
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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Introduction

This reference manual assumes that you have read the *simuPOP User's Guide* and know the basic concepts of simuPOP. It is also recommended 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 in module _simuPOP_la:

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 <module>
    #
IndexError: src/genoStru.h:477 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 <module>
    #
IndexError: src/population.h:448 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 optimized 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 <module>
    #
NameError: name 'alleleType' is not defined
>>> print optimized()
Traceback (most recent call last):
  File "refManual.py", line 1, in <module>
    #
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 reference to the existing 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 reference 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 `chromLocusPair(absIndex)` and `absLocusIndex(chrom, index)` 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)
1
>>> # index
>>> arr.index(2)
1
>>> # 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]
True
>>> # 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)
3
>>> 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 seriously 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

```
>>> print ListAllRNG()
('gfsr4', 'mt19937', 'mt19937_1999', 'mt19937_1998', 'r250', 'rand', 'rand48', 'random12
>>> # get system RNG
>>> print rng().name()
mt19937
>>> # set system RNG
>>> SetRNG("taus2", seed=10)
>>> print rng().name()
taus2
>>> # create a separate RNG instance
>>> r=RNG()
>>> for n in range(1,5):
...     print r.randBinomial(10, .7),
...
9 7 7 7
>>>
```

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 `rng().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.

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()`)
- 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. This object can not be created directly. It is created by a population.

Initialization

`SimuPOP::GenoStruTrait::GenoStruTrait`

```
GenoStruTrait()
```

Member Functions

x.absLocusIndex(chrom, locus) Return the absolute index of a locus on a chromosome. c.f. `chromLocusPair`

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.chromByName(name) Return the index of a chromosome by its name

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.chromName(chrom) Return the name of an chrom

x.chromNames() Return an array of chrom names

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()
5
>>> print pop.ploidy()
2
>>> print pop.ploidyName()
diploid
>>> print pop.numChrom()
2
>>> print pop.locusPos(2)
2.0
>>> print pop.alleleName(1)
C
>>> # get the fourth individual of the population
>>> ind = pop.individual(3)
>>> # access genotypic structure info
>>> print ind.ploidy()
2
>>> print ind.numChrom()
2
>>> print ind.numLoci(0)
5
>>> 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 supports subpopulations with boundary, and virtual subpopulations within 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, numbers and positions of loci on each chromosome etc. The most important components of a population are:

- subpopulations. 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 simuPOP uses one-level population structure, which means 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.

Initialization

Create a population object with given size and genotypic structure.

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

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, using `savePopulation` operator to save each generation to a file is a much better choice.

chromMap For MPI modules, currently unused.

chromNames An array of chromosome names.

infoFields Names of information fields that will be attached to each individual. For example, if you need to record the parents of each individual using operator `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 chromosome 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 the chromosome index and Y is the 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 the 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 Diploid population only. If this parameter is `True`, the last homologous chromosome will be treated as sex chromosome. (XY for male and XX for female.) If X and Y have different numbers of loci, the 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.

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.activateVirtualSubPop(id, vid=InvalidSubPopID) Activate a virtual subpopulation.

id subpopulation id

vid virtual subpopulation id

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 already exist, they will be re-initialized.

init initial value for the new fields.

x.ancestralDepth() Ancestral depth of the current population

Note: The return 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 in subPop

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.deactivateVirtualSubPop(subPop) Deactivate virtual subpopulations in a given subpopulation. In another word, all individuals will become visible.

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.hasActivatedVirtualSubPop() If a population has any activated virtual subpopulations

x.hasActivatedVirtualSubPop(subPop) If a subpopulation has any activated virtual subpopulation

x.hasVirtualSubPop(subpop) If a subpopulation has any virtual subpopulation

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 individual `ind` 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 after given positions

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

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 after a given position

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

x.insertBeforeLoci(idx, pos, names=[]) Insert loci before given positions

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 before a given position

`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`.

x.mergePopulationByLoci(pop, newNumLoci=[], newLociPos=[], byChromosome=False)
Merge populations by loci

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 `byChromosome=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.

byChromosome 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.numVirtualSubPop(subPop) Number of virtual subpopulation of a given subpopulation.

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.
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 achieve order 3,2,0,1, the rank should be 1 0 2 3.

x.rep() Current replicate in a simulator which is not meaningful for a stand-alone population

x.resize(newSubPopSizes, propagate=False) Resize current 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
idx
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, order=True) Set individual information for the given information field
name
 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, representing 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=[]) Move individuals to subpopulations according to individual subpopulation IDs
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.

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

x.setVirtualSplitter(vsp, sp) Set a virtual splitter to a given subpopulation.

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 subpopulation ID and relative index of an individual with absolute index ind

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.

x.virtualSubPopName(id, vid=InvalidSubPopID) Name of the given virtual subpopulation.

id subpopulation id

vid virtual subpopulation id

x.virtualSubPopSize(id, vid=InvalidSubPopID) return the size of virtual subpopulation subPop. if subPop is activated, and subPop does not specify which virtual subpopulation to count, the currently activated virtual subpop is returned. Therefore, When it is not certain if a subpopulation has activated virtual subpopulation, this function can be used.

id subpopulation id

vid virtual subpopulation id. If not given, current subpopulation, or current activated subpopulation size will be returned.

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])
>>>
>>> # 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()
5
>>> print pop.numSubPop()
2
>>> print pop.subPopSize(0)
2
>>> print pop.subPopSizes()
(2, 3)
>>> print pop.subPopBegin(1)
2
>>> print pop.subPopEnd(1)
5
>>> 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:   3
Loci positions:
                2 3 4
                0 2

Loci names:
                loc1-3 loc1-4 loc1-5
                loc2-1 loc2-2
population size:       5
Number of subPop:      4
Subpop sizes:          0 2 2 1
Number of ancestral populations:      0
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 ancestral 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.)

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      0.167200      0.020000
1      0.165900      0.019150
2      0.156600      0.016750
3      0.151800      0.014350
4      0.144900      0.014600
5      0.137150      0.013850
>>> # restore to the current generation
>>> pop.useAncestralPop(0)
>>>
```

2.2.3 Virtual subpopulations

simuPOP 0.8.2 introduces the concept of *virtual subpopulations*. Virtual subpopulations are collections of individuals in a subpopulation, defined by certain criterias. For example, all male individuals, all unaffected individuals, all individuals with information field age > 20, all individuals with genotype 0, 0 at a given locus, can form virtual subpopulations. Virtual subpopulations do not have to add up to the whole subpopulation, nor do they have to be distinct. Because properties of individuals are variable, virtual subpopulations do not have fixed sizes as subpopulations do.

Virtual subpopulations allow easy handling of heterogeneous populations, and can facilitate some computations that are previously very difficult to do. For example, mating schemes can work on virtual subpopulations. This allows complicated mating schemes such as mating in aged population, and mixed mating schemes. By limiting operators to virtual subpopulations, one can apply different genetic forces to different groups of individuals. It is also easy to calculate statistics at a finer scale, such as allele frequency of all males.

Virtual subpopulations are defined by virtual splitters. A splitter splits a subpopulation into pre-determined number of virtual subpopulations. It also assign a name, such as age=5 to each virtual subpopulation. For example

- A `duplicateSplitter` does not split the subpopulation at all. It presents the whole subpopulation as several virtual subpopulations. By applying different mating schemes to such virtual subpopulations, one can apply several mating schemes to the same subpopulation.
- A `infoSplitter` splits the population according to values of a given information field. It can split the population by given values, or by some cut-off values.
- A `proportionSplitter` splits the population with given proportions, and
- A `rangeSplitters` choose individuals from given ranges.
- A `genotypeSplitter` splits the population with genotype values at given loci.

The population class provies several functions to assign a splitter to a given subpopulation, retrieve virtual subpopulation sizes and names. Example 2.4 demonstrates how to assign virtual splitter, and how to use them.

Example 2.4: Virtual subpopulation related functions

```
>>> import random
>>> pop = population(1000, loci=[2, 3], infoFields=['age'])
>>> InitByFreq(pop, [0.2, 0.8])
>>> for ind in pop.individuals():
...     ind.setInfo(random.randint(0,5), 'age')
...
>>> # split by age
>>> pop.setVirtualSplitter(infoSplitter('age', values=[2,4]), 0)
>>> pop.virtualSubPopSize(0, 0)
163
>>> pop.virtualSubPopName(0, 1)
'age = 4'
>>>
>>> # split by genotype
>>> a = pop.setVirtualSplitter(
...     genotypeSplitter(locus=2, alleles=[[0,1], [1,1]], phase=True),
...     0)
>>> pop.virtualSubPopSize(0, 0)
129
>>> pop.virtualSubPopSize(0, 1)
652
>>>
```

2.2.4 Class nullSplitter

Details

This subpops does nothing. It treats the whole subpopulation as the only virtual subpopulation.

Initialization

SimuPOP::nullSplitter::nullSplitter

```
    nullSplitter()
```

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::nullSplitter::clone

x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.5 Class duplicateSplitter

Details

DuplicateSplitter does not split the parental subpopulation in any way. It presents the specified subpopulation as several subpopulations to the mating system, thus allow several different mating schemes to be applied to the same subpopulation. For example, a selfing-mating scheme can be applied to the subpopulation and populate half of the offspring subpopulation, and a random-mating scheme can be used to generate the rest of the offspring subpopulation.

Initialization

SimuPOP::duplicateSplitter::duplicateSplitter

```
    duplicateSplitter(num)
```

Member Functions

x.clone() SimuPOP::duplicateSplitter::clone

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.6 Class sexSplitter

Details

Split the population according to sex

Initialization

SimuPOP::sexSplitter::sexSplitter

```
sexSplitter()
```

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::sexSplitter::clone

x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.7 Class affectionSplitter

Details

Split the population according to affection status

Initialization

SimuPOP::affectionSplitter::affectionSplitter

```
affectionSplitter()
```

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::affectionSplitter::clone

x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.8 Class infoSplitter

Details

Split the population according to the value of an information field. A list of distinct values, or a cutoff vector can be given to determine how the virtual subpopulations are divided. Note that in the first case, an individual does not have to belong to any virtual subpopulation.

Initialization

SimuPOP::infoSplitter::infoSplitter

```
infoSplitter(info, values=[],info, cutoff=[])
```

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::infoSplitter::clone

x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.9 Class proportionSplitter

Details

Split the population according to a proportion

Initialization

SimuPOP::proportionSplitter::proportionSplitter

```
proportionSplitter(proportions=[])
```

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::proportionSplitter::clone

x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.

x.name(sp) Name of a virtual subpopulation

x.numVirtualSubPop() Number of virtual subpops of subpopulation sp

x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.10 Class rangeSplitter

Details

Split the population according to individual range

Initialization

SimuPOP::rangeSplitter::rangeSplitter

```
rangeSplitter(ranges)
```

range A shortcut for ranges=[range]

ranges A list of ranges

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.

x.clone() SimuPOP::rangeSplitter::clone
x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.
x.name(sp) Name of a virtual subpopulation
x.numVirtualSubPop() Number of virtual subpops of subpopulation sp
x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.11 Class genotypeSplitter

Details

Split the population according to given genotype

Initialization

SimuPOP::genotypeSplitter::genotypeSplitter

```
genotypeSplitter(loci, alleles, phase=False)
```

genotype A shortcut for genotypes=[genotype]

genotypes A list of genotypes

Member Functions

x.activate(pop, subPop) Mark individuals in the given vsp as visible, and others invisible.
x.clone() SimuPOP::genotypeSplitter::clone
x.deactivate(pop, sp) Deactivate. Namely make all individuals visible again.
x.name(sp) Name of a virtual subpopulation
x.numVirtualSubPop() Number of virtual subpops of subpopulation sp
x.size(pop, subPop) The size of a given virtual subpopulation.

2.2.12 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 2.5: Save population variables

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

2.2.13 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 2.6: 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 2.7 iterates through all individuals in subpopulation 2 using `population::individual()` function, while 2.8 uses `population::individuals()`. The latter is usually easier to use.

Example 2.7: Function `population::individual()`

```
for i in range(pop.subPopSize(2)):
    ind = pop.individual(i, 2)
    print ind.affected()
```

Example 2.8: Function `population::individuals()`

```
for ind in pop.individuals(2):
    # do something to ind
    print ind.affected()
```

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). Individuals are created by populations automatically. Do not call the constructor function directly.

Initialization

`SimuPOP::individual::individual`

```
individual()
```

Member Functions

`x.affected()` Whether or not an individual is affected

`x.affectedChar()` Return A (affected) or U (unaffected) 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 beginning 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 in 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 ploidy

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 carry 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) Return a carry with the genotypes of the p -th copy of the chromosomes

x.arrGenotype(p, ch) Return a carry with the genotypes of the ch -th chromosome in the p -th chromosome set

x.arrInfo() Return a carry of all information fields (of size `infoSize()`) 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 beginning 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 beginning of the ploidy p , ranging from 0 to `totNumLoci(p)`

p index of the ploidy

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 beginning 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 or Female.

x.setSubPopID(id) Set new subpopulation ID, `pop.rearrangeByIndID` will move this individual to that population

x.setVisible(visible) `SimuPOP::individual::setVisible`

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 belongs

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.visible() `SimuPOP::individual::visible`

Example

Example 2.9: 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()
2
>>> print ind.numChrom()
3
>>> # ...
>>> # as well as genotype
>>> print ind.allele(1)
0
>>> ind.setAllele(1,5)
>>> print ind.allele(1)
0
>>> # 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
0
>>> # other information
>>> print ind.affected()
False
>>> print ind.affectedChar()
U
>>> ind.setAffected(1)
>>> print ind.affectedChar()
A
>>> 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(newSubPopSize=[ ], newSubPopSizeExpr="", newSubPopSizeFunc=None,  
subPop=InvalidSubPopID, virtualSubPop=InvalidSubPopID, weight=0)
```

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.

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

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

newSubPopSizeFunc A function that takes parameters `gen` (generation number) and `oldsize` (an array of current population size) and return an array of subpopulation sizes of the next generation. This is usually easier to use than its expression version of this parameter.

subPop If this parameter is given, the mating scheme will be applied only to the given (virtual) subpopulation. This is only used in `heteroMating` where mating schemes are passed to.

weight When `subPop` is virtual, this is used to determine the number of offspring for this mating scheme. Weight can be

- 0 (default) the weight will be proportional to the current (virtual) subpopulation size. If other virtual subpopulation has non-zero weight, this virtual subpopulation will produce no offspring (weight 0).
- any positive number: the size will be determined by weights from other virtual subpopulations.

Member Functions

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

`x.mateSubPop(pop, subPop, offBegin, offEnd, ops)` `SimuPOP::mating::mateSubPop`

`x.subPop()` `SimuPOP::mating::subPop`

x.weight() SimuPOP::mating::weight

Example

Example 2.10: 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=[])
True
>>> 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., subpopulation size parameters will be ignored although some during-mating operators might be applied.

Initialization

Create a scheme with no mating

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

Note

All parameters are ignored!

Member Functions

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

2.4.3 Class binomialSelection

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 population is allowed.

Initialization

Create a binomial selection mating scheme

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

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. If 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,
             subPop=InvalidSubPopID, virtualSubPop=InvalidSubPopID, weight=0)
```

Please refer to class `mating` for descriptions of other parameters.

contWhenUniSex Continue when there is only one sex in the population. Default to True.

Member Functions

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

2.4.5 Class `selfMating`

A mating scheme of selfing

Details

In this mating scheme, a parent is chosen randomly, acts both as father and mother as in random mating.

Initialization

Create a self mating scheme

```
selfMating(numOffspring=1., numOffspringFunc=None, maxNumOffspring=0,
           mode=MATE_NumOffspring, newSubPopSize=[], newSubPopSizeFunc=None,
           newSubPopSizeExpr="", contWhenUniSex=True, subPop=InvalidSubPopID,
           virtualSubPop=InvalidSubPopID, weight=0)
```

Please refer to class `mating` for descriptions of other parameters.

contWhenUniSex Continue when there is only one sex in the population. Default to True.

Member Functions

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

2.4.6 Class pyMating

A Python mating scheme

Details

Hybrid mating scheme. This mating scheme takes a Python generator that generate parents that will be mated by the mating scheme. The mating scheme will generate offspring population (controlled by newSubPopSize etc), call this function repeatedly to get parents, perform the mating, produce a number of offspring (controlled by numOffspring etc), and apply given during mating operators. The parentsGenerator is not a usually Python function, rather a Python generator (use of yield keyword). Please refer to simuPOP user's guide for an example of how to use this mating scheme.

Initialization

Create a Python mating scheme

```
pyMating(chooser, generator, newSubPopSize=[], newSubPopSizeExpr="",
newSubPopSizeFunc=None, subPop=InvalidSubPopID, virtualSubPop=InvalidSubPopID,
weight=0)
```

Member Functions

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

2.4.7 Class heteroMating

SimuPOP::heteroMating

Initialization

Create a Python mating scheme

```
heteroMating(matingSchemes, newSubPopSize=[], newSubPopSizeExpr="",
newSubPopSizeFunc=None, subPop=InvalidSubPopID, virtualSubPop=InvalidSubPopID,
weight=0)
```

Member Functions

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

2.4.8 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

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

- **MATE_PoissonDistribution:** numOffspring or result of numOffspringFunc (evaluated at each generation) will be considered as p for a Poisson distribution. The number of offspring for each mating is determined by

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

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 $N = \text{maxNumOffspring}$, the number of offspring for each mating is determined by

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

- **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

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

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

2.4.9 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 [newsizes] instead of newsize when you do not have any subpopulation structure). The example of class Mating demonstrates the use of this parameter.

2.4.10 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 `initSize` to `endSize` after burnin, split the population at generation `split`. If `bottleneckGen` is specified, population size will be `bottleneckSize` at that generation.

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

Exponentially expand the population size from `initSize` 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)
```

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

2.4.11 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.

2.4.12 parent choosers

To implement more complex mating schemes, some concepts need to be understood. The first one is *parent chooser*. Parent chooser determines how parent or parents are chosen from a given subpopulation. There are several predefined parent choosers such as `randomParentChooser`, `randomParentsChooser`, and the most powerful one is called `pyParentsChooser`.

A `pyParentsChooser` accepts a Python generator function, instead of a normal python function. When this generator function is called, it returns a *generator* object that provides an iterator interface. Each time when the `next()` member function of this object is called, this function resumes where it was stopped last time, executes and returns what the next *yield* statement returns. An example of generator is given in `simuPOP` user's guide.

Example 2.11: A generator function that mimicks random mating

```
>>> from random import randint
>>>
>>> def randomChooser(pop, sp):
...     males = [x for x in range(pop.subPopSize(sp)) \
...               if pop.individual(x, sp).sex() == Male \
...               and pop.individual(x, sp).info('age') > 30]
...     females = [x for x in range(pop.subPopSize(sp)) \
...                 if pop.individual(x, sp).sex() == Female \
...                 and pop.individual(x, sp).info('age') > 30]
...     nm = len(males)
...     nf = len(females)
...     while True:
...         yield males[randint(0, nm-1)], females[randint(0, nf-1)]
...
>>> pop = population(subPop=[1000, 200], loci=[1], infoFields=['age'])
>>> # this will initialize sex randomly
>>> InitByFreq(pop, [0.2, 0.8])
>>> for ind in pop.individuals():
...     ind.setInfo(randint(0, 60), 'age')
...
>>> rc1 = randomChooser(pop, 0)
>>> for i in range(5):
...     print rc1.next(),
...
(262, 500) (592, 337) (581, 326) (205, 350) (796, 24)
>>> rc2 = randomChooser(pop, 1)
>>> for i in range(5):
...     print rc2.next(),
...
(113, 33) (171, 65) (48, 8) (53, 49) (188, 82)
>>>
```

A user defined parents chooser can be very complicated, involving user defined information such as geometric locations. An example is given in `scripts/demoNonRandomMating.py`. In example 2.11, the parents chooser `randomChooser` collects indexes of males and females that are over the age of 30 and return a pair of random male and female repeatedly. That is to say, individuals with age < 30 is not involved in mating. Of course, to completely implement age-dependent mating, other factors need to be considered. For example, a `pyTagger` is likely to be used to assign age to offspring.

It becomes obvious now that whereas a python function can return random male/female pair, the generator interface is much more efficient because the identification of two sex groups is done only once.

2.4.13 Class `randomParentChooser`

Choose a parent randomly

Initialization

`SimuPOP::randomParentChooser::randomParentChooser`

```
randomParentChooser()
```

Member Functions

```
x.chooseParent() SimuPOP::randomParentChooser::chooseParent  
x.clone() SimuPOP::randomParentChooser::clone  
x.initialize(pop, sp) SimuPOP::randomParentChooser::initialize
```

2.4.14 Class randomParentsChooser

Choose two parents randomly, considering selection

Initialization

SimuPOP::randomParentsChooser::randomParentsChooser

```
randomParentsChooser()
```

Member Functions

```
x.chooseParents() SimuPOP::randomParentsChooser::chooseParents  
x.clone() SimuPOP::randomParentsChooser::clone  
x.initialize(pop, sp) SimuPOP::randomParentsChooser::initialize  
x.numFemale() SimuPOP::randomParentsChooser::numFemale  
x.numMale() SimuPOP::randomParentsChooser::numMale
```

2.4.15 Class pyParentsChooser

Choose two parents using a Python generator does not consider selection

Initialization

SimuPOP::pyParentsChooser::pyParentsChooser

```
pyParentsChooser(parentsGenerator)
```

Member Functions

```
x.chooseParents() SimuPOP::pyParentsChooser::chooseParents  
x.clone() SimuPOP::pyParentsChooser::clone  
x.initialize(pop, sp) SimuPOP::pyParentsChooser::initialize
```

A parents chooser can yield a pair of parents, or a single parent. Obviously, a single diploid parent can not produce offspring using the usual Medelian fashion, so here comes another concept: *offspring generator*.

2.4.16 Offspring generator

An offspring generator determines how to produce offspring from given parent or parents. Currently, there are three standard offspring generators.

These offspring generator defines only the default way to fill offspring genotype. When a during-mating operator is involved, it may override what an offspring generator does. For example, a `recombinator` recombines parental chromosomes to fill offspring genotype. In the diploid case, it will behave the same for `cloneOffspringGenerator` and `selfingOffspringGenerator`.

2.4.17 Class cloneOffspringGenerator

SimuPOP::cloneOffspringGenerator

Initialization

SimuPOP::cloneOffspringGenerator::cloneOffspringGenerator

```
cloneOffspringGenerator(numOffspring=1, numOffspringFunc=None,  
maxNumOffspring=1, mode=MATE_NumOffspring)
```

Member Functions

x.clone() SimuPOP::cloneOffspringGenerator::clone

x.generateOffspring(pop, dad, mom, offBegin, offEnd, ops) Generate numOff offspring

2.4.18 Class selfingOffspringGenerator

SimuPOP::selfingOffspringGenerator

Initialization

SimuPOP::selfingOffspringGenerator::selfingOffspringGenerator

```
selfingOffspringGenerator(numOffspring=1, numOffspringFunc=None,  
maxNumOffspring=1, mode=MATE_NumOffspring)
```

Member Functions

x.clone() SimuPOP::selfingOffspringGenerator::clone

x.generateOffspring(pop, parent, , offBegin, offEnd, ops) Generate numOff offspring

2.4.19 Class mendelianOffspringGenerator

SimuPOP::mendelianOffspringGenerator

Initialization

SimuPOP::mendelianOffspringGenerator::mendelianOffspringGenerator

```
mendelianOffspringGenerator(numOffspring=1, numOffspringFunc=None,  
maxNumOffspring=1, mode=MATE_NumOffspring)
```

Member Functions

x.clone() SimuPOP::mendelianOffspringGenerator::clone

x.formOffspringGenotype(parent, it, ploidy, setSex) SimuPOP::mendelianOffspringGenerator::formOffspring

x.generateOffspring(pop, dad, mom, offBegin, offEnd, ops) Generate numOff offspring

x.initialize(pop, ops) Create an offspring generator, save information from pop and ops to speed up the calls to generateOffspring

2.4.20 Hybrid non-random mating scheme `pyMating`

Parent choosers and offspring generators can be combined to form non-standard mating schemes. The only limit is that they have to be compatible in that a parent chooser that choose one parent can not be used with an offspring generator that needs two parents. The basic usage of a `pyMating` operator is as follows

```
pyMating(randomParentChooser(),
         selfingOffspringGenerator(numOffspring=2))
```

or

```
pyMating(randomParentsChooser(),
         cloneOffspringGenerator())
```

2.4.21 Heterogeneous non-random mating scheme `heteroMating`

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 execution. Less efficient. For example, a hybrid mutator `pyMutator` will go through a population and mutate alleles with given mutation rate. How exactly the allele will be mutated is determined by a user-provided Python function. More specifically, this operator will pass the current allele to a user-provided Python function and take its return value as the mutant allele.
- pure Python: written in Python. The same speed as Python. For example, a `varPlotter` can plot Python variables that are set by other operators. Usually, an individual or a population object is passed to a user-provided Python function. Because arbitrary operations can be performed on the passed object, this operator is very flexible.

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 and/or ending generations (parameters `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 be counted 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);
- `"` suppress 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,
             grp, 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 parameters `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 2.12: 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,
...                  grp=[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
>>> # 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)
...     ]
... )
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 simulator 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 you 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 operators
- 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`.

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 population `rep`

By default return a cloned copy of population `rep` 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 referred 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 population `rep`, 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 2.13: 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")
>>>
```

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):

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

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.alleleFreq[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 2.14: 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]      0.19483333333333
    [1]      0.80516666666667
>>> # print number of allele 1 at locus 0
>>> print pop.vars()[ 'alleleNum' ][0][1]
4831
>>> print pop.dvars().alleleNum[0][1]
4831
>>> print pop.dvars().alleleFreq[0]
[0.19483333333333333, 0.8051666666666667]
>>> print pop.dvars(1).alleleNum[0][1]
3207
>>>
```

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::evaluate()` or `population::execute()`. For example:

Example 2.15: 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]')
6000
>>> pop.execute('newPopSize=int(popSize*1.5)')
>>> ListVars(pop.vars(), level=1, useWxPython=False)
```

```

newPopSize :    4500
grp :    -1
rep :    -1
popSize :        3000
numSubPop :      2
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 <module>
    #
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")
0
>>> print simu.population(1).evaluate("grp*2")
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 2.16: 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 41, myNum 82
gen 0, rep 1, num 39, myNum 78
gen 1, rep 0, num 45, myNum 90
gen 1, rep 1, num 33, myNum 66
gen 2, rep 0, num 51, myNum 102
gen 2, rep 1, num 39, myNum 78
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 array 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.setIndInfo(values, name, order)` set information fields of all individuals with values in an array.
- `pop.arrIndInfo(order)` return an array of all information fields
- `pop.arrIndInfo(subPop, order)` return an array of all information fields of subpopulation `subPop`.

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 array `f1, f2, f3` (assuming `infoSize()==3`) of individual `ind`. At a population level, `pop.arrIndInfo([subPop], order)` returns a array 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 2.18 is more efficient.

Example 2.17: 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)
(1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
>>>
```

Example 2.18: Use array information fields function

```
>>> pop = population(10, infoFields=['a', 'b'])
>>> aIdx = pop.infoIdx('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)
(1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0, 1.0)
>>>
```


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:
...             KamMutate(pop, maxAllele=2, rate=mu1, loci=[i])
...         else:
...             KamMutate(pop, maxAllele=2, rate=mu2, loci=[i])
...     return True
>>>

```

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
... )
0.400550      0.203100
0.407350      0.203450
0.408800      0.219250
0.410600      0.213150
True
>>>

```

pyOperator can also be a during-mating operator. You will need to define a function

```
def Func(pop, off, dad, mom, para)
```

or

```
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)
```

or

```
pyOperator(stage=DuringMating, func=shortFunc, param=someparam,
formOffGenotype=False, passOffspringOnly=True)
```

If your during-mating pyOperator 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.

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` or `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(
...     ops = [
...         pyIndOperator(func=indFunc, param=(3,2)),
...     ],
```

```

... )
2.0
2.0
2.0
2.0
2.0
2.0
True
>>>

```

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 initialize 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

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 frequencies must be 1; or for a matrix of allele frequencies, each row corresponds to a subpopulation or range.

identicalInds Whether or not make individual genotypes identical in all subpopulations. 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 population `pop`

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

Example

Example 3.4: Operator `initByFreq`

```
>>> simu = simulator(
...     population(subPop=[2,3], loci=[5,7], maxAllele=1),
...     randomMating(), rep=1)
>>> simu.step([
...     initByFreq(alleleFreq=[ [.2,.8],[.8,.2]]),
...     dumper(alleleOnly=True)
... ])
individual info:
sub population 0:
  0: FU 11111 1111111 | 11111 1111111
  1: FU 11111 0111111 | 11111 1111111
sub population 1:
  2: FU 00000 0000000 | 00000 0000000
  3: FU 10100 0000000 | 00000 0001000
  4: FU 00000 0000000 | 00000 0001000
End of individual info.

No ancestral 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 assigns 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 `value`. Each item of `value` will be assigned to each `subPop` or `indRange`.

Initialization

Initialize a population 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 `value`. 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 chromosomes). This parameter can also be an array of arrays of genotypes of one individual. If `value` is an array of values, it should have the length one, number of subpopulations, or the length of ranges of proportions.

Member Functions

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

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

Example

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 44444444 | 11111 44444444
sub population 1:
2: FU 33333 44444444 | 33333 2222222
3: FU 11111 44444444 | 11111 2222222
4: FU 11111 2222222 | 33333 2222222
End of individual info.

```

```

No ancestral population recorded.
True
>>>

```

3.2.4 Class spread (Function form: Spread)

Copy the genotype of an individual to all individuals

Details

Function `Spread(ind, subPop)` spreads the genotypes 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 population `pop`

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:        2
Maximum allele state:  255
Loci positions:
          1 2
Loci names:
          loc1-1 loc1-2
population size:       8
Number of subPop:      2
Subpop sizes:         4 4
Number of ancestral populations: 0

```

```

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

```

```

No ancestral population recorded.
>>>

```

3.2.5 Class `pyInit` (Function form: `PyInit`)

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

Details

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

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.

loci A vector of locus 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:
  0: MU   0  1  2  3  4   6  7  8  9 10 11 12 |   1  2  3  4  5   5  6  7  8  9 10 11
  1: MU   0  1  2  3  4   5  6  7  8  9 10 11 |   0  1  2  3  4   5  6  7  8  9 10 11
sub population 1:
  2: MU   1  2  3  4  5   6  7  8  9 10 11 12 |   1  2  3  4  5   7  8  9 10 11 12 13
  3: FU   1  2  3  4  5   6  7  8  9 10 11 12 |   1  2  3  4  5   7  8  9 10 11 12 13
  4: MU   2  3  4  5  6   6  7  8  9 10 11 12 |   2  3  4  5  6   7  8  9 10 11 12 13
End of individual info.

No ancestral 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 $r \times \text{size_of_subPop_a}$ 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 subpopulation with 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 subpopulation 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 subpopulation 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 sizes 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.

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

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

- `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 various 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 genotypes and parameters, 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

```
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)
>>>
```

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 Subpopulations 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 parameters, if needed, should be implemented by individual mutator classes.

There are numbers 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, do not call this constructor directly

```
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 models. The only differences between the following mutators are the 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 locus indexes. Will be ignored only when single rate is specified. Default to all loci.

maxAllele Maximum allowed allele. Interpreted by each sub mutator 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=[])
```

Please see class mutator for the descriptions of other parameters.

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 $rate/(K-1)$.

Member Functions

x.clone() Deep copy of a kamMutator

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

Example

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  0  0  0  0
  1: MU   2  0  5   0  0  0  2  0 |   0  0  0   0  0  0  1  0
  2: MU   0  0  3   0  0  0  4  0 |   0  0  2   0  0  0  0  0
  3: MU   0  0  8   0  0  0  0  0 |   6  0  7   0  0  0  0  0
  4: MU   0  0  0   0  0  0  0  0 |   0  0  5   0  0  0  0  0
End of individual info.
```

```

No ancestral 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 (VNTR) loci, 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 SMM is developed for allozymes. It provides better description for these kinds of evolutionary processes. Please see class `mutator` for the descriptions 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  2  0  0  1 |  1  2  0   0  0  0  1  1
  1: MU   1  2  1   0  0  0  2  1 |  0  2  2   2  2  2  2  1
  2: MU   2  2  1   2  1  0  2  2 |  2  1  1   0  0  1  2  2
End of individual info.

```

```

No ancestral population recorded.
individual info:
sub population 0:
  0: FU   1  2  1   3  3  1  1  2 |  2  1  1   0  1  0  2  2
  1: MU   0  3  2   0  1  1  3  2 |  1  1  3   3  1  3  1  2

```

```

    2: MU    3  3  2    3  2  1  1  3 |    3  2  2    1  1  2  1  3
End of individual info.

```

```

No ancestral 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 the 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 GSM model is developed for allozymes. It provides better description for these kinds of evolutionary processes. Please see class `mutator` for the descriptions 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

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

`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
  1: FU   2  2  0   1  2  2  2  0 |   2  2  1   2  0  0  2  0
  2: MU   1  2  2   2  2  0  2  2 |   1  2  2   0  0  2  1  0
End of individual info.

```

```

No ancestral population recorded.
individual info:
sub population 0:
  0: FU   4  2  2   3  1  3  0  3 |   3  0  3   2  1  1  3  0
  1: FU   3  3  1   2  3  3  3  1 |   4  3  0   3  1  1  4  2
  2: MU   2  3  3   3  1  1  3  3 |   0  3  4   1  1  3  0  1
End of individual info.

```

```

No ancestral 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   2  2  0  1  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 |   1  0  2   1  2  1  0  2
End of individual info.

```

```

No ancestral 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 ancestral 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   0  8  0  0  0
  1: MU   0  0  0   8  0  8  0  0 |   0  0  0   0  8  8  0  0
  2: MU   0  0  0   8  0  8  0  0 |   0  0  0   8  0  0  0  0
End of individual info.

No ancestral population recorded.
True
>>>
```

3.4.6 Class `pointMutator` (Function form: `PointMutate`)

Point mutator

Details

Mutate specified individuals at 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 class `mutator` for the descriptions of other parameters.

inds Individuals who will mutate

toAllele 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 of 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.
- it works for selfing. I.e., when only one parent is provided, it will be recombined twice, producing both maternal and paternal chromosomes of the offspring.

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 actual recombination rate between two loci is determined by $\text{intensity} \times \text{locus distance (between them)}$.

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

```
>>> simu = simulator(
...     population(4, loci=[4,5,6], maxAllele=9,
...     infoFields=['father_idx', 'mother_idx']),
...     randomMating())
>>> simu.step([
...     parentsTagger(),
...     ],
...     preOps = [initByFreq([.2,.2,.4,.2]), dumper(alleleOnly=True) ],
...     postOps = [ dumper(alleleOnly=True)]
... )
individual info:
sub population 0:
  0: MU 2200 03300 020102 | 1223 21120 022312
  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 ancestral population recorded.

```
individual info:
sub population 0:
  0: FU 0002 22133 011010 | 3122 20223 213032
  1: FU 2200 03300 020102 | 1231 20223 213032
  2: MU 1223 21120 020102 | 1231 20122 213032
```

```

    3: FU 1223 03300 020102 | 1231 20122 301231
End of individual info.

```

```

No ancestral population recorded.
True
>>> simu.step([
...     parentsTagger(),
...     recombinator(rate=[1,1,1], afterLocs=[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 ancestral 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 $f_i, i = 1, \dots, N$, 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 various selection intensities for different subpopulations). Then, a '*selector-aware*' mating scheme can select individuals according to their `fitness` information fields. This implies that

- only mating schemes can actually select individuals.
- a selector has to be a `PreMating` operator. This is not a problem when you use the operator form of the selector since its default stage is `PreMating`. However, if you use the function form of the selector 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.

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 the 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)
... ],
...     preOps=[ initByFreq(alleleFreq=[.2,.8])],
...     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

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

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 separates alleles into two groups: wildtype and diseased 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 genotypes AA, Aa, aa, while A stands for wildtype alleles.
- For a two-locus model, `fitness` is the fitness for genotypes AABB, AABb, AAbb, AaBB, AaBb, 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 `baseOperator` 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.

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.
- `wildtype` alleles 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-locus 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 one of the following values

- **SEL_Multiplicative**: the fitness is calculated as $f = \prod_i f_i$, where f_i is the single-locus fitness value.
- **SEL_Additive**: the fitness is calculated as $f = \max(0, 1 - \sum_i (1 - f_i))$. f will be set to 0 when $f < 0$.

Initialization

Create a multiple-locus 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

This selector assigns fitness values by calling a user provided function. It accepts a list of loci and a Python function `func`. For each individual, this operator will pass the genotypes at these loci, generation number, and optionally values at some information fields to this function. The return value is treated 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. More specifically, `func` can be

- `func(geno, gen)` if `infoFields` has length 0 or 1.
- `func(geno, gen, fields)` when `infoFields` has more than 1 fields. Values of fields 1, 2, ... will be passed. Both `geno` and `fields` should be a list.

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"])
```

func A Python function that accepts genotypes at specified loci, generation number, and optionally information fields. It returns the fitness value.

infoFields If specified, the first field should be the information field to save calculated fitness value (should be 'fitness' in most cases). The values of the rest of the information fields (if available) will also be passed to the user defined penetrance function.

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). 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 calculates the penetrance value of each offspring and assigns 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.

Penetrance values 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 the `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=[])
```

ancestralGen If this parameter is set to be `0`, apply penetrance to the current generation; if `-1`, apply to all generations; otherwise, apply to the specified numbers 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

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 locus 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__)`

penet 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 diseased alleles. Wildtype alleles are specified by parameter `wildtype` and any other alleles are considered as diseased alleles. `maPenetrance` accepts an array of penetrance for AA, Aa, aa in the single-locus case, and a longer table for the multi-locus 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 locus indexes. The genotypes of these loci will be examined.

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__)`

penet An array of penetrance values of AA, Aa, aa. A is the wild type group. In the case of multiple loci, penetrance should be in the order of AABB, 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 diseased 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

This is the 'multiple-locus' penetrance 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 locus penetrance operator

```
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

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

Example

Example 3.20: Operator mlPenetrance

```
>>> pop = population(1000, loci=[3])
>>> InitByFreq(pop, [0.3, 0.7])
>>> pen = []
>>> for loc in (0, 1, 2):
...     pen.append( maPenetrance(locus=loc, wildtype=[1],
...                             penetrance=[0, 0.3, 0.6] ) )
...
>>> # the multi-loci penetrance
```

```
>>> MlPenetrance(pop, mode=PEN_Multiplicative, peneOps=pen)
>>> Stat(pop, numOfAffected=True)
>>> print pop.dvars().numOfAffected
8
>>>
```

3.7.5 Class pyPenetrance (Function form: PyPenetrance)

Assign penetrance values by calling a user provided function

Details

For each individual, the penetrance is determined by a user-defined penetrance function `func`. This function takes genotypes at specified loci, and optionally values of specified information fields. The return value is considered as the penetrance for this individual. More specifically, `func` can be

- `func(geno)` if `infoFields` has length 0 or 1.
- `func(geno, fields)` when `infoFields` has more than 1 fields. Both parameters should be an list.

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 specified loci and return a penetrance value. The return value should be between 0 and 1.

infoFields If specified, the first field should be the information field to save calculated penetrance value. The values of the rest of the information fields (if available) will also be passed to the user defined penetrance function.

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 l in range(len(geno)/2):
...         p *= (geno[l*2]+geno[l*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 or functions were implemented to calculate quantitative traits for each individual and store the values in the information fields specified by the 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

```

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

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 return value is the sum of the trait plus $N(0, \sigma^2)$. 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 genotypes 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 $N(\text{mean}, \sigma^2)$. For multiple loci, the form is 'a-b|c-d|e-f' etc.

sigma Standard deviation of the environmental factor $N(0, \sigma^2)$.

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 diseased alleles. Wildtype alleles are specified by parameter `wildtype` and any other alleles are considered as diseased alleles. `maQuanTrait` accepts an array of fitness. Quantitative trait is then set for any given genotype. A standard normal distribution $N(0, \sigma^2)$ 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 wildtype 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 diseased 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-locus' 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 $f = \prod f_i$.
- QT_Additive: the mean of the quantitative trait is calculated as $f = \sum f_i$.

Note that all σ_i (for f_i) and σ (for f) will 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 σ to zero.

Initialization

Create a multiple locus quantitative trait operator

```
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

```
pyQuanTrait(loci, func, 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.

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

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 the ways of selecting individuals from a population. In `simuPOP`, ascertainment operators create sample populations that can be accessed from the population's local 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 an information field `oldindex`. This 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 parameter descriptions.

format Format to save the samples

name Name of the sample in the local namespace. This variable is an array of populations of size `times`. Default to `sample`.

nameExpr Expression version of parameter name. If both name and nameExpr are empty, sample populations will not be saved in the population's local namespace. 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 individual. Individuals with negative subpopulation IDs will be 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 individual subpopulation IDs

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. This sampler accepts a Python array with elements that will be assigned to individuals as their subpopulation IDs. Individuals with positive subpopulation IDs will then be picked out and form a sample.

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=[])
```

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 is given, keep all ancestral populations (default). If 0 is given, 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. This operator keeps samples in an array `name` in the local namespace. You may access them through `dvars()` or `vars()` functions.

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

Initialization

Draw a random sample, regardless of the affectedness 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 individuals 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 affectedness status is usually set by penetrance functions or 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 and 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 subpopulation

controls 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 genotypes, 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 *real random* 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.

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"])
```

Please refer to class `sample` for other parameter descriptions.

chooseUnaffected Instead of affected sibpairs, choose unaffected families.

countOnly Set variables about the 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 the population structure. Otherwise, specified numbers 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 the number of affected sibpairs, do not actually draw the sample.

maxOffspring The maximum number of offspring a parent may have

minAffected The minimal number of affected individuals in each pedigree. Default to 0.

minPedSize The 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` calculates various basic statistics for the population and set variables in the local namespace. Other operators or 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 or 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 disequilibrium 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=[], genoFreq_param={}, 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=[])
```

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 are:

- $F (F_{IT})$ 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 chosen 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,

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

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

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

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

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`.

- `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].`

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.

alleleFreq An array of loci at which all allele frequencies will be calculated (`alleleFreq=[loc1, loc2, ...]` where `loc1` etc. are loci where allele frequencies will be calculated). This parameter will set the following variables (array objects); for example, `alleleNum[1][2]` will be the number of allele 2 at locus 1:

- `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 chosen 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 chosen from the following options: `ChiSq`, `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

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

where p_i is the allele frequency of allele i . 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 chosen from the following options: `subpop` and `midValues`.

genoFreq An array of loci at which all genotype frequencies will be calculated (`genoFreq=[loc1, loc2, ...]` where `loc1` etc. are loci where genotype frequencies will be calculated). All the genotypes in the population will be counted. You may use `hasPhase` to set if a/b and b/a are the same genotype. This parameter will set the following dictionary variables. Note that unlike list used for `alleleFreq` etc., the indexes a, b of `genoFreq[a][b]` are dictionary keys, so you will get a *KeyError* when you used a wrong key. Usually, `genoNum.setdefault(a, {})` is preferred.

- `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`.
- `genoFreq_param` a dictionary of parameters of `phase = 0 or 1`.

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 sequences on loci `haplo`.
- `haploFreq[haplo]`, `subPop[sp]['haploFreq'][haplo]`, the frequency of allele sequences 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 **1x**, $x \neq 1$. Numbers and frequencies (proportions) of heterozygotes are calculated for each allele. `HeteroNum[loc]` and `HeteroFreq[loc]` are the overall heterozygosity number and frequency. I.e., the number and frequency of genotype **xy**, $x \neq y$. From these numbers, we can easily derive the number and frequency of homozygosity.

- `HeteroNum[loc]`, `subPop[sp]['HeteroNum'][loc]`, the overall heterozygote number.
- `HeteroFreq[loc]`, `subPop[sp]['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 frequency. 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 or 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/subpopulation.
- `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 chosen 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 (array objects of the numbers of alleles for *all loci*). Unrequested loci will have 0 distinct alleles.

- `numOfAlleles`, `subPop[sp]['numOfAlleles']` the 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 chosen from the following options: `numOfAffected`, `propOfAffected`, `numOfUnaffected`, `propOfUnaffected`.

numOfMale Whether or not count the numbers or 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 chosen 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.
- `popSize, subPop[sp]['popSize']` the 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.

relLoc 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 value.

rel_param A dictionary of parameters of relatedness statistics. Can be one or more items chosen from the following options: `Fst`, `Fis`, `Fit`, `AvgFst`, `AvgFis`, and `AvgFit`.

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 a 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 Chromosome(s) to display

dispWidth Number of characters to display an allele. Default to 1.

indRange Range(s) of individuals to display

infoOnly Only display genotypic information

loci Loci to display

max The maximum number of individuals to display. Default to 100. This is to avoid careless dump of huge populations.

output Output file. Default to the standard output.

outputExpr And other parameters: refer to `help(baseOperator.__init__)`

subPop Only display subpopulation(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

Save population

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

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

3.11.3 Class `pyOutput`

Output a given string.

Details

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

Initialization

Create a `pyOutput` operator that outputs a given string.

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

str String to be outputted

Member Functions

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 be 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

```
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 the current population as a variable named `pop`

expr The expression to be evaluated. The 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

stmts The statement that will be executed before the expression

Member Functions

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 executes them. No value will be returned or outputted.

Initialization

Evaluate statments in the local replicate namespace, no return value

```
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=[])
```

Please refer to class pyEval for parameter descriptions.

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

This is a during-mating operator that tags individuals with various information. Potential usages are:

- recording the parental information to track pedigree;
- tagging an individual/allele and monitoring 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=[])
```

Member Functions

x.clone() Deep copy of a
tagger

3.12.2 Class inheritTagger

Inherit tag from parents

Details

This during-mating operator will copy the tag (information field) 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 examining, at the last generation, how many offspring they have.

Initialization

Create an inheritTagger that inherits a tag from one or both parents

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

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 parentsTagger

Tagging according to parents' indexes

Details

This during-mating operator set 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, tagging information will be passed with individuals, and mating or population change etc. will not interfere with this simple tagging system.

Initialization

Create a parentsTagger

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

Member Functions

x.clone() Deep copy of a parentsTagger

3.12.4 Class pyTagger

Python tagger.

Details

This tagger takes some information fields from both parents, pass to a Python function and set the individual field with the return value. This operator can be used to trace the inheritance of trait values.

Initialization

Creates a pyTagger that works on specified information fields

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

func A Python 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 return value is assigned to fields 'A' and 'B' of the offspring. The return value has to be a list even if only one field is given.

infoFields Information fields. The user should guarantee 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

Terminators 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 value of 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 continueIf terminator

3.14 Conditional operator

3.14.1 Class ifElse

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`, `end`, `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 mechanism is to monitor the population statistics and act accordingly.

Initialization

Create a conditional operator

```
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 boolean 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 `ifElse`

```
>>> simu = simulator(
...     population(size=1000, loci=[1]),
...     randomMating(), rep=4)
>>> simu.evolve(
...     preOps = [ initByValue([1,1])],
...     ops = [
...         # penetrance, additive 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 0
No affected at gen 0
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.
- 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

Create a `turnOnDebug` operator

```
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

Create a `turnOffDebug` operator

```
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

Details

This operator does nothing.

Initialization

Create a `none` operator


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

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 pressing '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.

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 names 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.

TurnOnDebug(code=DBG_ALL)

Set debug codes. Default to turn on all debug codes. Only available in non-optimized modules.

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 configfile 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 from command 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 for user 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 determined from GUI, command line option or config file. This is useful for options that rarely need to be changed. Setting them to useDefault 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 of values 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 0x2a95589198>)

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 `SIMUOPTIMIZED`, and commandline option `-optimized` will be used if available. If nothing is defined, standard version will be used.

mpi currently unused

chromMap currently unused

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, suppress banner information when simuPOP is loaded.

debug a list of debug code (or string). If not set, environmental variable `SIMUDEBUG` will be used if available.

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)

Instantaneously 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

LargePeds_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.

LargePeds_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

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 $x \frac{m}{n-1} \frac{m}{n-1} \dots \frac{m}{n-1} x \dots \dots \frac{m}{n-1} \frac{m}{n-1} x$ where $x = 1-m$

MigrSteppingStoneRates (r, n, circular=False)

migration rate matrix, circular stepping stone model ($X=1-m$) $X \frac{m}{2} \frac{m}{2} \frac{m}{2} X \frac{m}{2} 0 0 \frac{m}{2} x \frac{m}{2}$
 $\dots 0 \dots \frac{m}{2} 0 \dots \frac{m}{2} X$ or non-circular $X \frac{m}{2} \frac{m}{2} \frac{m}{2} X \frac{m}{2} 0 0 \frac{m}{2} X \frac{m}{2} \dots 0 \dots \frac{m}{2} X$

```
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

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.

```
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

fields 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=1.0000000000000001e-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 affectedSibpairSample operator.

pop population to be saved. Must have ancestralDepth 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 information 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's local 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, adding this 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

```
Sibpair_LOD_gh (pop, sampleSize, penetrance=None, recRate=None, daf=None,  
gh='gh', keep_temp=False)
```

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 format but 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.

Sibpair_LOD_merlin (`pop`, `sampleSize`, `penetrance=None`, `merlin='merlin'`, `keep_temp=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.

Sibpair_TDT_gh (`pop`, `sampleSize`, `penetrance=None`, `recRate=None`, `daf=None`, `gh='gh'`, `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

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 format but 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

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, gen, migr=<simuPOP_std.noneOp; proxy  
  of <Swig Object of type 'simuPOP::noneOp *' at 0x2b9f4b0> >,  
  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 avoid rapid loss of genotype variation when population size is small.

endingSize ending population size

expand expanding method, can be linear or exponential

mergeAt when to merge population?

gen generations to evolve

recIntensity recombination intensity

mutRate mutation rate

step step at which to display statistics

keepParents whether or not keep parental 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 file should 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.

getMarkersFromRange (HapMap_dir, pops, chrom, startPos, endPos, maxNum, minAF, minDiffAF, minDist)

Get a population with markers from given range

HapMap_dir where HapMap data in simuPOP format is stored. The file should have been prepared by script-
s/loadHapMap.py.

pops HapMap populations to load

chrom chromosome number (1-based index)

startPos starting position (in cM)

endPos ending position (in cM). If 0, ignore this parameter.

maxNum maximum number of markers to get. If 0, ignore this parameter.

minAF minimal minor allele frequency

minDiffAF minimal allele frequency between HapMap populations.

minDist minimal distance between two adjacent markers, in cM

sample1DSL (pop, DSL, DA, pene, name, sampleSize)

Sample from the final population, using a single locus 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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