=1}^{N} w_n} = n_{11} \frac{w_{11}}{n_{11}w_{11} + n_{12}w_{12} + n_{22}w_{22}} = \frac{P_{11}w_{11}}{P_{11}w_{11} + P_{12}w_{12} + P_{22}w_{22}}$$

The same argument applies to the case of arbitrary number of genotypes and random mating.

The following operators, when applied, will set a variable fitness and an indicator so that selector-aware mating scheme can select individuals according to these values. This has two consequences:

- selector alone can not do selection! Only mating schemes can actually select on individuals.
- selector has to be PreMating operator. This is not a problem when you use the operator form of the selectors since their default stage is PreMating. However, if you use the function form of these selectors in a pyOperator, make sure to set the stage of pyOperator to PreMating.

### 3.6.2 Class selector

A base selection operator for all selectors.

#### Details

Genetic selection is tricky to simulate since there are many different *fitness* values and many different ways to apply selection. simuPOP employs an 'ability-to-mate' approach. Namely, the probability that an individual will be chosen for mating is proportional to its fitness value. More specifically,

- PreMating selectors assign fitness values to each individual, and mark part or all subpopulations as under selection.
- During sexless mating (e.g. binomialSelection mating scheme), individuals are chosen at probabilities that are proportional to their fitness values. If there are N individuals with fitness values  $f_i, i=1,...,N$ , individual i will have probability  $\frac{f_i}{\sum_j f_j}$  to be chosen and passed to the next generation.
- During randomMating, males and females are separated. They are chosen from their respective groups in the same manner as binomialSelection and mate.

All of the selection operators, when applied, will set an information field fitness (configurable) and then mark part or all subpopulations as under selection. (You can use different selectors to simulate varying selection intensity for different subpopulations). Then, a 'selector-aware' mating scheme can select individuals according to this fitness information field. This implies that

- Only mating schemes can actually select individuals.
- Selector has to be PreMating operator. This is not a problem when you use the operator form of the selectors since their default stage is PreMating. However, if you use the function form of these selectors in a pyOperator, make sure to set the stage of pyOperator to PreMating.

#### Note

You can not apply two selectors to the same subpopulation, because only one fitness value is allowed for each individual.

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#### Initialization

Create a selector

```
selector(subPops=[], stage=PreMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=["fitness"])
subPop A shortcut to subPops=[subPop]
subPops Subpopulations that the selector will apply to. Default to all.
```

### **Member Functions**

```
x.apply(pop) Set fitness to all individuals. No selection will happen!
```

```
x.clone() Deep copy of a selector
```

## 3.6.3 Class mapSelector (Function form: MapSelector)

Selection according to the genotype at one locus

### **Details**

This map selector implements selection at one locus. A user provided dictionary (map) of genotypes will be used in this selector to set each individual's fitness value.

#### Initialization

Create a map selector

```
mapSelector(loci, fitness, phase=False, subPops=[], stage=PreMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=["fitness"])
```

**fitness** A dictionary of fitness values. The genotype must be in the form of 'a-b' for a single locus, and 'a-b|c-d|e-f' for multi-loci.

**loci** The locus indexes. The genotypes at these loci will be used to determine fitness value.

```
locus The locus index. A shortcut to loci=[locus]
```

**output** And other parameters please refer to help(baseOperator.\_\_init\_\_)

phase If True, genotypes a-b and b-a will have different fitness values. Default to false.

#### **Member Functions**

x.clone() Deep copy of a map selector

## Example

```
Example 3.14: Operator mapSelector
```

```
>>> simu = simulator(
... population(size=1000, ploidy=2, loci=[1], infoFields=['fitness']),
... randomMating())
>>> s1 = .1
```

```
>>> s2 = .2
>>> simu.evolve([
        stat( alleleFreq=[0], genoFreq=[0]),
        mapSelector(locus=0, fitness=\{'0-0':(1-s1), '0-1':1, '1-1':(1-s2)\}),
        pyEval(r"'%.4f\n' % alleleFreq[0][1]", step=100)
        ],
. . .
                   initByFreq(alleleFreq=[.2,.8])],
        preOps=[
        end=300)
0.7740
0.3210
0.3380
0.3175
True
>>>
```

The example for class mapSelector is a typical example of heterozygote superiority. When  $w_{11} < w_{12} > w_{22}$ , the genotype frequencies will go to an equilibrium state. Theoretically, if

$$\begin{array}{rcl}
s_1 & = & w_{12} - w_{11} \\
s_2 & = & w_{12} - w_{22}
\end{array}$$

the stable allele frequency of allele 1 is

$$p = \frac{s_2}{s_1 + s_2}$$

Which is .677 in the example  $(s_1 = .1, s_2 = .2)$ .

## 3.6.4 Class maSelector (Function form: MaSelect)

Multiple allele selector (selection according to wildtype or diseased alleles)

### **Details**

This is called 'multiple-allele' selector. It separate alleles into two groups: wildtype and disease alleles. Wildtype alleles are specified by parameter wildtype and any other alleles are considered as diseased alleles. This selector accepts an array of fitness values:

- For single-locus, fitness is the fitness for genotype AA, Aa, aa, while A stands for wildtype alleles.
- For a two-locus model, fitness is the fitness for genotype AABB, AABb, AABb, AaBB, AbBb, Aabb, aaBB, aaBb and aaBb.
- For a model with more than two loci, use a table of length  $3\{n\}$  in a order similar to the two-locus model.

## Initialization

Create a multiple allele selector

```
maSelector(loci, fitness, wildtype, subPops=[], stage=PreMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=["fitness"])
```

Please refer to basicSelector for other parameter descriptions.

fitness For the single locus case, fitness is an array of fitness of AA, Aa, aa. A is the wildtype group. In the case of multiple loci, fitness should be in the order of AABB, AABb, AABb, AaBB, AaBb, AaBb, aaBb, aaBb, aabb.

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**output** And other parameters please refer to help(baseOperator.\_\_init\_\_)

wildtype An array of alleles in the wildtype group. Any other alleles are considered to be diseased alleles. Default to [0].

### Note

- maSelector only works for diploid populations now.
- wildtype at all loci are the same.

### **Member Functions**

x.clone() Deep copy of a maSelector

## **Example**

Example 3.15: Operator maSelector

```
>>> simu = simulator(
        population(size=1000, ploidy=2, loci=[1], infoFields=['fitness']),
        randomMating())
>>> s1 = .1
>>> s2 = .2
>>> simu.evolve(
        preOps=[initByFreq(alleleFreq=[.2,.8])],
        ops = [
            stat( alleleFreq=[0], genoFreq=[0]),
            maSelector(locus=0, fitness=[1-s1, 1, 1-s2]),
            pyEval(r"'%.4f\n' % alleleFreq[0][1]", step=100)
. . .
        ],
        end=300)
. . .
0.7975
0.3645
0.3085
0.3110
True
>>>
```

## 3.6.5 Class mlSelector (Function form: MlSelect)

Selection according to genotypes at multiple loci in a multiplicative model

#### **Details**

This selector is a 'multiple-loci model' selector. The selector takes a vector of selectors (can not be another mlSelector) and evaluate the fitness of an individual as the product or sum of individual fitness values. The mode is determined by parameter mode, which takes the value

- SEL\_Multiplicative: the fitness is calculated as  $f = \prod_i f_i$ .
- SEL\_Additive: the fitness is calculated as  $f = \max(0, 1 \sum_i (1 f_i)) = \max(0, 1 \sum_i s_i)$ . f will be set to 0 when f < 0. In this case,  $s_i$  are added, not  $f_i$  directly.

#### Initialization

Create a multi-loci selector

```
mlSelector(selectors, mode=SEL_Multiplicative, subPops=[],
stage=PreMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["fitness"])
```

Please refer to mapSelector for other parameter descriptions.

**selectors** A list of selectors

#### **Member Functions**

x.clone() Deep copy of a mlSelector

## **Example**

Example 3.16: Operator mlSelector

```
>>> simu = simulator(
        population(size=10, ploidy=2, loci=[2],
        infoFields=['fitness', 'spare']),
. . .
        randomMating())
>>> simu.evolve(
        [ mlSelector([
             mapSelector(locus=0, fitness=\{'0-0':1,'0-1':1,'1-1':.8\}),
             mapSelector(locus=1, fitness={'0-0':1,'0-1':1,'1-1':.8}),
              ], mode=SEL_Additive),
        ],
. . .
        preOps = [
             initByFreq(alleleFreq=[.2,.8])
        ],
        end=2
. . .
...)
True
>>>
```

## 3.6.6 Class pySelector (Function form: PySelect)

Selection using user provided function

#### **Details**

PYSELECTOR assigns fitness values by calling a user provided function. It accepts a list of susceptibility loci and a Python function. For each individual, this operator will pass the genotypes at these loci and the generation number and use the returned value as the fitness value. The genotypes are arranged in the order of 0-0, 0-1, 1-0, 1-1 etc. where X-Y represents locus X - ploidy Y.

### Initialization

Create a Python hybrid selector

```
pySelector(loci, func, subPops=[], stage=PreMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=["fitness"])
```

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func A Python function that accepts genotypes at susceptibility loci generation number, and return fitness value.

loci Susceptibility loci. The genotype at these loci will be passed to func.

output And other parameters please refer to help(baseOperator.\_\_init\_\_)

#### **Member Functions**

x.clone() Deep copy of a pySelector

#### **Example**

## Example 3.17: Operator pySelector

```
>>> simu = simulator(
        population(size=1000, ploidy=2, loci=[3], infoFields=['fitness'] ),
        randomMating())
>>>
>>> s1 = .2
>>> s2 = .3
>>> # the second parameter gen can be used for varying selection pressure
>>> def sel(arr, gen=0):
      if arr[0] == 1 and arr[1] == 1:
        return 1 - s1
. . .
      elif arr[0] == 1 and arr[1] == 2:
        return 1
      elif arr[0] == 2 and arr[1] == 1:
        return 1
. . .
      else:
        return 1 - s2
. . .
>>> # test func
>>> print sel([1,1])
0.8
>>>
>>> simu.evolve([
        stat( alleleFreq=[0], genoFreq=[0]),
        pySelector(loci=[0,1],func=sel),
. . .
        pyEval(r"'%.4f\n' % alleleFreq[0][1]", step=25)
. . .
        ],
        preOps=[
                   initByFreq(alleleFreq=[.2,.8])],
        end=100)
. . .
0.7980
1.0000
1.0000
1.0000
1.0000
True
>>>
```

## 3.7 Penetrance

## 3.7.1 Class penetrance

Base class of all penetrance operators.

#### **Details**

Penetrance is the probability that one will have the disease when he has certain genotype(s). Calculation and the parameter set of penetrance are similar to those of fitness. An individual will be randomly marked as affected/unaffected according to his/her penetrance value. For example, an individual will have probability 0.8 to be affected if the penetrance is 0.8.

Penetrance can be applied at any stage (default to DuringMating). When a penetrance operator is applied, it calculate the penetrance value of each offspring and assign affected status accordingly. Penetrance can also be used PreMating or PostMating. In these cases, the affected status will be set to all individuals according to their penetrance values. Pentrance values are used to set the affectedness of individuals, and are usually not saved. If you would like to know the penetrance value, you need to

- use addInfoField('penetrance') to the population to analyze. (Or use infoFields parameter of the population constructor), and
- use e.g., mlPenetrance(..., infoFields=['penetrance']) to add the penetrance field to the penetrance operator you use. You may choose a name other than 'penetrance' as long as the field names for the operator and population match.

Penetrance functions can be applied to the current, all, or certain number of ancestral generations. This is controlled by the ancestralGen parameter, which is default to -1 (all available ancestral generations). You can set it to 0 if you only need affection status for the current generation, or specify a number n for the number of ancestral generations (n + 1 total generations) to process. Note that ancestralGen parameter is ignored if the penetrance operator is used as a during mating operator.

## Initialization

Create a penetrance operator

```
penetrance(ancestralGen=-1, stage=DuringMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

default to be always active.

**ancestralGen** If this parameter is set to be 0, then apply penetrance to the current generation; if -1, apply to all generations; otherwise, apply to the specified number of ancestral generations

**infoFields** If one field is specified, it will be used to store penetrance values.

stage Specify the stage this operator will be applied, default to DuringMating.

### **Member Functions**

**x.apply(pop)** Set penetrance to all individuals and record penetrance if requested

x.clone() Deep copy of a penetrance operator

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## 3.7.2 Class mapPenetrance (Function form: MapPenetrance)

Penetrance according to the genotype at one locus

#### **Details**

Assign penetrance using a table with keys 'X-Y' where X and Y are allele numbers.

#### **Initialization**

Create a map penetrance operator

```
mapPenetrance(loci, penet, phase=False, ancestralGen=-1,
stage=DuringMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

**loci** The loci indexes. The genotypes of these loci will be used to determine penetrance.

**locus** The locus index. Shortcut to loci=[locus]

**output** And other parameters please refer to help(baseOperator. init )

penetrance A dictionary of penetrance. The genotype must be in the form of 'a-b' for a single locus.

**phase** If True, a/b and b/a will have different penetrance values. Default to False.

#### **Member Functions**

**x.clone()** Deep copy of a map penetrance operator

#### **Example**

## Example 3.18: Operator mapPenetrance

```
>>> pop = population(size=10, ploidy=2, loci=[2], subPop=[2, 8])
>>> InitByFreq(pop, [.2, .8])
>>> MapPenetrance(pop, locus=0,
...     penetrance={'0-0':0, '0-1':1, '1-1':1})
>>> Stat(pop, numOfAffected=1)
>>>
```

## 3.7.3 Class maPenetrance (Function form: MaPenetrance)

Multiple allele penetrance operator

## **Details**

This is called 'multiple-allele' penetrance. It separates alleles into two groups: wildtype and disease alleles. Wildtype alleles are specified by parameter wildtype and any other alleles are considered as diseased alleles. maPenetrance accepts an array of fitness for AA, Aa, aa in the single-locus case, and a longer table for multilocus case. Penetrance is then set for any given genotype.

### Initialization

Create a multiple allele penetrance operator (penetrance according to diseased or wildtype alleles)

```
maPenetrance(loci, penet, wildtype, ancestralGen=-1,
stage=DuringMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

**loci** The loci indexes. The genotypes of these loci will be examed.

**locus** The locus index. The genotype of this locus will be used to determine penetrance.

```
output And other parameters please refer to help(baseOperator.__init__)
```

**penetrance** An array of penetrance values of AA, Aa, aa. A is the wild type group. In the case of multiple loci, fitness should be in the order of AABB, AABb, AABb, AaBb, AaBb, aaBb, aaBb, aabb.

**wildtype** An array of alleles in the wildtype group. Any other alleles will be considered as in the disease allele group.

#### **Member Functions**

x.clone() Deep copy of a multi-allele penetrance operator

### **Example**

## Example 3.19: Operator maPenetrance

```
>>> pop = population(size=10, ploidy=2, loci=[2], subPop=[2, 8])
>>> InitByFreq(pop, [.2, .8])
>>> MaPenetrance(pop, locus=0, wildtype=0, penetrance=[0, 1, 1])
>>> Stat(pop, numOfAffected=1)
>>>
```

## 3.7.4 Class mlPenetrance (Function form: MlPenetrance)

Penetrance according to the genotype according to a multiple loci multiplicative model

## **Details**

MLPENTRANCE is the 'multiple-locus' penetrnace calculator. It accepts a list of penetrances and combine them according to the mode parameter, which takes one of the following values:

- PEN\_Multiplicative: the penetrance is calculated as  $f = \prod f_i$ .
- PEN\_Additive: the penetrance is calculated as  $f = \min(1, \sum f_i)$ . f will be set to 1 when f < 0. In this case,  $s_i$  are added, not  $f_i$  directly.
- PEN\_Heterogeneity: the penetrance is calculated as  $f=1-\prod{(1-f_i)}$ .

Please refer to Neil Risch (1990) for detailed information about these models.

### **Initialization**

Create a multiple loci penetrance operator using a multiplicative model

```
mlPenetrance(peneOps, mode=PEN_Multiplicative, ancestralGen=-1,
    stage=DuringMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
    grp=GRP_ALL, infoFields=[])

mode Can be one of PEN_Multiplicative, PEN_Additive, and PEN_Heterogeneity
```

peneOps A list of penetrance operators

### **Member Functions**

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#### x.clone() Deep copy of a multi-loci penetrance operator

### **Example**

## Example 3.20: Operator mlPenetrance

## 3.7.5 Class pyPenetrance (Function form: PyPenetrance)

Assign penetrance values by calling a user provided function

#### **Details**

For each individual, users provide a function to calculate penetrance. This method is very flexible but will be slower than previous operators since a function will be called for each individual.

#### Initialization

Provide locus and penetrance for 11, 12, 13 (in the form of dictionary)

```
pyPenetrance(loci, func, ancestralGen=-1, stage=DuringMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

**func** A user-defined Python function that accepts an array of genotypes at susceptibility loci and return a penetrance value. The returned value should be between 0 and 1.

**loci** Disease susceptibility loci. The genotypes at these loci will be passed to the provided Python function in the form of loc1\_1, loc1\_2, loc2\_1, loc2\_2, ... if the individuals are diploid.

**output** And other parameters please refer to help(baseOperator.\_\_init\_\_)

#### **Member Functions**

x.clone() Deep copy of a Python penetrance operator

#### **Example**

#### Example 3.21: Operator pyPenetrance

```
>>> pop = population(1000, loci=[3])
>>> InitByFreq(pop, [0.3, 0.7])
>>> def peneFunc(geno):
```

```
p = 1
        for 1 in range(len(geno)/2):
            p *= (qeno[1*2]+qeno[1*2+1])*0.3
        return p
. . .
>>> PyPenetrance(pop, func=peneFunc, loci=(0, 1, 2))
>>> Stat(pop, numOfAffected=True)
>>> print pop.dvars().numOfAffected
62
>>> #
>>> # You can also define a function, that returns a penetrance
>>> # function using given parameters
>>> def peneFunc(table):
        def func(geno):
          return table[geno[0]][geno[1]]
        return func
. . .
>>> # then, given a table, you can do
>>> PyPenetrance(pop, loci=(0, 1, 2),
        func=peneFunc(((0,0.5),(0.3,0.8))))
>>>
```

## 3.8 Quantitative Trait

## 3.8.1 Class quanTrait

Base class of quantitative trait

#### **Details**

Quantitative trait is the measure of certain phenotype for given genotype. Quantitative trait is similar to penetrance in that the consequence of penetrance is binary: affected or unaffected; while it is continuous for quantitative trait.

In simuPOP, different operators/functions were implemented to calculate quantitative traits for each individual and store the values in the information fields specified by user (default to qtrait). The quantitative trait operators also accept the ancestralGen parameter to control the number of generations for which the qtrait information field will be set.

## Initialization

Create a quantitative trait operator, default to be always active

```
quanTrait(ancestralGen=-1, stage=PostMating, begin=0, end=-1, step=1,
at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=["qtrait"])
```

### **Member Functions**

```
x.apply(pop) Set qtrait to all individual
x.clone() Deep copy of a quantitative trait operator
```

## 3.8.2 Class mapQuanTrait (Function form: MapQuanTrait)

Quantitative trait according to genotype at one locus

3.8. Quantitative Trait

#### **Details**

Assign quantitative trait using a table with keys 'X-Y' where X and Y are allele numbers. If parameter sigma is not zero, the returned value is the sum of the trait plus  $N\left(0,\sigma^2\right)$ . This random part is usually considered as the environmental factor of the trait.

#### Initialization

Create a map quantitative trait operator

```
mapQuanTrait(loci, qtrait, sigma=0, phase=False, ancestralGen=-1,
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["qtrait"])
```

**loci** An array of locus indexes. The quantitative trait is determined by genotype at these loci.

locus The locus index. The quantitative trait is determined by genotype at this locus.

**output** And other parameters please refer to help(baseOperator.\_\_init\_\_)

phase If True, a/b and b/a will have different quantitative trait values. Default to False.

**qtrait** A dictionary of quantitative traits. The genotype must be in the form of 'a-b'. This is the mean of the quantitative trait. The actual trait value will be N(mean, sigma2). For multiple loci, the form is 'a-b|c-d|e-f' etc.

sigma Standard deviation of the environmental factor N(0, sigma2).

#### **Member Functions**

**x.clone()** Deep copy of a map quantitative trait operator

## 3.8.3 Class maQuanTrait (Function form: MaQuanTrait)

Multiple allele quantitative trait (quantitative trait according to disease or wildtype alleles)

### **Details**

This is called 'multiple-allele' quantitative trait. It separates alleles into two groups: wildtype and disease susceptibility alleles. Wildtype alleles are specified by parameter wildtype and any other alleles are considered as disease alleles. maQuanTrait accepts an array of fitness. Quantitative trait is then set for any given genotype. A standard normal distribution  $N\left(0,\sigma^2\right)$  will be added to the returned trait value.

#### Initialization

Create a multiple allele quantitative trait operator

```
maQuanTrait(loci, qtrait, wildtype, sigma=[], ancestralGen=-1,
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["qtrait"])
```

Please refer to quanTrait for other parameter descriptions.

```
output And other parameters please refer to help(baseOperator.__init__)
```

qtrait An array of quantitative traits of AA, Aa, aa. A is the wild type group

sigma An array of standard deviations for each of the trait genotype (AA, Aa, aa)

wildtype An array of alleles in the wildtype group. Any other alleles will be considered as disease alleles. Default to [0].

#### **Member Functions**

**x.clone()** Deep copy of a multiple allele quantitative trait

## 3.8.4 Class mlQuanTrait (Function form: MlQuanTrait)

Quantitative trait according to genotypes from a multiple loci multiplicative model

#### **Details**

Operator mlQuanTrait is a 'multiple-loci' quantitative trait calculator. It accepts a list of quantitative traits and combine them according to the mode parameter, which takes one of the following values

- QT\_Multiplicative: the mean of the quantitative trait is calculated as  $f = \prod f_i$ .
- ullet QT\_Additive: the mean of the quantitative trait is calculated as  $f=\sum f_i$ .

Note that all  $\sigma_i$  (for  $f_i$ ) and  $\sigma$  (for f) will all be considered. I.e, the trait value should be

$$f = \sum_{i} (f_i + N(0, \sigma_i^2)) + \sigma^2$$

for QT\_Additive case. If this is not desired, you can set some of the  $\sigma$  to zero.

## Initialization

Multiple loci quantitative trait using a multiplicative model

```
mlQuanTrait(qtraits, mode=QT_Multiplicative, sigma=0,
ancestralGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=["qtrait"])
```

Please refer to quanTrait for other parameter descriptions.

```
mode Can be one of QT_Multiplicative and QT_Additive
qtraits A list of quantitative traits
```

#### **Member Functions**

x.clone() Deep copy of a multiple loci quantitative trait operator

## 3.8.5 Class pyQuanTrait (Function form: PyQuanTrait)

Quantitative trait using a user provided function

### **Details**

For each individual, a user provided function is used to calculate quantitative trait.

#### **Initialization**

Create a Python quantitative trait operator

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```
pyQuanTrait(loci, func, ancestralGen=-1, stage=PostMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=["gtrait"])
```

Please refer to quanTrait for other parameter descriptions.

func A Python function that accepts genotypes at susceptibility loci and returns the quantitative trait value.

loci Susceptibility loci. The genotypes at these loci will be passed to func.

output And other parameters please refer to help(baseOperator.\_\_init\_\_)

#### **Member Functions**

**x.clone()** Deep copy of a Python quantitative trait operator

## 3.9 Ascertainment

## 3.9.1 Class sample

Base class of other sample operator

#### **Details**

Ascertainment/sampling refers to ways to select individuals from a population. In simuPOP, ascerntainment operators form separate populations in a population's namespace. All the ascertainment operators work like this except for pySubset which shrink the population itself.

Individuals in sampled populations may or may not keep their original order but their indexes in the whole population are stored in a information field oldindex. That is to say, you can use ind.info('oldindex') to check the original position of an individual.

Two forms of sample size specification are supported: with or without subpopulation structure. For example, the size parameter of randomSample can be a number or an array (which has the length of the number of subpopulations). If a number is given, a sample will be drawn from the whole population, regardless of the population structure. If an array is given, individuals will be drawn from each subpopulation sp according to size[sp].

An important special case of sample size specification occurs when size=[] (default). In this case, usually all qualified individuals will be returned.

The function forms of these operators are a little different from others. They do return a value: an array of samples.

#### **Initialization**

Draw a sample

```
sample(name="sample", nameExpr="", times=1, saveAs="", saveAsExpr="",
format="auto", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

Please refer to baseOperator::\_\_init\_\_ for other parameters.

**format** Format to save the samples

**name** Name of the sample in local namespace. This variable is an array of populations of size times. Default to sample. If name=" is set, samples will not be saved in local namespace.

**nameExpr** Expression version of parameter name. If both name and nameExpr are empty, do not store pop. This expression will be evaluated dynamically in population's local namespace.

saveAs Filename to save the samples

**saveAsExpr** Expression version of parameter saveAs. It will be evaluated dynamically in population's local namespace.

**times** How many times to sample from the population. This is usually 1, but we may want to take several random samples.

#### **Member Functions**

```
x.apply(pop) Apply the sample operator
x.clone() Deep copy of a sample operator
x.samples(pop) Return the samples
```

## 3.9.2 Class pySubset (Function form: PySubset)

Shrink population

#### **Details**

This operator shrinks a population according to a given array or the subPopID() value of each indvidual. individuals with negative subPop ID are removed.

#### Initialization

Create a pySubset operator

```
pySubset(keep=[], stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

**keep** An array of subpopulation IDs for each individual.

#### **Member Functions**

```
x.apply(pop) Apply the pySubset operator
x.clone() Deep copy of a pySubset operator
```

## 3.9.3 Class pySample (Function form: PySample)

Python sampler.

#### **Details**

A Python sampler that generate a sample with given individuals.

## Initialization

Create a Python sampler

```
pySample(keep, keepAncestralPops=-1, name="sample", nameExpr="",
times=1, saveAs="", saveAsExpr="", format="auto", stage=PostMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

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This sampler accepts a Python array which will be assigned to each individual as subPOP ID. Individuals with positive subPOPID will then be picked out and form a sample. Please refer to class sample for other parameter descriptions.

keep Subpopulation IDs of all individuals

**keepAncestralPop** The number of ancestral populations that will be kept. If -1, keep all ancestral populations (default). If 0, no ancestral population will be kept.

#### **Member Functions**

```
x.clone() Deep copy of a Python sampler
x.drawsample(pop) Draw a Python sample
```

## 3.9.4 Class randomSample (Function form: RandomSample)

Randomly draw a sample from a population

#### **Details**

This operator will randomly choose size individuals (or size[i] individuals from subpopulation i) and return a new population. The function form of this operator returns the samples directly. The operator keeps samples in an array name in the local namespace. You may access them through dvars() or vars() functions.

The original subpopulation structure/boundary is kept in the samples.

#### Initialization

Draw a random sample, regardless of the affected status

```
randomSample(size=[], name="sample", nameExpr="", times=1, saveAs="",
saveAsExpr="", format="auto", stage=PostMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

Please refer to class sample for other parameter descriptions.

**size** Size of the sample. It can be either a number which represents the overall sample size, regardless of the population structure; or an array which represents the number of samples drawn from each subpopulation.

#### Note

Ancestral populations will not be copied to the samples.

### **Member Functions**

x.clone() Deep copy of a randomSample operator

## 3.9.5 Class caseControlSample (Function form: CaseControlSample)

Draw a case-control sample from a population

#### **Details**

This operator will randomly choose cases affected individuals and controls unaffected individuals as a sample. The affected status is usually set by penetrance functions/operators. The sample populations will have two subpopulations: cases and controls.

You may specify the number of cases and the number of controls from each subpopulation using the array form of the parameters. The sample population will still have only two subpoulations (cases/controls) though.

A special case of this sampling scheme occurs when one of or both cases and controls are omitted (zeros). In this case, all cases and/or controls are chosen. If both parameters are omitted, the sample is effectively the same population with affected and unaffected individuals separated into two subpopulations.

#### Initialization

Draw cases and controls as a sample

```
caseControlSample(cases=[], controls=[], spSample=False,
name="sample", nameExpr="", times=1, saveAs="", saveAsExpr="",
format="auto", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

Please refer to class sample for other parameter descriptions.

cases The number of cases, or an array of the numbers of cases from each subpopulationcontrols The number of controls, or an array of the numbers of controls from each subpopulation

#### **Member Functions**

```
x.clone() Deep copy of a caseControlSample operator
```

## 3.9.6 Class affectedSibpairSample (Function form: AffectedSibpairSample)

Draw an affected sibling pair sample

#### **Details**

Special preparation for the population is needed in order to use this operator. Obviously, to obtain affected sibling pairs, we need to know the parents and the affectedness status of each individual. Furthermore, to get parental genotype, the population should have ancestralDepth at least 1. The most important problem, however, comes from the mating scheme we are using.

randomMating() is usually used for diploid populations. The *realrandom* mating requires that a mating will generate only one offspring. Since parents are chosen with replacement, a parent can have multiple offspring with different parents. On the other hand, it is very unlikely that two offspring will have the same parents. The probability of having a sibling for an offspring is  $\frac{1}{N^2}$  (if do not consider selection). Therefore, we will have to allow multiple offspring per mating at the cost of small effective population size.

All these requirements come at a cost: multiple ancestral populations, determining affectedness status and tagging will slow down evolution; multiple offspring will reduce effective population size. Fortunately, simuPOP is flexible enough to let all these happen only at the last several generations.

## Initialization

Draw an affected sibling pair sample

```
affectedSibpairSample(size=[], chooseUnaffected=False,
countOnly=False, name="sample", nameExpr="", times=1, saveAs="",
saveAsExpr="", format="auto", stage=PostMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=["father_idx",
"mother idx"])
```

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Please refer to class sample for other parameter descriptions.

**chooseUnaffected** Instead of affected sibpairs, choose unaffected families.

countOnly Set variables about number of affected sibpairs, do not actually draw the sample

**size** The number of affected sibling pairs to be sampled. Can be a number or an array. If a number is given, it is the total number of sibpairs, ignoring population structure. Otherwise, given number of sibpairs are sampled from subpopulations. If size is unspecified, this operator will return all affected sibpairs.

#### **Member Functions**

- x.clone() Deep copy of a affectedSibpairSample operator
- x.drawsample(pop) Draw a sample
- **x.prepareSample(pop)** Preparation before drawing a sample

## 3.9.7 Class largePedigreeSample

Draw a large pedigree sample

#### Initialization

Draw a large pedigree sample

```
largePedigreeSample(size=[], minTotalSize=0, maxOffspring=5,
minPedSize=5, minAffected=0, countOnly=False, name="sample",
nameExpr="", times=1, saveAs="", saveAsExpr="", format="auto",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["father_idx", "mother_idx"])
```

Please refer to class sample for other parameter descriptions.

```
countOnly Set variables about number of affected sibpairs, do not actually draw the sample.
maxOffspring The maximum number of offspring a parent may have
minAffected Minimal number of affected individuals in each pedigree, default to 0
minPedSize Minimal pedigree size, default to 5
minTotalSize The minimum number of individuals in the sample
```

### **Member Functions**

- x.clone() Deep copy of a largePedigreeSample operator
- x.drawsample(pop) Draw a a large pedigree sample
- **x.prepareSample(pop)** Preparation before drawing a sample

## 3.9.8 Class nuclearFamilySample

Draw a nuclear family sample

### Initialization

Draw a nuclear family sample

```
nuclearFamilySample(size=[], minTotalSize=0, maxOffspring=5,
minPedSize=5, minAffected=0, countOnly=False, name="sample",
nameExpr="", times=1, saveAs="", saveAsExpr="", format="auto",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["father_idx", "mother_idx"])
```

Please refer to class sample for parameter descriptions.

#### **Member Functions**

```
x.clone() Deep copy of a nuclearFamilySample operator
x.drawsample(pop) Draw a nuclear family sample
x.prepareSample(pop) Preparation before drawing a sample
```

## 3.10 Statistics Calculation

### 3.10.1 Class stator

Base class of all the statistics calculator

#### **Details**

Operator stator calculate various basic statistics for the population and set variables in the local namespace. Other operators/functions can refer to the results from the namespace after stat is applied.

### Initialization

Create a stator

```
stator(output="", outputExpr="", stage=PostMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

### **Member Functions**

```
x.clone() Deep copy of a stator
```

## 3.10.2 Class stat (Function form: Stat)

Calculate statistics

### **Details**

Operator stat calculates various basic statistics for the population and sets variables in the local namespace. Other operators/functions can refer to the results from the namespace after stat is applied. Stat is the function form of the operator.

Note that these statistics are dependent to each other. For example, heterotype and allele frequencies of related loci will be automatically calculated if linkage diseqilibrium is requested.

#### **Initialization**

Create an stat operator

```
stat(popSize=False, numOfMale=False, numOfMale_param={},
numOfAffected=False, numOfAffected_param={}, numOfAlleles=[],
numOfAlleles_param={}, alleleFreq=[], alleleFreq_param={},
heteroFreq=[], expHetero=[], expHetero_param={}, homoFreq=[],
genoFreq=[], haploFreq=[], LD=[], LD_param={}, association=[],
association_param={}, Fst=[], Fst_param={}, relGroups=[], relLoci=[],
rel_param={}, relBySubPop=False, relMethod=[], relMinScored=10,
hasPhase=False, midValues=False, output="", outputExpr="",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

If only one item is specified, the outer [] can be ignored. I.e., LD=[loc1, loc2] is acceptable. This parameter will set the following variables. Please note that the difference between the data structures used for ld and LD. The names are potentially very confusing but I have no better idea.

- ld['loc1-loc2']['allele1-allele2'],subPop[sp]['ld']['loc1-loc2']['allele1-allele2']
- ld\_prime['loc1-loc2']['allele1-allele2'], subPop[sp]['ld\_prime']['loc1-loc2']['allele1-allele2']
- r2['loc1-loc2']['allele1-allele2'], subPop[sp]['r2']['loc1-loc2']['allele1-allele2']
- LD[loc1][loc2], subPop[sp]['LD'][loc1][loc2]
- LD\_prime[loc1][loc2], subPop[sp]['LD\_prime'][loc1][loc2]
- R2[loc1][loc2], subPop[sp]['R2'][loc1][loc2]

Fst Calculate  $F_{st}$ ,  $F_{is}$ ,  $F_{it}$ . For example, Fst = [0,1,2] will calculate  $F_{st}$ ,  $F_{is}$ ,  $F_{it}$  based on alleles at loci 0, 1, 2. The locus-specific values will be used to calculate AvgFst, which is an average value over all alleles (Weir & Cockerham, 1984). Terms and values that match Weir & Cockerham:

- $F(F_{IT})$  the correlation of genes within individuals (inbreeding);
- $\theta$  (  $F_{ST}$ ) the correlation of genes of difference individuals in the same population (will evaluate for each subpopulation and the whole population)
- $f(F_{IS})$  the correlation of genes within individuals within populations.

This parameter will set the following variables:

- Fst[loc], Fis[loc], Fit[loc]
- AvgFst, AvgFis, AvgFit.

**Fst\_param** A dictionary of parameters of Fst statistics. Can be one or more items choosen from the following options: Fst, Fis, Fit, AvgFst, AvgFis, and AvgFit.

**LD** Calculate linkage disequilibria LD, LD' and  $r^2$ , given LD=[ [loc1, loc2], [ loc1, loc2, allele1, allele2], ... ] For each item [loc1, loc2, allele1, allele2], D, D' and  $r^2$  will be calculated based on allele1 at loc1 and allele2 at loc2. If only two loci are given, the LD values are averaged over all allele pairs. For example, for allele A at locus 1 and allele B at locus 2,

$$D = P_{AB} - P_A P_B$$

$$D' = D/D_{max}$$

$$D_{max} = \min(P_A (1 - P_B), (1 - P_A) P_B) \text{ if } D > 0 \min(P_A P_B, (1 - P_A) (1 - P_B)) \text{ if } D < 0$$

$$r^2 = \frac{D^2}{P_A (1 - P_A) P_B (1 - P_B)}$$

- **LD\_param** A dictionary of parameters of LD statistics. Can have key stat which is a list of statistics to calculate. Default to all. If any statistics is specified, only those specified will be calculated. For example, you may use LD\_param={LD\_prime} to calculate D' only, where LD\_prime is a shortcut for 'stat':['LD\_prime']. Other parameters that you may use are:
  - subPop, whether or not calculate statistics for subpopulations
  - midValues, whether or not keep intermediate results.
- - alleleNum[a], subPop[sp]['alleleNum'][a]
  - alleleFreq[a], subPop[sp]['alleleFreq'][a].
- **alleleFreq\_param** A dictionary of parameters of alleleFreq statistics. Can be one or more items choosen from the following options: numOfAlleles, alleleNum, and alleleFreq.

association Association measures

- **association\_param** A dictionary of parameters of association statistics. Can be one or more items choosen from the following options: ChiSq\_P, UC\_U, and CramerV.
- **expHetero** An array of loci at which the expected heterozygosities will be calculated (expHetero=[loc1, loc2, ...]). The expected heterozygosity is calculated by

$$h_{exp} = 1 - p_i^2.$$

The following variables will be set:

- expHetero[loc], subPop[sp]['expHetero'][loc].
- **expHetero\_param** A dictionary of parameters of expHetero statistics. Can be one or more items choosen from the following options: subpop and midValues.
- - genoNum[a][geno] and subPop[sp]['genoNum'][a][geno], the number of genotype geno at allele a. geno has the form x-y.
  - genoFreq[a][geno] and subPop[sp]['genoFreq'][a][geno], the frequency of genotype geno at allele a.
- haploFreq A matrix of haplotypes (allele sequences on different loci) to count. For example, haploFreq = [ 0,1,2 ], [1,2] ] will count all haplotypes on loci 0,1 and 2; and all haplotypes on loci 1, 2. If only one haplotype is specified, the outer [] can be omitted. I.e., haploFreq=[0,1] is acceptable. The following dictionary variables will be set with keys 0-1-2 etc. For example, haploNum['1-2']['5-6'] is the number of allele pair 5,6 (on loci 1 and 2 respectively) in the population.

- haploNum[haplo] and subPop[sp]['haploNum'][haplo], the number of allele sequencies on loci haplo.
- haploFreq[haplo], subPop[sp]['haploFreq'][haplo], the frequency of allele sequencies on loci haplo.

**hasPhase** If a/b and b/a are the same genotype. Default to False.

- heteroFreq An array of loci to calculate observed heterozygosities and expected heterozygosities (heteroFreq=[loc1, loc2, ...]). This parameter will set the following variables (arrays of observed heterozygosities). Note that heteroNum[loc][1] is the number of heterozygote  $\mathbf{1x}, x \neq 1$ . Numbers and frequencies (proportions) of heterozygotes are calculated for each allele. HeteroNum[loc] and HeterFreq[loc] are the overall heterozygosity number and frequency. I.e., the number/frequency of genotype  $\mathbf{xy}, x \neq y$ . From this number, we can easily derive the number of homozygosity.
  - HeteroNum[loc], subPop[sp]['HeteroNum'][loc], the overall heterozygote number
  - $\bullet \ \ \texttt{HeteroFreq[loc]}, \ subPop[sp]['\ \texttt{HeteroFreq'}][loc], \ the \ overall \ heterozygote \ frequency$
  - heteroNum[loc][allele], subPop[sp]['heteroNum'][loc][allele]
  - heteroFreq[loc][allele], subPop[sp]['heteroFreq'][loc][allele]
- homoFreq An array of loci to calculate observed homozygosities and expected homozygosities (homoFreq=[loc1, loc2, ...]). This parameter will calculate the numbers and frequencies of homozygotes **xx** and set the following variables:
  - homoNum[loc], subPop[sp]['homoNum'][loc],
  - homoFreq[loc], subPop[sp]['homoFreq'][loc].
- midValues Whether or not post intermediate results. Default to False. For example, Fst will need to calculate allele frequencise. If midValues is set to True, allele frequencies will be posted as well. This will be helpful in debugging and sometimes in deriving statistics.
- **numOfAffected** Whether or not count the numbers/proportions of affected and unaffected individuals. This parameter can set the following variables by user's specification:
  - numOfAffected, subPop[sp]['numOfAffected'] the number of affected individuals in the population/subpopulation
  - numOfUnaffected, subPop[sp]['numOfUnAffected'] the number of unaffected individuals in the population
  - propOfAffected, subPop[sp]['propOfAffected'] the proportion of affected individuals in the population/subpopulation
  - propOfUnaffected, subPop[sp]['propOfUnAffected'] the proportion of unaffected individuals in the population/subpopulation
- **numOfAffected\_param** A dictionary of parameters of numOfAffected statistics. Can be one or more items choosen from the following options: numOfAffected, propOfAffected, numOfUnaffected, propOfUnaffected.
- **numOfAlleles** An array of loci at which the numbers of distinct alleles will be counted (numOfAlleles=[loc1, loc2, ...] where loc1 etc. are absolute locus indexes). This is done through the calculation of allele frequencies. Therefore, allele frequencies will also be calculated if this statistics is requested. This parameter will set the following variables (carray objects of the numbers of alleles for *allloci*. Unrequested loci will have 0 distinct alleles.):
  - numOfAlleles, subPop[sp]['numOfAlleles'], number of distinct alleles at each locus. (Calculated only at requested loci.)

- **numOfAlleles\_param** A dictionary of parameters of numOfAlleles statistics. Can be one or more items choosen from the following options: numOfAffected, propOfAffected, numOfUnaffected, propOfUnaffected.
- **numOfMale** Whether or not count the numbers/proportions of males and females. This parameter can set the following variables by user's specification:
  - numOfMale, subPop[sp]['numOfMale'] the number of males in the population/subpopulation
  - numOfFemale, subPop[sp]['numOfFemale'] the number of females in the population/subpopulation
  - propOfMale, subPop[sp]['propOfMale'] the proportion of males in the population/subpopulation
  - propOfFemale, subPop[sp]['propOfFemale'] the proportion of females in the population/subpopulation
- **numOfMale\_param** A dictionary of parameters of numOfMale statistics. Can be one or more items choosen from the following options: numOfMale, propOfMale, numOfFemale, and propOfFemale.

**popSize** Whether or not calculate population sizes. This parameter will set the following variables:

- numSubPop the number of subpopulations
- subPopSize an array of subpopulation sizes. Not available for subpopulations.
- popSize, subPop[sp]['popSize'] population/subpopulation size.
- **relGroups** Calculate pairwise relatedness between groups. Can be in the form of either [[1,2,3],[5,6,7],[8,9]] or [2,3,4]. The first one specifies groups of individuals, while the second specifies subpopulations. By default, relatedness between subpopulations is calculated.

relLoci Loci on which relatedness values are calculated

- relMethod Method used to calculate relatedness. Can be either REL\_Queller or REL\_Lynch. The relatedness values between two individuals, or two groups of individuals are calculated according to Queller & Goodnight (1989) (method=REL\_Queller) and Lynch et al. (1999) (method=REL\_Lynch). The results are pairwise relatedness values, in the form of a matrix. Original group or subpopulation numbers are discarded. relatedness[grp1][grp2] is the relatedness value between grp1 and grp2. There is no subpopulation level relatedness values.
- **rel\_param** A dictionary of parameters of relatedness statistics. Can be one or more items choosen from the following options: Fst, Fis, Fit, AvqFst, AvqFis, and AvqFit.

### **Member Functions**

- x.apply(pop) Apply the stat operator
- **x.clone()** Deep copy of a stat operator

# 3.11 Expression and Statements

## 3.11.1 Class dumper

Dump the content of a population.

## Initialization

Dump population

```
dumper(alleleOnly=False, infoOnly=False, ancestralPops=False,
     dispWidth=1, max=100, chrom=[], loci=[], subPop=[], indRange=[],
     output=">", outputExpr="", stage=PostMating, begin=0, end=-1, step=1,
     at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
   alleleOnly Only display allele
   ancestralPops Whether or not display ancestral populations, default to False
   chrom Chromsoome(s) to display
   dispWidth Width of allele display, default to 1
   indRange Range(s) of individuals to display
   infoOnly Only display info
   loci Loci to display
   max Max number of individuals to display, default to 100. This is to avoid careless dump of huge populations.
   output Output file, default to standard output.
   outputExpr And other parameters: refer to help(baseOperator.__init__)
   subPop Only display subPop(s)
Member Functions
x.alleleOnly() Only show alleles (not structure, gene information?
x.apply(pop) Apply to one population. It does not check if the operator is activated.
x.clone() Deep copy of an operator
x.infoOnly() Only show info
x.setAlleleOnly(alleleOnly) SimuPOP::dumper::setAlleleOnly
x.setInfoOnly(infoOnly) SimuPOP::dumper::setInfoOnly
3.11.2 Class savePopulation
Save population to a file
Initialization
SimuPOP::savePopulation::savePopulation
     savePopulation(output="", outputExpr="", format="bin", compress=True,
```

**x.apply(pop)** Apply to one population. It does not check if the operator is activated.

stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP\_ALL,

x.clone() Deep copy of an operator

grp=GRP\_ALL, infoFields=[])

## 3.11.3 Class pyOutput

Output a given string.

#### **Details**

A common usage is outputting a new line for the last replicate.

#### Initialization

Create a pyOutput operator that output a given string.

```
pyOutput(str="", output=">", outputExpr="", stage=PostMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

#### **Member Functions**

str String to be outputted

```
x.apply(pop) Simply output some info
x.clone() Deep copy of an operator
x.setString(str) Set output string.
```

## 3.11.4 Class pyEval (Function form: PyEval)

Evaluate an expression

### **Details**

Python expressions/statements will be executed when pyEval is applied to a population by using parameters expr/stmts. Statements can also been executed when pyEval is created and destroyed or before expr is executed. The corresponding parameters are preStmts, postStmts and stmts. For example, operator varPlotter uses this feature to initialize R plots and save plots to a file when finished.

### Initialization

Evaluate expressions/statments in the local namespace of a replicate

stmts The statement that will be executed before the expression

```
pyEval(expr="", stmts="", preStmts="", postStmts="", exposePop=False,
    name="", output=">", outputExpr="", stage=PostMating, begin=0,
    end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])

exposePop If true, expose current population as variable pop

expr The expression to be evaluated. Its result will be sent to output.

name Used to let pure Python operator to identify themselves

output Default to >. I.e., output to standard output.

postStmts The statement that will be executed when the operator is destroyed

preStmts The statement that will be executed when the operator is constructed
```

- **x.apply(pop)** Apply the pyEval operator
- x.clone() Deep copy of a pyEval operator
- x.name() Return the name of an expression

The name of a pyEval operator is given by an optional parameter name. It can be used to identify this pyEval operator in debug output, or in the dryrun mode of simulator::evolve.

## 3.11.5 Class pyExec (Function form: PyExec)

Execute a Python statement

#### **Details**

This operator takes a list of statements and execute them. No value will be returned or outputted.

### Initialization

Evaluate statments in the local replicate namespace, no return value

**exposePop** If true, expose current population as variable pop

```
pyExec(stmts="", preStmts="", postStmts="", exposePop=False, name="",
  output=">", outputExpr="", stage=PostMating, begin=0, end=-1, step=1,
  at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
default To >. I.e., output to standard output.
```

postStmts The statement that will be executed when the operator is destroyed

preStmts The statement that will be executed when the operator is constructed

**stmts** The statements (a single or multi-line string) that will be executed when this operator is applied.

#### **Member Functions**

x.clone() Deep copy of a pyExec operator

# 3.12 Tagging (used for pedigree tracking)

## 3.12.1 Class tagger

Base class of tagging individuals

#### **Details**

TAGGER is a during mating operator that tag individuals with various information. Potential usages are:

- recording parental information to track pedigree;
- tagging an individual/allele and monitor its spread in the population etc.

## Initialization

Create a tagger, default to be always active but no output

```
tagger(begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

```
x.clone() Deep copy of a
tagger
```

## 3.12.2 Class inheritTagger

Inherite tag from parents.

#### **Details**

This during-mating operator will copy the tag information from his/her parents. Depending on mode parameter, this tagger will obtain tag from his/her father (two tag fields), mother (two tag fields) or both (first tag field from both father and mother). An example may be tagging one or a few parents and see, at the last generation, how many offspring they have.

#### Initialization

Create an inheritTagger, default to be always active

```
inheritTagger(mode=TAG_Paternal, begin=0, end=-1, step=1,
at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=["paternal_tag",
"maternal_tag"])
```

Create a inheritTagger that inherit a tag from one or both parents. A tag is actually a information field whose value will be copied from parents to offspring. By default, paternal tag is copied to offspring's using the specified information field. If mode=TAG\_Both, two tags will be copied from parents (info1 from father, and info2 from mother).

```
mode Can be one of TAG_Paternal, TAG_Maternal, and TAG_Both
```

### **Member Functions**

x.clone() Deep copy of a inheritTagger

## 3.12.3 Class parents Tagger

Tagging according to parents' indexes

## **Details**

This during-mating operator set

c tag(), currently a pair of numbers, of each individual with indexes of his/her parents in the parental population. This information will be used by pedigree-related operators like affectedSibpairSample to track the pedigree information. Since parental population will be discarded or stored after mating, and tagging information will be passed with individuals, mating/population change etc. will not interfere with this simple tagging system.

#### Initialization

Create a parentsTagger, default to be always active

```
parentsTagger(begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=["father_idx", "mother_idx"])
```

x.clone() Deep copy of a parentsTagger

#### **Details**

This tagger takes some information fields from both parents, pass to a Python function and set the individual field with the returned value.

This operator can be used to trace the inheritance of trait values.

#### Initialization

```
pyTagger(func=None, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

Creates a pyTagger that work on specified information fields.

**func** A Pyton function that returns a list to assign the information fields. e.g., if fields=['A', 'B'], the function will pass values of fields 'A' and 'B' of father, followed by mother if there is one, to this function. The returned value is assigned to fields 'A' and 'B' of the offspring. The returned value has to be a list even if only one field is given.

**infoFields** Information fields. The user should gurantee the existence of these fields.

### **Member Functions**

```
x.clone() Deep copy of a pyTagger
```

## 3.13 Terminator

## 3.13.1 Class terminator

Base class of all terminators.

#### **Details**

These operators are used to see if an evolution is running as expected, and terminate the evolution if a certain condition fails.

## Initialization

Create a terminator

```
terminator(message="", output=">", outputExpr="", stage=PostMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

message A message that will be displayed when the evolution is terminated.

## **Member Functions**

x.clone() Deep copy of a terminator

## 3.13.2 Class terminateIf

Terminate according to a condition

## **Details**

This operator terminates the evolution under certain conditions. For example, terminateIf(condition='alleleFreq[0][1]<0.05', begin=100) terminates the evolution if the allele frequency of allele 1 at locus 0 is less than 0.05. Of course, to make this operator work, you will need to use a stat operator before it so that variable alleleFreq exists in the local namespace.

When the condition is true, a shared variable var="terminate" will be set to the current generation.

#### **Initialization**

Create a terminateIf terminator

```
terminateIf(condition="", message="", var="terminate", output="",
outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

#### **Member Functions**

```
x.apply(pop) Apply the terminateIf terminator
```

x.clone() Deep copy of a terminateIf terminator

## 3.13.3 Class continueIf

Terminate according to a condition failure

#### **Details**

The same as terminateIf but continue if the condition is True.

## Initialization

Create a continueIf terminator

```
continueIf(condition="", message="", var="terminate", output="",
outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

### **Member Functions**

```
x.apply(pop) Apply this operator
```

x.clone() Deep copy of a continue If terminator

# 3.14 Conditional operator

### 3.14.1 Class if Else

Conditional operator

## Details

This operator accepts

- an expression that will be evaluated when this operator is applied;
- an operator that will be applied if the expression is True (default to null);
- an operator that will be applied if the expression is False (default to null).

When this operator is applied to a population, it will evaluate the expression and depending on its value, apply the supplied operator. Note that the begin, at, step, and at parameters of ifOp and elseOp will be ignored. For example, you can mimic the at parameter of an operator by ifElse('rep in [2,5,9]' operator). The real use of this machanism is to monitor the population statistics and act accordingly.

#### Initialization

SimuPOP::ifElse::ifElse

```
ifElse(cond, ifOp=None, elseOp=None, output=">", outputExpr="",
stage=PostMating, begin=0, end=-1, step=1, at=[], rep=REP_ALL,
grp=GRP_ALL, infoFields=[])
```

cond Expression that will be treated as a bool variable

elseOp An operator that will be applied when cond is False

ifOp An operator that will be applied when cond is True

#### **Member Functions**

```
x.apply(pop) Apply the ifElse operator to one population
```

x.clone() Deep copy of an ifElse operator

#### **Example**

### Example 3.22: Operator if Else

```
>>> simu = simulator(
       population(size=1000, loci=[1]),
        randomMating(), rep=4)
>>> simu.evolve(
     preOps = [ initByValue([1,1])],
     ops = [
        # penetrance, additve penetrance
        maPenetrance(locus=0, wildtype=[1], penetrance=[0,0.5,1]),
        # count number of affected
. . .
        stat(numOfAffected=True),
        # introduce disease if no one is affected
        ifElse(cond='numOfAffected==0',
          ifOp=kamMutator(rate=0.01, maxAllele=2)),
        ifElse(cond='numOfAffected==0',
            ifOp=pyEval(r'"No affected at gen %d\n" % gen'))
      ],
      end=50
. . .
...)
No affected at gen 0
```

```
No affected at gen 11
No affected at gen 12
No affected at gen 41
True
>>>
```

## 3.15 Debug-related operators/functions

Standard simuPOP module can print out lots of debug information upon request. These are mostly used for internal debugging purposes but you can also use them when error happens. For example, the following code will crash simuPOP:

```
>>> population(1).individual(0).arrAllele()
```

It is not clear why this simple line will cause us trouble, instead of outputting the genotype of the only individual of this population. However, the reason is clear if you turn on debug information:

Example 3.23: Turn on/off debug information

```
>>> TurnOnDebug(DBG_ALL)
Debug code DBG_ALL is turned on. cf. listDebugCode(), turnOffDebug()
>>> population(1).individual(0).arrAlleles()
Constructor of Population is called
Population size 1
Destructor of Population is called
Segmentation fault (core dumped)
```

population(1) creates a temporary object that is destroyed right after the execution of the input. When Python tries to display the genotype, it will refer to an invalid location. The right way to do this is to create a persistent population object:

```
>>> pop = population(1)
>>> pop.individual(0).arrAllele()
```

If the output is overwhelming after you turn on all debug information, you can turn on certain part of the information by using the following functions:

- ListDebugCode() list all debug code.
- turnOnDebug(), TurnOnDebug(code) turn on debug codes.
- turnOffDebug(), TurnOffDebug(code) turn off debug codes.

turnOnDebug() and turnOffDebug() are operators and accept all operator parameters begin, step etc. Usually, you can use turnOnDebug to output more information about a potential bug before simuPOP starts to misbehave.

Another useful debug code is DBG\_PROFILE. When turned on, it will display running time of each operator. This will give you a good sense of which operator runs slowly (or simply the order of operator execution if you are not sure). If most of the execution time is spent on a pure-Python operator, you may want to rewrite it in C++. Note that DBG\_PROFILE is suitable for measuring individual operator performance. If you would like to measure the execution time of all operators in several generations, ticToc operator is better.

## 3.15.1 Class turnOnDebug (Function form: TurnOnDebug)

Set debug on

#### **Details**

Turn on debug. There are several ways to turn on debug information for non-optimized modules, namely

- set environment variable SIMUDEBUG
- use simuOpt.setOptions(debug) function, or
- use TurnOnDebug or TurnOnDebugByName function
- use this turnOnDebug operator

The advantage of using this operator is that you can turn on debug at given generations.

#### **Initialization**

SimuPOP::turnOnDebug::turnOnDebug

```
turnOnDebug(code, stage=PreMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

#### **Member Functions**

- x.apply(pop) Apply the turnOnDebug operator to one population
- x.clone() Deep copy of a turnOnDebug operator

## 3.15.2 Class turnOffDebug (Function form: TurnOffDebug)

Set debug off

#### **Details**

Turn off debug.

#### Initialization

SimuPOP::turnOffDebug::turnOffDebug

```
turnOffDebug(code, stage=PreMating, begin=0, end=-1, step=1, at=[],
rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

#### **Member Functions**

- **x.apply(pop)** Apply the turnOffDebug operator to one population
- **x.clone()** Deep copy of a turnOffDebug operator

## 3.16 Miscellaneous

## 3.16.1 Class noneOp

None operator

## Initialization

```
noneOp(output=">", outputExpr="", stage=PostMating, begin=0, end=0,
step=1, at=[], rep=REP ALL, grp=GRP ALL, infoFields=[])
```

This operator does nothing.

#### **Member Functions**

- **x.apply(pop)** Apply the noneOp operator to one population
- x.clone() Deep copy of a noneOp operator

## **Example**

#### Example 3.24: Operator noneOp

```
>>> # this may be set from command line option
>>> savePop = False
>>> # then, saveOp is defined accordingly
>>> if savePop:
... saveOp = savePopulation(output='a.txt')
... else:
... saveOp = noneOp()
...
>>> simu = simulator(population(10), randomMating())
>>> simu.step([saveOp])
True
>>>
```

## 3.16.2 Class pause

Pause a simulator

## Details

This operator pauses the evolution of a simulator at given generations or at a key stroke, using stopOnKeyStroke=True option. Users can use 'q' to stop an evolution. When a simulator is stopped, press any other key to resume the simulation or escape to a Python shell to examine the status of the simulation by press 's'.

There are two ways to use this operator, the first one is to pause the simulation at specified generations, using the usual operator parameters such as at. Another way is to pause a simulation with any key stroke, using the stopOnKeyStroke parameter. This feature is useful for a presentation or an interactive simulation. When 's' is pressed, this operator expose the current population to the main Python dictionary as variable pop and enter an interactive Python session. The way current population is exposed can be controlled by parameter exposePop and popName. This feature is useful when you want to examine the properties of a population during evolution.

#### **Initialization**

Stop a simulation. Press 'q' to exit or any other key to continue.

```
pause(prompt=True, stopOnKeyStroke=False, exposePop=True,
popName="pop", output=">", outputExpr="", stage=PostMating, begin=0,
end=-1, step=1, at=[], rep=REP_LAST, grp=GRP_ALL, infoFields=[])
```

**exposePop** Whether or not expose pop to user namespace, only useful when user choose 's' at pause. Default to True.

popName By which name the population is exposed. Default to pop.

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```
prompt If True (default), print prompt message
stopOnKeyStroke If True, stop only when a key was pressed
```

#### **Member Functions**

- x.apply(pop) Apply the pause operator to one population
- x.clone() Deep copy of a pause operator

## 3.16.3 Class ticToc (Function form: TicToc)

Timer operator

#### **Details**

This operator, when called, output the difference between current and the last called clock time. This can be used to estimate execution time of each generation. Similar information can also be obtained from turnOnDebug(DBG\_PROFILE), but this operator has the advantage of measuring the duration between several generations by setting step parameter.

#### Initialization

Create a timer

```
ticToc(output=">", outputExpr="", stage=PreMating, begin=0, end=-1,
step=1, at=[], rep=REP_ALL, grp=GRP_ALL, infoFields=[])
```

#### **Member Functions**

- x.apply(pop) Apply the ticToc operator to one population
- x.clone() Deep copy of a ticToc operator

## 3.16.4 Class setAncestralDepth

Set ancestral depth

#### Details

This operator set the number of ancestral generations to keep in a population. It is usually called like setAncestral(at=[-2]) to start recording ancestral generations to a population at the end of the evolution. This is useful when constructing pedigree trees from a population.

## Initialization

Create a setAncestralDepth operator

```
setAncestralDepth(depth, output=">", outputExpr="", stage=PreMating,
begin=0, end=-1, step=1, at=[], rep=REP_ALL, grp=GRP_ALL,
infoFields=[])
```

#### **Member Functions**

- **x.apply(pop)** Apply the setAncestralDepth operator to one population
- **x.clone()** Deep copy of a setAncestralDepth operator

# Global and Python Utility functions

## 4.1 Global functions

## AlleleType()

Return the allele type of the current module. Can be binary, short, or long.

#### Limits()

Print out system limits

#### ListAllRNG()

List the name of all available random number generators

#### ListDebugCode()

List all debug codes

#### LoadPopulation(file, format="auto")

Load a population from a file. The file format is by default determined by file extension (format="auto"). Otherwise, format can be one of txt, bin, or xml.

## LoadSimulator(file, mate, format="auto")

Load a simulator from a file with the specified mating scheme. The file format is by default determined by file extension (format="auto"). Otherwise, format can be one of txt, bin, or xml.

## MaxAllele()

Return 1,  $2^8 - 1$ ,  $2^{16} - 1$  for binary, short, or long allele modules, respectively

#### MergePopulations(pops, newSubPopSizes=[], keepAncestralPops=-1)

Merge several populations with the same genotypic structure and create a new population

## MergePopulationsByLoci(pops, newNumLoci=[], newLociPos=[], byChromosome=False)

Merge several populations of the same size by loci and create a new population

#### ModuleCompiler()

Return the compiler used to compile this simuPOP module

#### ModuleDate()

Return the date when this simuPOP module is compiled

## ModulePlatForm()

Return the platform on which this simuPOP module is compiled

#### ModulePyVersion()

Return the Python version this simuPOP module is compiled for

## Optimized()

Return True if this simuPOP module is optimized

## SetRNG(rng="", seed=0)

Set random number generator. If seed=0 (default), a random seed will be given. If rng="", seed will be set to the current random number generator.

#### TurnOffDebug(code=DBG\_ALL)

Turn off debug information. Default to turn off all debug codes. Only available in non-optimized modules. Do not mix this function with turnOffDebug(), which creates an operator

#### TurnOnDebug(code=DBG ALL)

Set debug codes. Default to turn on all debug codes. Only available in non-optimized modules. Do not mix this function with turnOnDebug(), which creates an operator

#### rng()

Return the currently used random number generator

#### simuRev()

Return the revision number of this simuPOP module. Can be used to test if a feature is available.

#### simuVer()

Return the version of this simuPOP module

## 4.2 Utility Modules

Several utility modules are distributed with simuPOP. They provide important functions and extensions to simuPOP and serve as good examples on how simuPOP can be used.

Compared to simuPOP kernel functions, these utility functions are less tested, and are subject to more frequent changes. Please report to simuPOP mailing list if any function stops working.

## 4.2.1 Module simuOpt

Module simuOpt can be used to control which simuPOP module to load, and how it is loaded using function setOptions. It also provides a simple way to set simulation options, from user input, command line, configuration file or a parameter dialog. All you need to do is to define an option description list that lists all parameters in a given format, and call the getParam function. This module, if loaded, pre-process the command line options. More specifically, it checks command line option:

- -c configfile read from a configuration file
- --config configgile the same as -c
- --optimized load optimized modules, unless setOption explicitly use non-optimizedmodules.
- -q Do not display banner information when simuPOP is loaded
- --quiet the same as -q

- **--useTkinter** force the use of Tcl/Tk dialog even when wxPython is available. By default, wxPython is used whenever possible.
- **--noDialog** do not use option dialog. If the options can not be obtained fromcommand line or configuration file, users will be asked to input them interactively.

Because these options are reserved, you can not use them in your simuPOP script.

#### **Module Functions**

## getParam (options=[], doc=", details=", noDialog=False, checkUnprocessedArgs=True, verbose=False, nCol=1)

Get parameters from either

- a Tcl/Tk based, or wxPython based parameter dialog (wxPython is used if it is available)
- command line argument
- configuration file specified by -c file (-config file), or
- prompt for user input

The option description list consists of dictionaries with some predefined keys. Each dictionary defines an option. Each option description item can have the following keys:

- arg short command line option name. 'h' checks the presence of argument -h. If an argument is expected, add a comma to the option name. For example, 'p:' matches command line option -p=100 or -p 100
- longarg long command line option name. 'help' checks the presence of argument '-help'. 'mu=' matches command line option -mu=0.001 or -mu 0.001.
- **label** The label of the input field in a parameter dialog, and as the prompt foruser input.
- **default** default value for this parameter. It is used to as the default value in the parameter dialog, and as the option value when a user presses 'Enter' directly during interactive parameter input.
- **useDefault** use default value without asking, if the value can not be determinedfrom GUI, command line option or config file. This is useful for options that rarely need to be changed. Setting them to useDfault allows shorter command lines, and easy user input.
- **description** a long description of this parameter, will be put into the usage information, which will be displayed with ( -h , -help command line option, or help button in parameter dialog).
- **allowedTypes** acceptable types of this option. If allowedTypes is types.ListType or types.TupleType and the user's input is a scalar, the input will be converted to a list automatically. If the conversion can not be done, this option will not be accepted.
- validate a function to validate the parameter. You can define your own functions or use the ones defined in this module.
- **chooseOneOf** if specified, simuOpt will choose one from a list of values using a listbox (Tk) or a combo box (wxPython).
- **chooseFrom** if specified, simuOpt will choose one or more items from a list ofvalues using a listbox (tk) or a combo box (wxPython).
- **separator** if specified, a blue label will be used to separate groups of parameters.
- jump it is used to skip some parameters when doing the interactive user input. For example, getParam will skip the rest of the parameters if -h is specified if parameter -h has item 'jump':-1 which means jumping to the end. Another situation of using this value is when you have a hierarchical parameter set. For example, if mutation is on, specify mutation rate, otherwise proceed.
- jumpIfFalse The same as jump but jump if current parameter is False.

This function will first check command line argument. If the argument is available, use its value. Otherwise check if a config file is specified. If so, get the value from the config file. If both failed, prompt user to input a value. All input will be checked against types, if exists, an array of allowed types. Parameters of this function are:

options a list of option description dictionaries

doc short description put to the top of parameter dialog

**details** module help. Usually set to doc .

noDialog do not use a parameter dialog, used in batch mode. Default to False.

checkUnprocessedArgs check args, avoid misspelling of arg name

verbose whether or not print detailed info

nCol number of columns in the parameter dialog.

## printConfig (opt, param, out=<open file '<stdout>', mode 'w' at 0x2a955940a0>)

Print configuration.

opt option description list

param parameters returned from getParam()

out output

#### requireRevision (rev)

Compare the revision of this simuPOP module with given revision. Raise an exception if current module is out of date.

## saveConfig (opt, file, param)

Write a configuration file. This file can be later read with command line option -c or -config.

opt the option description list

file output file

param parameters returned from getParam

## setOptions (optimized=None, mpi=None, chromMap=[], alleleType=None, quiet=None, debug=[])

set options before simuPOP is loaded to control which simuPOP module to load, and how the module should be loaded.

**optimized** whether or not load optimized version of a module. If not set, environmental variable SIMUOP-TIMIZED, and commandline option –optimized will be used if available. If nothing is defined, standard version will be used.

**alleleType** 'binary', 'short', or 'long'. 'standard' can be used as 'short' for backward compatibility. If not set, environmental variable SIMUALLELETYPE will be used if available. if it is not defined, the short allele version will be used.

quiet If True, supress banner information when simuPOP is loaded.

debug a list of debug code (or string). If not set, environmental variableSIMUDEBUG will be used if available.

mpi currently unused

chromMap currently unused

#### usage (options, before=")

Print usage information from the option description list. Used with -h (or -help) option, and in the parameter input dialog.

options option description list.

before optional information

#### valueAnd (t1, t2)

Return a function that returns true if passed option passes validator t1 and t2

#### valueBetween (a, b)

Return a function that returns true if passed option is between value a and b (a and b included)

#### valueEqual (a)

Return a function that returns true if passed option equals a

#### valueGE (a)

Return a function that returns true if passed option is greater than or equal to a

## valueGT (a)

Return a function that returns true if passed option is greater than a

#### valueIsList ()

Return a function that returns true if passed option is a list (or tuple)

#### valueIsNum ()

Return a function that returns true if passed option is a number (int, long or float)

#### valueLE (a)

Return a function that returns true if passed option is less than or equal to a

## valueLT (a)

Return a function that returns true if passed option is less than a

#### valueListOf (t)

Return a function that returns true if passed option val is a list of type t. If t is a function (validator), check if all v in val pass t(v)

## valueNot (t)

Return a function that returns true if passed option does not passes validator t

#### valueNotEqual (a)

Return a function that returns true if passed option does not equal a

## valueOneOf (t)

Return a function that returns true if passed option is one of the values list in t

#### valueOr (t1, t2)

Return a function that returns true if passed option passes validator t1 or t2

#### valueTrueFalse ()

Return a function that returns true if passed option is True or False

#### valueValidDir ()

Return a function that returns true if passed option val if a valid directory

#### valueValidFile ()

Return a function that returns true if passed option val if a valid file

## 4.2.2 Module simuUtil

This module provides some commonly used operators and format conversion utilities.

#### **Module Functions**

#### CaseControl\_ChiSq (pop, sampleSize, penetrance=None)

Draw affected sibpair sample from pop, run TDT using GENEHUNTER

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

**pene** penetrance function, if not given (None), existing affectionstatus will be used.

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

keep\_temp if True, do not remove sample data. Default to False.

### ChiSq\_test (pop)

perform case control test

**pop** loaded population, or population file in simuPOP format. This function assumes that pop has two sub-populations, cases and controls, and have 0 as wildtype and 1 as disease allele. pop can also be an loaded population object.

Return value A list of p-value at each locus.

Note this function requires rpy module.

#### ConstSize (size, split=0, numSubPop=1, bottleneckGen=-1, bottleneckSize=0)

The population size is constant, but will split into numSubPop subpopulations at generation split

## ExponentialExpansion (initSize, endSize, end, burnin=0, split=0, numSubPop=1, bottleneckGen=-1, bottleneckSize=0)

Exponentially expand population size from intiSize to endSize after burnin, split the population at generation split.

## InstantExpansion (initSize, endSize, end, burnin=0, split=0, numSubPop=1, bottleneckGen=-1, bottleneckSize=0)

Instaneously expand population size from intiSize to endSize after burnin, split the population at generation split.

#### LOD gh (file, gh='gh')

Analyze data using the linkage method of genehunter. Note that this function may not work under platforms other than linux, and may not work with your version of genehunter. As a matter of fact, it is almost unrelated to simuPOP and is provided only as an example how to use python to analyze data.

#### Parameters

**file** file to analyze. This function will look for file.dat and file.pre in linkage format.

loci a list of loci at which p-value will be returned. If the list is empty, all p-values are returned.

gh name (or full path) of genehunter executable. Default to 'gh'

**Return value** A list (for each chromosome) of list (for each locus) of p-values.

## LOD\_merlin (file, merlin='merlin')

run multi-point non-parametric linkage analysis using merlin

## 

Draw affected sibpair sample from pop, run TDT using GENEHUNTER

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

**gtrait** a function to calculate quantitative trait

infoField information field to store quantitative trait. Default to 'qtrait'

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

merlin executable name of merlin, full path name can be given.

**keep\_temp** if True, do not remove sample data. Default to False.

## 

Draw affected sibpair sample from pop, run TDT using GENEHUNTER

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

qtrait a function to calculate quantitative trait

infoField information field to store quantitative trait. Default to 'qtrait'

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

merlin executable name of merlin, full path name can be given.

keep\_temp if True, do not remove sample data. Default to False.

## LinearExpansion (initSize, endSize, end, burnin=0, split=0, numSubPop=1, bottleneckGen=-1, bottleneckSize=0)

Linearly expand population size from intiSize to endSize after burnin, split the population at generation split.

## ListVars (var, level=-1, name=", subPop=True, useWxPython=True)

list a variable in tree format, either in text format or in a wxPython window.

var any variable to be viewed. Can be a dw object returned by dvars() function

**level** level of display.

name only view certain variable

subPop whether or not display info in subPop

**useWxPython** if True, use terminal output even if wxPython is available.

## LoadFstat (file, loci=[])

load population from fstat file 'file' since fstat does not have chromosome structure an additional parameter can be given

## MigrIslandRates (r, n)

```
migration rate matrix x m/(n-1) m/(n-1) .... m/(n-1) x ..... m/(n-1) m/(n-1) x where x = 1-m
```

## MigrSteppingStoneRates (r, n, circular=False)

```
migration rate matrix, circular step stone model (X=1-m) X m/2 m/2 m/2 X m/2 0 0 m/2 x m/2 .....0 ... m/2 0 .... m/2 X or non-circular X m/2 m/2 X m/2 0 0 m/2 X m/2 .....0 ... m X
```

```
QtraitSibs_Reg_merlin (pop, sampleSize, qtrait=None, infoField='qtrait',
     merlin='merlin-regress', keep_temp=False)
     Draw affected sibpair sample from pop, run TDT using GENEHUNTER
     pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least
          one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the
          Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles
     qtrait a function to calculate quantitative trait
     infoField information field to store quantitative trait. Default to 'qtrait'
     sampleSize total sample size N. N/4 is the number of families to ascertain.
     merlin executable name of merlin, full path name can be given.
     keep temp if True, do not remove sample data. Default to False.
QtraitSibs VC merlin (pop, sampleSize, qtrait=None, infoField='qtrait',
     merlin='merlin', keep_temp=False)
     Draw affected sibpair sample from pop, run TDT using GENEHUNTER
     pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least
          one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the
          Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles
     gtrait a function to calculate quantitative trait
     infoField information field to store quantitative trait. Default to 'qtrait'
     sampleSize total sample size N. N/4 is the number of families to ascertain.
     merlin executable name of merlin, full path name can be given.
     keep_temp if True, do not remove sample data. Default to False.
Regression_merlin (file, merlin='merlin-regress')
     run merlin regression method
SaveCSV (pop, output=", outputExpr=", fields=['sex', 'affection'], loci=[],
     combine=None, shift=1, **kwargs)
     save file in CSV format
     fileds information fields, 'sex' and 'affection' are special fields that is treated differently.
     genotype list of loci to output, default to all.
     combine how to combine the markers. Default to None. A function can be specified, that takes the form
     def func(markers) return markers[0]+markers[1]
     shift since alleles in simuPOP is 0-based, shift=1 is usually needed to output alleles starting from allele 1.
          This parameter is ignored if combine is used.
SaveFstat (pop, output=", outputExpr=", maxAllele=0, loci=[], shift=1,
     combine=None)
     # save file in FSTAT format
SaveLinkage (pop, output=", outputExpr=", loci=[], shift=1, combine=None,
     fields=[], recombination=1.00000000000001e-05, penetrance=[0, 0.25,
     0.5], affectionCode=['1', '2'], pre=True, daf=0.001)
     save population in Linkage format. Currently only support affected sibpairs sampled with affectedSibpairSam-
     ple operator.
```

```
pop population to be saved. Must have ancestral Depth 1 paired individuals are sibs. Parental population are
          corresponding parents. If pop is a filename, it will be loaded.
     output output.dat and output.ped will be the data and pedigree file.You may need to rename them to be
          analyzed by LINKAGE. This allows saving multiple files.
     outputExpr expression version of output.
     affectionCode default to '1'
     pre True. pedigree format to be fed to makeped. Non-pre format it is likely to be wrong now for non-sibpair
          families.
     Note the first child is always the proband.
SaveMerlinDatFile (pop, output=", outputExpr=", loci=[], fields=[],
     outputAffection=False)
     Output a .dat file readable by merlin
SaveMerlinMapFile (pop, output=", outputExpr=", loci=[])
     Output a .map file readable by merlin
SaveMerlinPedFile (pop, output=", outputExpr=", loci=[], fields=[],
     header=False, outputAffection=False, affectionCode=['U', 'A'],
     combine=None, shift=1, **kwargs)
     Output a .ped file readable by merlin
SaveQTDT (pop, output=", outputExpr=", loci=[], header=False,
     affectionCode=['U', 'A'], fields=[], combine=None, shift=1, **kwargs)
     save population in Merlin/QTDT format. The population must have pedindex, father_idx and mother_idx infor-
     mation fields.
     pop population to be saved. If pop is a filename, it will be loaded.
```

**output** base filename.

**outputExpr** expression for base filename, will be evaluated in pop'slocal namespace.

**affectionCode** code for unaffected and affected. '1', '2' are default,but 'U', and 'A' or others can be specified.

loci loci to output

**header** whether or not put head line in the ped file.

fields information fields to output

**combine** an optional function to combine two alleles of a diploid individual.

**shift** if combine is not given, output two alleles directly, addingthis value (default to 1).

```
SaveSolarFrqFile (pop, output=", outputExpr=", loci=[], calcFreq=True)
```

Output a frequency file, in a format readable by solar

calcFreq whether or not calculate allele frequency

Draw affected sibpair sample from pop, run Linkage analysis using GENEHUNTER

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

**pene** penetrance function, if not given (None), existing affectionstatus will be used.

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

recRate recombination rate, used in the Linkage file. If not given,pop.dvars().recRate[0] will be used. If there is no such variable, 0.0001 is used.

daf disease allele frequency. This is needed for the linkage formatbut I am not sure if it is used by TDT.

gh executable name of genehunter, full path name can be given.

**keep\_temp** if True, do not remove sample data. Default to False.

## 

Draw affected sibpair sample from pop, run multi-point linkage analysis using merlin

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

**pene** penetrance function, if not given (None), existing affectionstatus will be used.

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

merlin executable name of merlin, full path name can be given.

keep\_temp if True, do not remove sample data. Default to False.

## 

Draw affected sibpair sample from pop, run TDT using GENEHUNTER

pop simuPOP population. It can be a string if path to a file is given. This population must 1. have at least one ancestral generation (parental generation) 2. have a variable DSL (pop.dvars().DSL) indicating the Disease susceptibility loci. These DSL will be removed from the samples. 3. has only binary alleles

**pene** penetrance function, if not given (None), existing affectionstatus will be used.

**sampleSize** total sample size N. N/4 is the number of families to ascertain.

**recRate** recombination rate, used in the Linkage file. If not given,pop.dvars().recRate[0] will be used. If there is no such variable, 0.0001 is used.

daf disease allele frequency. This is needed for the linkage formatbut I am not sure if it is used by TDT.

gh executable name of genehunter, full path name can be given.

**keep\_temp** if True, do not remove sample data. Default to False.

#### TDT\_gh (file, gh='gh')

Analyze data using genehunter/TDT. Note that this function may not work under platforms other than linux, and may not work with your version of genehunter. As a matter of fact, it is almost unrelated to simuPOP and is provided only as an example how to use python to analyze data.

#### Parameters

file file to analyze. This function will look for file.dat and file.pre in linkage format.

**loci** a list of loci at which p-value will be returned. If the list is empty, all p-values are returned.

gh name (or full path) of genehunter executable. Default to 'gh'

**Return value** A list (for each chromosome) of list (for each locus) of p-values.

#### VC merlin (file, merlin='merlin')

run variance component method

**file** file.ped, file.dat, file.map and file,mdl are expected.file can contain directory name.

```
dataAggregator (self, maxRecord=0, recordSize=0)
```

EXPERIMENTAL collect variables so that plotters can plot them all at once You can of course put it in other uses

```
\textbf{Usage} \ \ a = dataAggregator(\ maxRecord=0, recordSize=0)
```

maxRecord if more data is pushed, the old ones are discarded

recordSize size of recorda.push(gen, data, idx=-1)

gen generation number

data one record (will set recordSize if the first time), or

idx if idx!=-1, set data at idx.a.clear() a.range() # return min, max of all data a.data[i] # column i of the data a.gen # a.ready() # if all column has the same length, so data is ready

Internal data storage self.gen [....] self.data column1 [......] column2 [......] ....... each record is pushed at the end of

Initialization

maxRecord maxRecorddow size. I.e., maximum generations of data to keep

```
saveFstat (output=", outputExpr=", **kwargs)
```

operator version of the function SaveFstat

```
saveLinkage (output=", outputExpr=", **kwargs)
```

An operator to save population in linkage format

## 4.2.3 Module simuRPy

This module helps the use of rpy package with simuPOP. It defines an operator varPlotter that can be used to plot population expressions when rpy is installed.

#### **Module Functions**

```
rmatrix (mat)
```

Convert a Python 2d list to r matrix format that can be passed to functions like image directly.

```
varPlotter (self, expr, history=True, varDim=1, numRep=1, win=0, ylim=[0, 0],
    update=1, title=", xlab='generation', ylab=", axes=True, lty=[], col=[],
    mfrow=[1, 1], separate=False, byRep=False, byVal=False, plotType='plot',
    level=20, saveAs=", leaveOpen=True, dev=", width=0, height=0, *args,
    **kwargs)
```

Plotting with history plot a number in the form of a variable or expression, use

```
>>> varPlotter(var='expr')
```

plot a vector in the same window and there is only one replicate in the simulator, use

```
>>> varPlotter(var='expr', varDim=len)
```

where len is the dimension of your variable or expression. Each line in the figure represents the history of an item in the array. plot a vector in the same window and there are several replicates, use

```
>>> varPlotter(var='expr', varDim=len, numRep=nr, byRep=1)
```

varPlotter will try to use an appropriate layout for your subplots (for example, use 3x4 if numRep=10). You can also specify parameter mfrow to change the layout. if you would like to plot each item of your array variables in a subplot, use

```
>>> varPlotter(var='expr', varDim=len, byVal=1)
```

or in case of a single replicate

```
>>> varPlotter(var='expr', varDim=len, byVal=1, numRep=nr)
```

There will be numRep lines in each subplot. Use option history=False to plot with history. Parameters byVal, varDim etc. will be ignored. Other options are

title, xtitle, ytitle title of your figure(s). title is default to your expression, xtitle is defaulted to generation.

win window of generations. I.e., how many generations to keep in a figure. This is useful when you want to keep track of only recent changes.

**update** update figure after update generations. This is used when you do not want to update the figure at every generation.

**saveAs** save figures in files saveAs#gen.eps. For example, if saveAs='demo', you will get files demo1.eps, demo2.eps etc.

**separate** plot data lines in separate panels.

**image** use R image function to plot image, instead of lines.

level level of image colors (default to 20).

**leaveOpen** whether or not leave the plot open when plotting is done. Default to True. Initialization

## 4.2.4 Module hapMapUtil

Utility functions to manipulate HapMap data. These functions are provided as samples on how to load and evolve the HapMap dataset. They tend to change frequently so do not call these functions directly. It is recommended that you copy these function to your script when you need to use them.

#### **Module Functions**

```
evolveHapMap (pop, endingSize, endGen, migr=<simuPOP_std.noneOp; proxy
   of <Swig Object of type 'simuPOP::noneOp *' at 0x5a06990> >,
    expand='exponential', mergeAt=10000, initMultiple=1, recIntensity=0.01,
   mutRate=9.9999999999999995e-08, step=10, keepParents=False,
   numOffspring=1)
   Evolve and expand the hapmap population
   gen total evolution generation
```

**initMultiple** copy each individual initMultiple times, to avoidrapid loss of genotype variation when population size is small.

endingSize ending poplation size

expand expanding method, can be linear or exponential

mergeAt when to merge population?

endGen endingGeneration

recIntensity recombination intensity

mutRate mutation rate

step step at which to display statistics

 ${\tt keepParents}\ \ {\tt whether}\ {\tt or}\ {\tt not}\ {\tt keep}\ {\tt parental}\ {\tt generations}$ 

**numOffspring** number of offspring at the last generation

**migr** a migrator to be used.

```
getMarkersFromName (hapmap_dir, names, chroms=[])
```

Get population from marker names. This function returns a tuple with a population with found markers and names of markers that can not be located in the HapMap data. The returned population has three subpopulations, corresponding to CEU, YRI and JPT+CHB hapmap populations.

**hapmap\_dir** where hapmap data in simuPOP format is stored. The filesshould have been prepared by script-s/loadHapMap.py.

names names of markers

**chroms** a list of chromosomes to look in. If empty, all 22 autosomes will be tried.

## 

Get a population with markers from given range

**hapmap\_dir** where hapmap data in simuPOP format is stored. The filesshould have been prepared by script-s/loadHapMap.py.

**chrom** chromosome number (1-based index)

startPos starting position (in cM)

endPos ending position (in cM)

maxNum maximum number of markers to get

minAF minimal minor allele frequency

minDist minimal distance between two adjacent markers, in cM

## sample1DSL (pop, DSL, DA, pene, name, sampleSize)

Sample from the final population, using a single lcous penetrance model.

DSL disease locus

DA disease allele

pene penetrance

name name of directory to save (it must exist)

sampleSize sample size, in this case, sampleSize/4 is the number of families

## sample2DSL (pop, DSL, pene, name, size)

Sample from the final population, using a two locus penetrance model

**DSL** disease loci (two locus)

pene penetrance value, assuming a two-locus model

name name to save sample

size sample size

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