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# 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 a wide variety of tools (Splus/R, Python/SciPy, Matplotlib etc.) to perform tasks like statistical analysis, gene mapping and visualization. Depend on machine configuration, simuPOP can simulate large (think in millions) populations at reasonable speed.

This is a reference manual to all variables, functions, and operators. This should be read after you learned the structure of simuPOP and how to write a simuPOP script from 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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# Genotypic structure

Genotypic structure refers to

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

Here information fields refer to the numbers attached to each individual, such as fitness value, parent index, age etc. Individuals may need some information fields to use certain operators. For example, 'fitness' field is required by all selectors.

Example 1 creates a population and displays some of genotypic information.

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## Example 1 Genotype structure functions

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Individuals in the same population share the same genotypic structure. Consequently, *genotypic information can be retrieved from individual, population and simulator* (consists of populations with the same genotypic structure) *level*.

---

## Example 2 Calling genotype structure functions from individual or simulator

---

You may have noticed that locus Indices start from 0. **As a matter of fact, all arrays in simuPOP start at index 0.** To avoid confusion, I will refer the first locus as locus zero, second locus as locus one; first individual in a population as individual zero, and so on. The reason why zero-based indices are used is because C++ and Python, using which simuPOP is built, are both zero-based.

Another concern is how we should refer to loci on different chromosomes. The solution is that we almost always use *absolute index* and seldom use *relative index*. For example, if there are five and seven loci on the first two chromosomes, the absolute indices of loci will be (0,1,2,3,4), (5,6,7,8,9,10,11). It may feel confusing at first but this avoids the trouble of having to use two numbers (chrom, index) to refer to a locus. If relative index is needed, functions `chromLocusPair(absIndex)` and `absLocusIndex(chrom, index)` can be used.

## 1.1 Genotype structure functions

A full list of genotypic structure related functions, please use `help(population)` or `help(individual)` or directly `help(GenoStruTrait)`. (You may notice that both `population` and `individual` classes are inherited from `GenoStruTrait` class. )

### Genotypic structure related functions

function	description
<code>ploidy()</code>	number of copies of chromosomes
<code>ploidyName()</code>	haploid, diploid, triploid etc
<code>numLoci(chrom)</code>	number of loci on a chromosome
<code>sexChrom()</code>	whether or not the last chromosome is sex chromosome
<code>totNumLoci()</code>	total number of loci on all chromosomes
<code>genoSize()</code>	<code>totNumLoci()*ploidy()</code>
<code>locusPos(loc)</code>	the position of a locus
<code>arrLociPos()</code>	return an (editable) array of loci positions
<code>numChrom()</code>	number of chromosomes
<code>chromBegin(chrom)</code>	index of the first locus on a chromosome
<code>chromEnd(chrom)</code>	index of the last locus on a chromosome + 1
<code>absLocusIndex(chrom, loc)</code>	absolute index of a locus on a chromosome
<code>chromLocusPair(loc)</code>	(chrom, loc) pair of an absolute index
<code>alleleName(allele)</code>	name of an allele (if previously specified)
<code>alleleNames()</code>	array of names of alleles, the first one is for missing value
<code>locusName(loc)</code>	name of a locus
<code>maxAllele()</code>	maximum allele state for all loci
<code>setMaxAllele(max)</code>	set maximum allele state for all loci
<code>infoIdx(name)</code>	index of the field name.
<code>infoField(idx)</code>	name of the field <code>idx</code>
<code>infoFields()</code>	all information fields

## 1.2 Sex chromosome

If `sexChrom()` is false, all chromosomes are assumed to be autosomes. You can also create population/individuals with a sex chromosome. Please note that we currently only model the XY chromosomes in diploid population. Consequently,

- 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, recombination may still occur at this unused part of chromosome to simplify implementation and usage.
- It is assumed that male has XY and female has XX chromosomes. The sex chromosomes of male individuals will be arranged in the order of XY.

## 1.3 Information fields

An individual will by default have genotype, sex and affectedness information, but other information is needed for some operations. For example, the fitness value of an individual is needed for selection, one or more trait values may be needed to calculate quantitative traits; and age may be needed if age-dependent mating schemes are used. Since 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.

Operators may require certain information field 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 index of the parents of each individual in the parental generation. You do need to add these fields to the `infoFields` parameter of the population constructor. If you forget, an error message will appear and tells you to add certain field when a field is needed by some operators.

The information fields can be access from each individual (c.f. `info(idx)`, `info(name)`, `setInfo(value, idx)`, `setInfo(value, name)`, `arrInfo()` of individuals), or from the population as a whole (c.f. `setindInfo(value)`, `arrIndInfo(subPop)`). Some operators allows you to specify which information field(s) to use. Just to show what you can do with information fields, one can

- create a population with 5 trait values and some risk factors
- assign risk factors (environmental maybe) manually, or through some operators
- calculate each trait values using different quantitative trait operators, some gene may contribute to more than one trait values
- calualte a final trait values from these information fields.



# Population

population objects are essential to simuPOP. They are composed of subpopulations each with certain number of individuals, all have the same genotypic structure. A population can store arbitrary number of ancestral populations to facilitate pedigree analysis.

## 2.1 Population overview

simuPOP uses one-level population structure. That is to say, there is no sub-subpopulation or families in subpopulations. Mating is within subpopulations only. Exchange 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, total population size will not be changed.
- Mating can fill any population/subpopulation structure with offsprings. Both population and subpopulation sizes can be changed. Since mating is within subpopulation, you can not create new subpopulation through mating.
- A special operator `pySubset` can shrink population size. It removes individuals according to their `subPopID()` status. (Will explain later.) This can be used to model sudden population decrease due to natural disaster.
- Subpopulations can be split or merged.

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

Every population has its own variable space, or *local namespaces* 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 in these namespaces and store their results in them. For example, function `Stat` set variables like `alleleFreq[loc]` and you can access them like `pop.dvars().alleleFreq[loc][allele]`.

Population has a large number of member functions, ranging from reviewing simple property to generating new population from the current one. However, you do not have to know all the member functions to use a population. As a matter of fact, you will only use a small portion of these functions unless you need to write pure python functions/operators that involves complicated manipulation of populations.

## 2.2 Population related functions

The following table lists all population related functions. Functions that are prefixed by `'p.'` are member functions. That is to say, they should be called in the form of `pop.function()` where `pop` is a population object created by

functions like `population(...)` or `LoadPopulation(...)`.

### Population related functions

ref	function	description
2.2.1	<code>population()</code>	Create a population. Note that this is technically the <code>__init__</code> function of the population object.
2.2.1	<code>p.clone()</code>	Deep copy of a population. (In python, <code>pop1 = pop</code> will only create a reference to <code>pop</code> .)
2.5	<code>p.numSubPop()</code>	Number of subpopulations in a population
2.5	<code>p.subPopSize(sp)</code>	Size of a subpopulation
2.5	<code>p.subPopSizes()</code>	Return an array of subpopulation sizes
2.5	<code>p.popSize()</code>	Total population size
2.5	<code>p.absIndIndex(ind, sp)</code>	Return the absolute index of an individual in a subpopulation
2.5	<code>p.subPopIndPair(ind)</code>	Return the (sp,idx) pair from an absolute index of an individual
2.5	<code>p.subPopBegin(sp)</code>	Index of the first individual of a subpopulation
2.5	<code>p.subPopEnd(sp)</code>	Index of the last individual of a subpopulation + 1
2.6	<code>p.individual(ind)</code>	Return an individual
2.6	<code>p.individual(ind, sp)</code>	Return an individual from a subpopulation
8.2.1	<code>p.arrGenotype()</code>	Return an editable array of all genotype of the population. You need to know how these genotype are organized to safely read/write genotype directly.
8.2.1	<code>p.arrGenotype(sp)</code>	Return an editable array of all genotype of a subpopulation.
8.2.1	<code>p.arrInfo(sp)</code>	Return the editable array of all information field of a subpopulation (default to the whole population). Note that the order of individuals within each subpopulation is not honored.
	<code>p.indInfo(idx or field, [subPop])</code>	Get information of all individuals (or in a subpopulation), the information does not have to be in the same order as the individuals.
	<code>p.setIndInfo(values, [subPop])</code>	Set individual information for the given information field (index or name), for the given subpopulation (default to all population).
	<code>p.addInfoField(field)</code>	Add a information field, for example, 'penetrance', for the analysis of an existing population.
	<code>p.setInfoFields(fields)</code>	set the information fields of an existing population. The existing fields will be removed.
8.2.1	<code>p.exposeAffectedness(name='affected')</code>	Expose (not editable) the effectedness field of all individuals
8.2.1	<code>p.setIndSubPopID(info)</code>	Set info field of all individuals using an array of size <code>popSize()</code>
8.2.1	<code>p.setIndSubPopIDWithID()</code>	Fill info field of all individuals using their respective subpopulation ID.
8.2.1	<code>p.setSubPopByIndID(info=[])</code>	Rearrange individual and set subpopulation structure, using the info value of each individual as subpopulation ID. Individuals with negative info value will be removed.
8.2.1	<code>p.splitSubPop(which, sizes, subPopID=[])</code>	Split a subpopulation into subpopulations of gives sizes. (The sum of sizes should equal the size of which subpopulation.) Subpopulation IDs can be specified.
8.2.1	<code>p.setSubPopStru(newSubPops, allowPopSizeChange=False)</code>	Set subpopulation structure. Population size may be changed but all genotype may be lost.
8.2.1	<code>p.splitSubPopByProportion(which, proportions, subPopID=[])</code>	Split a subpopulation into subpopulations of given proportions. (The sum of proportions should add up to one). Subpopulation IDs can be specified.
8.2.1	<code>p.removeEmptySubPops()</code>	Remove empty subpopulations by adjusting subpopulation IDs.



ref	function	description
8.2.1	<code>p.removeSubPops( subPops=[], shiftSubPopID=True, removeEmptySubPops=False)</code>	Remove some subpopulations (and all individuals within). If <code>shiftSubPopID</code> is false, <code>subPopID</code> will be keep intact.
8.2.1	<code>p.removeIndividuals( inds, subPop=-1)</code>	Remove individuals. If a valid <code>subPop</code> is given, remove individuals from this subpopulation.
8.2.1	<code>p.mergeSubPops( subPops, removeEmptySubPops=False)</code>	Merge subpopulations, using the first subpopulation ID.
8.2.1	<code>p.reorderSubPops( order, rank, removeEmptySubPops=False)</code>	Reorder subpopulations by order or by rank. FIXME: details.
8.2.1	<code>p.newPopByIndInfo( keepAncestralPops=True, removeEmptySubPops=False)</code>	FIXME: details.
8.2.1	<code>p.removeLoci( remove=[], keep=[])</code>	Remove some loci from the current population. One of <code>remove</code> or <code>keep</code> can be specified.
8.2.1	<code>p.newPopWithPartialLoci( remove=[], keep=[])</code>	Copy current population to a new one and remove its loci. (Current population untouched)
8.2.1	<code>p.pushAndDiscard(pop)</code>	(Almost) Internal use only.
2.10	<code>p.ancestralDepth()</code>	Ancestral depth of current population.
2.10	<code>p.setAncestralDepth(depth)</code>	Set ancestral depth. 0 for none, -1 for unlimited.
2.10	<code>p.ancestralPop()</code>	Current ancestral population selected. (0 for latest generation)
2.10	<code>p.useAncestralPop(idx)</code>	Use an ancestral population. 0 for latest generation.
	<code>p.equalTo(pop)</code>	Compare two populations.
2.11	<code>p.savePopulation( filename, format='auto', compress=True)</code>	Save a population.
	<code>SavePopulation( pop, filename, format='auto', compress=True)</code>	Save a population.
	<code>SavePopulations(pops, filename, format='auto')</code>	Save an array of populations to a file.
2.11	<code>p.loadPopulation( filename)</code>	Load a population and replace the current one. (Use <code>LoadPopulation</code> instead)
2.11	<code>LoadPopulation( filename)</code>	Load a population and return it. Format can be 'bin', 'xml', 'text' or 'auto'. If auto is specified, file format is determined by file extension '.bin', '.xml' or '.txt'.
	<code>LoadPopulations( filename)</code>	Load an array of populations from a single file.
	<code>p.rep()</code>	Current replicate in a simulator
	<code>p.grp()</code>	Current group ID in a simulator
	<code>p.gen()</code>	Current generation during evolution.
2.7	<code>p.vars()</code>	Return a dictionary of attached Python namespace.
2.7	<code>p.vars(sp)</code>	Return the namespace for a subpopulation
2.7	<code>p.dvars()</code>	Return the dictionary <code>vars()</code> with keys mapped to attributes. I.e., you can access <code>pop.vars()['LD']</code> as <code>pop.dvars().LD</code> .
2.7	<code>p.dvars(sp)</code>	Return the attribute version of <code>vars(sp)</code>
2.7	<code>p.hasVar( name)</code>	Whether or not a variable exists in the local namespace

ref	function	description
2.7	<code>ListVars( var, level=-1, subpop=True, useWxPython=True)</code>	List a dictionary returned by functions like <code>pop.dvars()</code> or <code>pop.vars(sp)</code> , up to certain level (default to all). You may use name parameter if you know the variable name, and set <code>subPop=False</code> if you are only interested in the overall population. <code>wxPython</code> will be automatically used if available, unless you set <code>useWxPython=False</code> .
2.7	<code>p.evaluate(expr, stmts="")</code>	Evaluate an expression and return its result. Optionally run statement first.
2.7	<code>p.execute(stmts)</code>	Evaluate a statement (can be multi-line string).

## 2.2.1 Creating a population

A population can be created through

- call `population` function to create an instance of population from `population` class.
- call `LoadPopulation`, `LoadFstat` etc to load a population from a saved file.
- generated as a subset of an existing population by operators like `randomSample`, `caseControlSample` or equivalent functions `RandomSample`, `CaseControlSample`.
- Obtained from an existing simulator through `simulator::getPopulation()`

Help contents of all functions of population class can be displayed by `help(population)`. Help on a member function can be viewed by `help(population.func)`. In Python, constructor is named `__init__` and you can use class name to create an instance of the class. Therefore, to display parameters of `population` function, you need to run

```
help(population.__init__)
```

Some notes about the parameters:

- `size`, `subPop`: `size` can be ignored if `subPop` is specified. If both parameters are provided, `subPop` should add up to `size`.
- `loci`: number of loci on each chromosome. The length of parameter `loci` determines number of chromosomes. The last chromosome can be sex chromosome. In this case, please specify the maximum number of loci on X and Y. I.e., if there are 3 loci on Y chromosome and 5 on X chromosome, use 5.
- `sexChrom`: true or false. Diploid population only. If true, the last homologous chromosomes will be treated as sex chromosomes. (XY for male and XX for female.) If X and Y have different number of loci, you should use the longer one as loci number of the last (sex) chromosome.
- `lociPos`: a 1-d or 2-d array specifying positions of loci on 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 locations, although they are usually interpreted as base pairs or centiMorgans, depending on types of simulation being performed. Currently, loci location is used only for specifying recombination intensity. The actual recombination rate is intensity times loci distance between adjacent loci.

- `ancestralDepth`: number of most recent ancestral generations to keep during evolution. Default to 0. 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 populations may quickly exhaust your computer RAM. If you really need to do that, use `savePopulation` operator to save each generation to a file is a much better choice.
- `alleleNames`: Names of the alleles. They are used only for output.
- `maxAllele`: maximum allele state for the whole population. This will set a cap for all loci. For individual locus, you can specify `maxAllele` in mutation models, which can be smaller than global `maxAllele` but not larger. Note that this number is the number of allele states minus 1 since allele number starts from 0.

Example 4 shows a few examples of using the population function to create populations.

---

**Example 4** Use of population function

---

## 2.3 Copying a population

Like many other python operations,

```
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()
```

This scenario also apply to simulator (see later sections), if `simu` is a simulator with several replicates,

```
pop = simu.population(idx)
```

will get a reference to one of the replicates. You can, although not recommended, modify simulator through this `pop` reference. Note that this `pop` reference will become invalid when the simulator is destroyed so the following calling sequence will crash python.

```
pop = simu.population(idx)
simu = simulator(...)
pop.savePopulation(...)
```

If you would like to get a real copy, use

```
pop = simu.getPopulation(idx)
```

## 2.4 Interaction with Operators and Functions

Operators are objects that can be applied to populations. They have special attributes like at which generations to be active, at what stage of a evolutionary life cycle to be applied. Usually, an operator is created and passed as a parameter to a simulator. When `simulator::evolve` (or `step`, `apply`) is called, the simulator will call the `apply()` function of these operators at appropriate times.

For example, operators `initByFreq`, `stat` and two copies of `kamMutator` are created in example 5. During evolution, `simu` will apply `initByFreq` once to each replicate of the simulator; apply the first `kamMutator` to the first replicate and the second `kamMutator` to the second replicate at every generation; apply `stat` to count allele frequency and calculate  $F_{st}$  every 10 generations. More details about operators will be described later.

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( [0.3, .2, .5] ).apply(pop)
```

or dump the content of a population by

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

This style of calling 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 6** Function `InitByFreq`

---

Note that

1. The following two calling sequences have different consequences:

```
pop = population(10)
simu = simulator(pop, randomMating(), rep=3)
simu.evolve( preOps = [initByFreq([.8,.2]) ] )
```

initialize three replicates of the population independently, (`initByFreq` object is applied to three populations.)  
but

```
pop = population(10)
InitByFreq(pop, [.8, .2])
simu = simulator(pop, randomMating(), rep=3)
```

initialize a population once and create a simulator with three copies of the initialized population.

2. If you are going to call such a function many times, it is more efficient to do

```
init = initByFreq([.8,.2])
for i in range(0,1000):
    init.apply(pop[i])
```

than

```
for i in range(0,1000):  
    InitByFreq(pop[i], [.8,.2])
```

The difference is that the second method creates and destroys an `initByFreq` object each time it calls the function.

Because `initByFreq` and `dumper` will be frequently used in this manual, I will briefly describe them here.

- `initByFreq` takes an array of probabilities (must add up to one). When applying to a population, each allele will be assigned 0,1,2,3,... etc according to the provided probabilities. `InitByFreq(pop,...)` is its function form.
- `dumper` will simply display the population. The output format for each individual is: individual index, tag, sex, affected status, alleles on copy 1,2,... of all chromosomes, separated by |. Its function form is named `Dump(pop)`.

Example 7 demonstrates the use of these two operators:

---

**Example 7** Operator `dumper` and `initByFreq`

---

## 2.5 Population Structure

subpopulation structure can be accessed through the following member functions:

- `pop.popSize()`, total population size
- `pop.numSubPop()`, number of subpopulations
- `pop.subPopSize(sp)`, size of subpopulation, which can be zero. Note that `sp` is zero-indexed.
- `pop.subPopBegin(sp)`, the index of the first individual in subpopulation `sp`
- `pop.subPopEnd(sp)`, the index of the last individual in subpopulation `sp` plus one.
- `pop.subPopIndPair(ind)`, return the subpopulation and relative index of individual `ind`.
- `pop.absIndIndex(ind, sp)`. return the absolute index of an individual

---

**Example 8** population structure functions

---

There are another set of functions that deal with population/subpopulation size changes. In these functions, the `info` field of each individual plays an important role. This field represents an individual's (new) subpopulation ID most of the times. For example, function `rearrangeByIndID()` rearrange individuals in the order of their `info` values. Similar functions are

- `pop.setIndSubPopID(info)`, set individual `info` using a vector of size of the population
- `pop.setIndSubPopIDWithID()`, use subpopulation id to set individual `info`

- `pop.setSubPopByIndID( )`, rearrange individual and set subpopulation structure according individual info values
- `pop.removeEmptySubPops( )`, remove empty subpopulations.
- `pop.removeSubPops(subPops)`, remove subpopulation
- `pop.reorderSubPops(order, rank, removeEmptySubPops=False)`,
- `pop.newPopByIndID(keepAncestralPops=True, info=[ ])`,
- `pop.removeLoci(remove=[ ], keep=[ ])`, remove some loci from the population
- `pop.newPopWithPartialLoci(remove=[ ], keep=[ ])`, return a new reduced population
- `pop.splitSubPop(which, subPopSizes, subPopID)`, split subpopulation which according to subPopSizes
- `pop.splitSubPopByProportion(which, proportions, subPopID)`, use proportion
- `pop.mergeSubPop(subPops)`. merge subpopulations

These functions may look useful and appealing but you will almost never use them directly. All these operations will be performed by various operators, in a more user-friendly way. Only when you begin to write your own operators will you have to read about the details of these functions.

Example 9 demonstrate the use of functions `setIndSubPopID`, `setSubPopByIndID` and `removeLoci`.

---

#### Example 9 population structure functions

---

## 2.6 Individuals

You can access individuals of a population through `individual( )` function. There are two forms of this function, one with and one without parameter `subPop`,

- `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.

The returned `individual` object also has its own member functions. You can retrieve genotypic information of an individual through the same set of functions. You can also get/set genotype of an individual. Note that you can not create an individual object directly.

---

#### Example 10 Individual member functions

---

Again, you will very seldom have to use these functions directly unless when you write pure python operators.

The following table lists all individual related functions. They are all member functions so they have to be access through an individual object in the form of `ind.function( )`.

#### Individual related functions

function	description
<code>i.arrGenotype()</code>	Return an editable array of the genotype of an individual. The layout of this array is explained in section 8.2. Although this function is not as easy to use as other allele-access functions, it is the fastest one since you can read/write genotype directly after you get the handle of all genotype through this function.
<code>i.arrGenotype(p)</code>	Return only the p-th copy of the chromosome.
<code>i.arrGenotype(p, ch)</code>	Return only the ch-th chromosome of the p-th copy.
<code>i.allele(idx)</code>	Return the allele at locus <code>idx</code>
<code>i.allele(idx, p)</code>	Return the allele at locus <code>idx</code> of the p-th copy of the chromosomes,
<code>i.allele(idx, p, ch)</code>	Return the allele at locus <code>idx</code> of the ch-th chromosome of the p-th chromosome set
<code>i.alleleChar(idx)</code>	Return the name of allele <code>allele(idx)</code>
<code>i.alleleChar(idx, p)</code>	Return the name of allele <code>allele(idx, p)</code>
<code>i.alleleChar(idx, p, ch)</code>	Return the name of allele <code>allele(idx, p, ch)</code>
<code>i.setAllele(allele, idx)</code>	Set the allele at locus <code>idx</code>
<code>i.setAllele(allele, idx, p)</code>	Set the allele at locus <code>idx</code> of the p-th copy of the chromosomes,
<code>i.setAllele(allele, idx, p, ch)</code>	Set the allele at locus <code>idx</code> of the ch-th chromosome of the p-th chromosome set
<code>i.info(idx or name)</code>	Get the the value of info field (indexed by <code>idx</code> or <code>name</code> ).
<code>i.setInfo(value, idx or name)</code>	Set the value of info field (indexed by <code>idx</code> or <code>name</code> )
<code>i.arrInfo()</code>	Return an editable array of all information fields.
<code>i.sex()</code>	Return the sex of an individual, <b>1 for Male and 2 for Female</b> . However, this is not guranteed so please use <code>sexChar()</code>
<code>i.sexChar()</code>	Return the sex of an individual <b>M/F</b>
<code>i.setSex(sex)</code>	Set the sex. You should use <code>setSex(Male)</code> or <code>setSex(Female)</code> instead of 1 and 2.
<code>i.affected()</code>	Whether or not an individual is affected
<code>i.unaffected()</code>	Not affected()
<code>i.affectedChar()</code>	Return 'A' or 'U' for affectedness status.
<code>i.setAffected(aff)</code>	Set affectedness status.
<code>i.subPopID()</code>	Return the info field of an individual
<code>i.setSubPopID()</code>	Set the info field of an individual

## 2.7 Population Variables

Populations are associated with python variables. These variables are usually set by various operators. For example, `stat` operator calculates many population statistics and store results in population namespace. Example 2.7 demonstrates how `stat` set variables `popSize`, `alleleFreq` etc.

You can refer to these variables using `population::vars()` or `population::dvars()` function. The returned value of `vars()` and `dvars()` reflects the same dictionary. However, `dvars()` uses a little Python magic so that you can use attribute syntax to access dictionary keys. Since `a.alleleFreq[0]` is a lot easier to read than `a['alleleFre'][0]`, `dvars()` is always preferred to `vars()`. A function `ListVars` defined in `simuUtil` can be used to display the variables. With `wxPython` installed, this function will open a nice window with a tree representing the variables. Without `wxPython` (or use parameter `useWxPython=False`), variables will be displayed in a indented form. Several parameters can be used to limit your display. They are

- `level`: level of tree, further nested variables will not be displayed

- name: name of variable to display.
- subPop: whether or not display variables for each subpopulations

---

### Example 11 Population variables

---

These variables form a Python dictionary, and furthermore a local namespace for functions like `population::evaluate`. *Local namespace* means that you can use dictionary items as variables during evaluation. For example:

---

### Example 12 Local namespaces of populations

---

As you can see, these variables are *local* to the population and is not directly accessible from the main namespace. `vars(subPop)` and `dvars(subPop)` function can be used. Both functions takes an optional `subPop` option. If ignored, they will return population dictionary; otherwise, they will return dictionary for subpopulation `subPop`. This is a very convenient feature, because subpopulations and populations have similar keys, you can calculate the same statistics for the whole population and individual subpopulations, just by specifying different namespaces.

## 2.8 Sample from a Population

Sampling (or ascertainment) is a complicated issue. `simuPOP` provides several methods to generate samples from an existing population. Details please refer to Chapter 7.12.

## 2.9 Information fields

The information fields are information that is attached to each individual. For example, an individual may need `father_idx` and `mother_idx` to track pedigree information, may need `penetrance` to set affectedness.

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

- `pop.setInfoFields(fields)`
- `pop.addIndField(field)`

Note that changing `infoField` for a simulator is dangerous since all populations in a simulator share the same genotypic structure. You should `addIndField` to all populations to avoid potential problems.

One can set/retrieve information at the level of individuals

- `ind.info(idx or field)`
- `ind.setInfo(idx or field)`
- `ind.arrInfo()`

or set the population level

- `pop.indInfo(idx or field, [subPop])`



- `pop.setIndInfo(idx or field, [subPop])`
- `pop.arrIndInfo([subPop]`

Idx or field means that you can use field index obtained from `infoIdx(field)`, or use field name directly. field is easier to use but idx is faster.

For each individual, `ind.arrInfo()` will return `f1, f2, f3, ...` etc for that individual. From a population point of view, `pop.arrIndInfo([subPop])` will return a list of `f1, f2, f3, ..., f1, f2, f3, ...`. Note that the order of individuals may not be kept in this (sub)population-wise array. That is to say, `pop.arrIndInfo()[0]` does not have to be the first field of the first individual. This property is also true for `setIndInfo(values, idx or name)`. That is to say, if you want to set information field for individuals in a population unordered, you can use

```
setIndInfo(values, idx)
```

Otherwise, you will have to use the less efficient way:

```
for i in range(pop.popSize()):
    pop.individual(i).setInfo(values[i], idx)
```

Note that `indInfo` is more convenient but it is less efficient (fields must be copied out) than `arrIndInfo`. To handle the return value of `arrIndInfo`, you would usually do:

```
idx = pop.infoIdx('trait2')
step = pop.infoSize()
arr = pop.arrIndInfo(subPop=2)
for i in range(pop.subPopSize(2)):
    # note again that arr is writable.
    arr[idx + step*i] = something
```

## 2.10 Ancestral populations

By default, a population object only hold 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 number of generations to keep. This parameter is default to zero, meaning keeping no ancestral population. You can specify a positive number to store most recent ancestry generations; or -1 to store all populations.

Several important usage of ancestral populations:

- `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 save the last three generations in populations so that pedigree based sampling schemes can sample from the population.

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

A typical use of this function is demonstrated in example 13. 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 afterwards. (Note that this is not the best way to examine the changes of allele frequencies, a `stat` operator should be used.)

---

**Example 13** Ancestral populations

---

## 2.11 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 human 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.

---

**Example 14** Save and load population

---

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`.

It is also possible to save a bunch of populations in a single file, provided that they have the same genotypic structure. The functions are

- `SavePopulations([pop1,pop2,...], filename, format='auto', compress=True)`
- `LoadPopulations(filename)`

Shared variables will also be saved (except for big objects like samples). Since the number of shared variables can be big, it may be 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

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

## 2.12 View a population (GUI, wxPython required)

Introduced in ver 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,

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



# Mating Scheme

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 choose parent(s) to generate offsprings to fill the next generation.
- During-mating operators are applied to all offsprings.
- Apply selection if applicable.

## 3.1 Create a Mating Scheme

Most mating schemes take the following parameters:

- `numOffsprings` number of offsprings or  $p$  for a random distribution. default to 1. This parameter determines number of offsprings a mating event will produce so it determines family size.
- `numOffspringsFunc` a python function that return number of offspring or  $p$ .
- `maxNumOffsprings` used when `numOffsprings` is generated from a binomial distribution.
- `mode` One of `MATE_NumOffspring`, `MATE_NumOffspringsEachFamily`, `MATE_GeometricDistribution`, `MATE_PoissonDistribution`, `MATE_BinomialDistribution`.
- `newSubPopSize` an array of sizes of subpopulations.
- `newSubPopSizeExpr` an expression that will return the new subpopulation size. Details about python expression will be discussed later.
- `newSubPopSizeFunc` Added for more convenience. This should be a function that accept a int parameter (generation), an array of current population size and return an array of subpopulation sizes. This is usually easier to use than the expression version of this parameter.

## 3.2 Determine number of offsprings during mating

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

The method to determine the number of offsprings are set by `mode` parameter:

- `MATE_NumOffsprings`: if `numOffspringsFunc` is not given, number of offsprings will be constant `numOffsprings` all the time. Otherwise, `numOffspringsFunc(gen)` will be called **once** for each generation to get the number of offsprings for the matings happen in this generation.
- `MATE_NumOffspringsEachFamily`: `numOffspringsFunc` has to be given and will be called whenever a mating happens. Since `numOffspringsFunc` can be **any** python function, this mode allows arbitrary model of assigning number of offsprings during mating. The mode can be slow though.
- `MATE_GeometricDistribution`: `numOffsprings` or result of `numOffspringsFunc` (evaluated at each generation) will be considered as  $p$  for a geometric distribution. The number of offsprings for each mating is determined by

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

- `MATE_PoissonDistribution`: `numOffsprings` or result of `numOffspringsFunc` (evaluated at each generation) will be considered as  $p$  for a Poisson distribution. The number of offsprings for each mating is determined by

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

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. (FIXME: this part needs more consideration.)

- `MATE_BinomialDistribution`: `numOffsprings` or result of `numOffspringsFunc` (evaluated at each generation) will be considered as  $p$  for a Binomial distribution. Let  $N = \text{maxNumOffsprings}$ , the number of offsprings for each mating is determined by

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

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

### 3.3 Determine subpopulation sizes of next generation

The default behavior of `simuPOP` is to use the same population/subpopulation sizes as 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 size can be easily calculated through an expression, you can use `newSubPopSizeExpr` to determine the new subpopulation sizes. For example `newSubPopSizeExpr='[gen+10]'` uses generation number + 10 as the new population size. More complicated expression can be used, maybe along with `pyExec` operators, but in this case, a specialized function and `newSubPopSizeFunc` is recommended. Note that the expression uses variables from local namespace.
- 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 take two parameters: generation number and current subpopulation sizes and return an array of new subpopulation sizes. (return `[newsize]` instead of `newsize` when you do not have any subpopulation structure). For example, the following function defines a linear expansion demographic scenario where a real example where a single population is splitted at 200 generations (using a `splitPopulation` operator).

```
def lin_exp(gen, oldSize=[]):
    if gen < 200:    # burn in, constant population size
        return [1000]
    else:           # increase subpopulation sizes
        incSize = (10000-1000)/(500-200)/len(oldSize)
        return [oldSize[x]+incSize for x in range(0, len(oldSize))]
```

you can then use this function as follows

```
...randomMating(newSubPopSizeFunc=lin_exp) ...
```

## 3.4 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 burnin and split to equal sized subpopulations. For all these function, 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 burnin. Population size change happens **after** burnin (start at burn+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 population size from `intiSize` to `endSize` after burnin, split the population at generation `split`. If `bottleneckGen` is specified, population size will be `bottleneckSize` at that generation.

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

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

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

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

## 3.5 Different Mating Schemes

Currently, simuPOP provides the following mating schemes:

- `noMating()` parent generation will be considered as offspring generation. subpop sizes will be ignored although some during-mating operators can be applied.
- `binomialSelection()` no sex is involved. Offspring is chosen from parental generation by random or according to fitness values.
- `randomMating()` sexed random mating. A parameter (`contIfUniSex`) can be set to determine the behavior when only one sex exists in a subpopulation. Default is continue without warning.
- `pyMating()` (**not usable right now**) Hybrid mating scheme. This mating scheme takes two parameters: `mateFunc` and `keepSubPopStru`. `mateFunc` should be a python function that accept a (parental) population and return parent indices for each offspring. If `keepSubPopStru=True` (default), parents should come from the same subpopulation and the offspring population will have subpopulation structure. Otherwise, mating can across subpopulation structure.

Detailed information of each mating scheme can be found through `help(...)` function.

## 3.6 Sex chromosomes

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

Recombinations on sex chromosomes of females (XX) is just like those on autosomes. However, this is not true in male. 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.



# Operators

Operators are objects that act on populations. They (there are exceptions) can be applied to populations directly using `apply()` member function, but most of the time they are managed and applied by a simulator.

## 4.1 Type of operators

There are three kinds of operators:

- *built-in*: written in C++, 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 python function during simulation. Less efficient. For example, a hybrid mutator `pyMutator` will determine if an allele will be mutated and call a user-defined Python function to mutate it.
- *pure python*: written in python. Same speed as python. For example, a `varPlotter` can plot python variables that are set by other operators.

You do not have to know the type of an operator to use them. The interface of them are all the same. Note that although it is possible to write pure python operators to operate directly on populations, it might work very slowly compared to the built-in ones.

### 4.1.1 Applicable Stages

Operators can be applied at different stage(s) of a life cycle. More specifically, at pre-, during- or post mating stage(s). Note that it is possible for an operator to apply multiple times in a life cycle. For example, an save-to-file operator might be applied before and after mating to trace parental information. Applicable stages are usually set by default but you can change it by setting `stage=(PreMating|PostMating|DuringMating|PrePostMating)` parameter. Note that some operators ignore `stage` parameter since they only work at one stage.

---

**Example 15** Operator stage

---

### 4.1.2 Active Generations

Operators do not have to be applied at all generations. You can specify starting generation, ending generation, gaps between applicable generations, or even specific generations to apply. For example, you might want to start applying

migrations after certain burn-in generation; or you want to calculate every 10 generations. Operators take the following parameters during initialization:

- `begin` start generation. default to 1. negative number is interpreted as `endGeneration + begin`
- `end` stop applying after this generation. negative number is allowed
- `step` number of generations between active generations. default to 1
- `at` an array of active generations. If given, `begin`, `end`, `step` will be ignored.

For example

---

**Example 16** Set active generations of an operator

---

The last example displays variable `gen` for each replicate. Note that you can use negative generation number whenever you specifies the `end` parameter of `evolve`. In this case, generation -1 is the last generation (`end`), -2 is `end-1`, and so on.

### 4.1.3 Replicates and Groups

Most operators are applied to every replicate of a simulator during evolution. However, you can apply operators to one or a group of replicates only. For example, you can initialize different replicates with different initial values and then start evolution. c.f. `simulator::setGroup`.

The most useful example is

```
output( '\n', rep=REP_LAST)
```

that will output `\n` at the end of each generation. Here is an example of using replicate groups:

---

**Example 17** Replicate group

---

### 4.1.4 Output Specification

Operators can have outputs. Output can be standard output (terminal) or a file, which can be constant, or change with generation or replicate. Different operators can append to the same file to form table-like outputs.

Filename can have the following format:

- `'filename'` this file will be closed after each use. I.e., if several 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 close at the end. Several operators can output to this file to form a table.
- `'>>>filename'` The same as `'>>filename'` except that the file will not be cleared at the beginning of evolution if it is not empty.
- `'>'` out put to standard output.

---

**Example 18** log/operatoroutput

---

- " suppress output.

The following example shows the difference between ">" and ">>"

In the first simulator, all operators uses "a.txt" (the same as ">a.txt"). This file is repeatedly covered by other operators so what we finally get is a newline written by output("\n"). The second simulator works fine by using ">>a.txt".

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

---

**Example 19** log/operatoroutputexpr

---

## 4.2 Python expression and statistics calculation

### 4.2.1 Expressions and Statements

Expressions are used extensively in operators so basic knowledge of python is required. If you know almost nothing about Python, please spend some time on the Python tutorial from python website.

Unlike C/C++, assignments in Python do not return values. This is the biggest difference between Python expression and statement:

- expressions consist of constants, variables, operators, functions, but *no* assignments, condition, loop etc. Expression returns a value when executed. An example of expression is `range(1,5)+10`.
- statements consist of arbitrary valid python code. Statement does *not* return a value when executed. An example of statement is `a=range(1,5)`.

### 4.2.2 simuPOP variables

All populations have their own attached variables. We have seen the structure of a population dictionary: it starts empty and will have many variables created by various operators. You can access local namespace of each replicate through a simulator's `vars(rep)` function:

<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>	

It is important to know that

- `simulator::vars(0)`, `vars(1)` etc are the *local namespaces* for each replicate.
- `subPop[0]`, `subPop[1]` etc have almost the same set of keys as those for the whole population. This is because `stat` operator calculate statistics of each replicate of population, and all subpopulations.

To list these variables, you can use the `ListVars()` function defined in `simuUtil.py`. For example

```
ListVars(simu.vars(0), level=2)
```

list all variables for the first replicate. `Level=2` stops `ListVars` from expanding lists and dictionaries after two levels.

Two functions can be used to access simulator and population variables: `vars()` and `dvars()`. We have known `population::vars()` and `population::dvars()`, `simulator::vars()` and `simulator::dvars()` work in almost the same way.

- `simulator::vars(rep)`, `dvars(rep)`: return replicate `rep`'s local namespace
- `simulator::vars(rep, subPop)`, `dvars(rep, subPop)`: return the namespace of `subPop` sub-population of replicate `rep`.

The return values of `vars()` and `dvars()` are different. `vars()` returns a Python dictionary. You should access their keys in the usual Python way. `dvars()` returns a 'wrapped' Python dictionary. You can access dictionary keys as attributes. `dvars()` is usually considered to be easier to use.

### 4.2.3 evaluate function and `pyEval` and `pyExec` operators

Function `population::evaluate` and operator `pyEval/pyExec` will work in local namespaces. For example, if there are `a` and `b` in the main namespace and `a` in `pop`, `pop.evaluate('a')` will return `pop.vars()['a']`, `pop.evaluate('b')` will return global `b` since there is no `b` in the local namespace. If this is still too abstract, here is a real example

---

**Example 20** python expression

---

- `simulator` creates a simulator with two replicates 0 and 1.
- We evaluate `grp*2` in different replicates and get different results.
- `gen` is not in either replicate's namespace so the global one will be used.
- Using statements can create variables in local namespaces. (You can use `global` statement to create global variable if you are familiar with python.)

`pyEval/pyExec` operators execute python expression/statements, *using local namespaces*.

- `pyEval` (operator) evaluate a Python expression and return its value, optional execute a list of statements beforehand.
- `pyExec` (operator) execute a list of statements in the form of a multi-line string. No return value or output.

Here, `expr` is a simple string containing an expression that will return a value when executed; `stmts` is a string of statements, separated by `'\n'`.

For example, you can return a string of “gen:rep” using the following function

```
pop.evaluate(r"%d:%d" % (gen,rep))
```

but if you would like to change/create variables, you have to use statements like

```
pop.evalulate(r"myval", stmts=r"myval=rep+1")
```

Since you are executing Python statements, you can of course do it directly in python. For example, the above function does exactly the following

```
pop.vars()['myval'] = pop.vars()['rep'] + 1
pop.vars()['myvar']
```

As a matter of fact, we seldom use `evaluate` function directly (maybe for debugging), usually

- we use expressions for dynamic parameters. For example:

```
newSubPopSizeExpr="range(10,20)*1.2"
outputExpr= ' "saveAt%s.txt" % gen'
```

These parameters will be evaluated whenever they are referred.

- we use expression/statements in `pyEval/pyExec` operators. These statements will work in local namespaces. For example:

---

**Example 21** Expression evaluation

---

Because of the interactive nature of python, it is very easy to write short programs, quote them in `r" 'program' "` and put them in to `pyEval/pyExec` operators.



# Simulator

Simulators combine three important components of simuPOP: population, mating scheme and operators together. A simulator is usually created with an instance of population, a replicate number and a mating scheme. It makes 'rep' replicates of this population and control the evolution process of these populations.

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

## 5.1 Generation Number

Several aspects of generation number may cause confusion:

- generation starts from zero
- a generation number presents a 'to-be-evolved' generation
- 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 three times. Generation 0, generation 1, and generation 2. At the end of 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`).

When you use `start=0`, `step=5`, `end=10` for your operator, it will be applied at generations 0, 5, 10 etc.

## 5.2 Operator calling sequence

Simulators separate operators into pre-, during- and post- mating operators. During evolution, simulator first apply all PreMating operators and then call the `mate()` function of the given mating scheme, which will call

DuringMating operators during the birth of each offspring. After the new generation is generated, PostMating operators are applied in the order they appear in the operator list.

Anyway, operators are not always active. They can be applied to certain generations or certain replicate(s) of population. A simulator will always apply preOps and postOps operators, but will ask if an operator is active (by providing rep, grp, gen information) before its is called.

The order of applying operators usually does not matter but errors can occur if you are not careful. For example, stat(...) calculate the statistics of 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 post-mating population. However, it 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 real evolution is always a good idea.

## 5.3 Evolution

Simulators can evolve a given number of generations (the 'end' parameter of evolve), or evolve indefinitely using a certain type of operators called terminators. 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. Useful simulator functions are

- gen() return current generation number
- setGen() set current generation. Usually used to reset a simulator
- population() return temporary reference of one of the populations. 'Reference' means that the changes to the referred population will reflect to the one in simulator. 'Temporary' means that the referred population might be invalid after evolution.
- evolve() evolve all replicates of the population
- apply() apply a list of operators to all populations.
- step() evolve one generation.

The most useful function is of course evolve, which takes parameters

- preOps: operators that will be applied before evolution
- ops: operators that will be applied at each generation.
- postOps: operators that will be applied after evolution.
- end: ending generation. Default to -1. In this case, a simulator will only be ended by a terminator.
- dryrun: dryrun mode. see previous section
- saveAs: saveAt, format: see next section



## 5.4 Save and Load

A simulator can be saved to a file in the format of `'txt'`, `'bin'`, or `'xml'`. This enables us to stop a simulation and resume it at another time or on another machine. It is also a good idea to save a snapshot of a simulation every several generations. Note that mating scheme can not be saved and has to be re-specified in `LoadSimulator()`.

simulators can also be saved during evolution. Three relevant parameters of `evolve()` function are:

- `saveAs`: filename to save the simulator. Default to `simu`.
- `saveAt`: generations at which to save the simulator. Generation can be negative, meaning counting backwards.
- `format`: format. Default to `'bin'`.

During evolution, simulator will be saved at `saveAt` generations with filenames `saveAs+gen+format` (for example `simu1000.bin`).

It is also possible to build a simulator from a bunch of populations:

- `SimulatorFromPops(pops, mating)`, build a simulator with given populations and mating scheme
- `SimulatorFromFiles(files, mating)`, load populations from a given list of files (population images) and build a simulator with given mating scheme.



# Writing simuPOP scripts

## 6.1 Conventions of simuPOP scripts

A simuPOP script is usually composed of the following parts:

1. First line:

```
#!/usr/bin/env python
```

2. Introduction to the whole script:

```
'''
This script simulates ....
'''
```

These comments can be accessed as module `__doc__` and will be displayed as help message.

3. Options: (see the next section)

```
options = [
... a dictionary of all user input parameters ...
]
```

These parameters will be handled by simuPOP automatically. Users will be able to set them through command line, configuration file, Tkinter- or wxPython-based GUI.

4. Auxillary functions

5. Evolution function

```
def simulation(...)
```

6. Executable part:

```
if __name__ == '__main__':
    allParam = simuOpt.getParam(options,
        ''' A short description ''', __doc__)
    # if user press cancel,
    if len(allParam) == 0:
        sys.exit(1)
    # -h or --help
    if allParam[0]:
        print simuOpt.usage(options, __doc__)
```

```

    sys.exit(0)
# save configuration, something like
if allParam[-2] != None:
    simuOpt.saveConfig(options, allParam[-2]+' .cfg', allParam)
# get the parameters, something like
N = allParam[1]
# run the simulation
simulation(N)

```

You will notice that `simuOpt` does all the housekeeping things for you, including parameter reading, conversion, validation, print usage, save configuration file. Since most of the parts are pretty standard, you can actually copy any of the scripts under the `scripts` directory as a template for your new script.

Note that these scripts, if proper written, can also be imported. Other scripts (or interactive session) can import a script and call its simulation function directly.

## 6.2 Parameter handling and user input

Although `simuPOP` scripts, simply Python scripts, can be in any valid Python style, it is highly recommended that all `simuPOP` scripts follow the same writing style and provide a uniform interface to users. From a user's point of view, a `simuPOP` script `cmd.py` should

1. Start a Tk/wxPython dialog to accept user input when `--noDialog` is not specified.
2. List all commandline/config file options through `-h` or `--help` option.
3. Accept `-c` or `--config` parameter to read a configuration file and set parameters.
4. Be able to use command line arguments to set parameters if `--useDefault` is not specified.
5. When `--noDialog` and `--useDefault` is specified, use default values for all parameters, if they can not be obtained from commandline parameters, configuration file, and have a default value.
6. Accept `--saveconfig file` to save current configuration (input my commandline argument) into file.
7. Be able to make use of optimized libraries through the use of command line parameter (`--optimized`), config file entry (`optimized=True`) or environment variable (`SIMUOPTIMIZED`).
8. Be able to make use of longallele libraries through the use of command line parameter (`--longallele`), config file entry (`longallele=True`) or environment variable (`SIMULONGALLELE`).

To alleviate trouble of doing all these, `simuPOP` has provided a set of functions. Here is how parameters should be handled. The first step is describe each parameter in details. This includes (not all is necessary) short and long argument name, entry on a configuration file, prompt when asking for user input, default value, description that will be shown in usage, allowed types of parameter, function to validate the input value. All these should be put in a list of dictionaries like follows:

```

options = [
    { 'arg':'h', 'longarg':'help', 'default':False,
      'allowedTypes':[IntType],
      'description':'print this message'},
    { 'longarg':'saveconfig=', 'default':"", 'allowedTypes':[StringType],
      'description':'Save current configuration in a file.'},

```

```
{ 'arg':'m', 'longarg':'mu', 'label'='mutationRate',
  'default':0.005,
  'validate': simuOpt.valueBetween(0,1),
  'description':'mutation rate (a number or an array of numbers) at each loci'
} ]
```

The entries:

- `arg` and `longarg` are command line argument format. For example,
  - `arg: 'h'` checks the presence of argument `-h`, return `True` if succeeds
  - `arg: 'f: '` checks the presence of argument pair `-f something`, return `something` if succeeds
  - `longarg: 'help'` checks the presence of argument `--longarg`, return `True` if succeeds
  - `longarg: 'mu= '` checks the presence of argument pair `--mu number`, return `number` if succeeds.
- `label` will be used as the label of input field in a parameter dialog, and as the prompt for user input.
- `default` is used when prompt is empty, or when user press enter directly.
- `description` is the description of this parameter, will be put into usage information. ( `-h` or help button in parameter dialog).
- `allowedTypes` is the accepted types. If `allowedTypes` is `types.ListType` or `types.TupleType` and user input is a scalar, the input will be converted to a list automatically.
- `validate` is a function to validate the parameter. You can define your own functions or use the following from `simuOpt`
  - `valueGT(a), valueLT(a), valueGE(a), valueLE(a)`: check greater than, less than, greater equal, less equal to a value `a`.
  - `valueBetween(a,b), valueOneOf(list)`: check if the value is between `a` and `b` or is one of `list`
  - `valueValidFile(), valueValidDir()`: check if the parameter is a valid file/directory name.
  - `valueIsNum()`: check if the parameter is a number.
  - `valueListOf()`: check if parameter is a list of given type, in a list of types, or pass a validator. For example, you can use `valueListOf(types.IntType)`, `valueListOf([types.IntType, types.LongType])` or `valueListOf( valueValidFile() )`. As you can see, validators can be nested.
  - `valueOr(validator), valueAnd(val1, val2), valueOr(val1,val2)` accepts other validators and perform respective logical calculation. For example  
`valueOr( valueGT(0), valueListOf( valueGT(0) ) )`  
 accept a positive number, or a list of positive number.
- `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`: `jump` is used to skip some parameter when doing interactive user input. For example, `getParam` will skip the rest of the parameters if `-h` is specified since parameter `-h` has item `'jump':-1` which means jump to the end. Another use of this value is when you have a hierarchical parameter sets. For example, if mutation is on, specify mutation rate, otherwise proceed....

- `jumpIfFalse`: The same as `jump` but jump if current parameter is false.

With all these information at hand, the rest is routine, if you follow the coding conventions.

# Operator and Function References

This chapter will list all functions, types and operators by category.

## 7.1 Library-dependent functions/constants

Several functions and constants are defined for each library

- `alleleType()`: return 'binary', 'short', or 'long'.
- `MaxAllele`: 1 for binary libraries, usually 255 for short libraries and  $2^{32} - 1$  for long libraries. Note that this number for short and long libraries might change on different platforms.
- `simuVer()`: return 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 became available.

## 7.2 `carray` type

The return value of simuPOP functions that start with `arr` is of a special python type `carray`. This object reflects the underlying C/C++ array and you can read/write array element just as a regular list. Only a small subset of list member functions, `count`, `index` to be exact, are available. This is because you are not allowed to change the size of underlying C/C++ vector. The following is the operations allowed:

```
# 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
str(arr)
# count
arr.count(2)
# index
arr.index, 2)
# can read write
arr[0] = 0.5
# convert to list
arr.tolist()
# or simply
```

```

list(arr)
# compare to list directly
arr == [0.5, 1.0, 3.0, 3.5, 5.0, 6.0, 7.0]
# you can also convert and compare
list(arr) == [0.5, 1.0, 3.0, 3.5, 5.0, 6.0, 7.0])
# slice
arr[:] = [1,2,3,4,5,6,7]
# arr1 is 1,2,3
arr1 = arr[:3]
# assign slice from a number
# IMPORTANT NOTE that arr will also be affected
# since arr1 point to a part of arr
arr1[:] = 10
# assign vector of the same length
arr1[:] = [30,40]
# assign from another part
arr[1:3] = arr[3:5]

```

No other operation is allowed.

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

## 7.3 Use of R (RPy) in Python

Most of the info can be found in rpy manual. One function in `simuRPy` may help though:

```

def rmatrix(mat):
    ' convert a python 2d list to r.matrix object'
    return with_mode(NO_CONVERSION, r.do_call)('rbind',mat)

```

with this function, you can easily handle matrices in R. (List and array has been easy enough to be handled).

```

>>> a = [[1,2],[4,5]]
>>> r.image( rmatrix(a))

```

With the help of this function, you can call almost any R function directly, maybe except some R-only syntax like formula, expression etc. In this case, you can always do

```

>>> r("'whatever R expression'")

```

Since `Rpy` is not always available, you may see the following scenario again and again in `simuPOP` scripts:

```

try:
    from simuRPy import *
except:
    hasRPy = False
else:
    hasRPy = True
...
if hasRPy:
    r.....

```



## 7.4 Operator (Hybrid) pyOperator

This is the single most powerful hybrid operator. Whenever you think that something is too complicated to be done by standard operators, you can do it here in python. This operator accepts a Python function which accepts a population and optionally a parameter. To use this operator, 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. para be ommitted.

- use pyOperator like

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

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

When pyOperator is called, it will simply pass the accepted population to the function. If your function returns False, the simulation will be stopped.

This operator allows implementation of arbitrarily complicated operators, at a cost of efficiency. Of course, 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 frequency.

---

**Example 23** define a python operator

---

---

**Example 24** use of python operator

---

Note that

- Currently, pyOperator does not support parameter output and outputExpr. This is because of the incompatibility between the Python way and underlying C++ way of handling file I/O stream. Consequently, you will have to handle file input/output by yourself through param parameter. Be careful that you **can not** mix output of pyOperator with those of other (normal) operators.
- If parameter param is ignored, myOperator must be without para as well. Note that you can pass arbitrary number of parameters by putting them into a tuple and pass to myOpeartor .
- Since you can attach any information to a population, you can in practise use pop.dvars( ) to pass parameters.
- pyOperator is a post-mating operator by default. Remember to use stage parameter to change this when necessary.

pyOperator can also be a DuringMating 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)
```

The two additional parameters are:

- `formOffGenotype`: (default to `False`) By default, a mating scheme will set the genotype of offspring by copy one of the parental chromosomes. However, if `formOffGenotype` is true, the mating scheme will let you do the job. You will have to set offspring genotype and sex by yourself.
- `passOffspringOnly`: In case that your function will only deal with offspring, you can set this parameter to true and use a shorter form of the function.

Note that if your `duringMating` `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 big.

An example of `duringMating` `pyOperator` can be found in `scripts/demoPyOperator.py`.

## 7.5 Initialization

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 genotype, and the last one calls a user-defined function.

### 7.5.1 Operator (C++) `initByFreq`, function `InitByFreq`

`initByFreq` operator accepts `alleleFreq` or `alleleFreqs`. The first one ignores subpopulation structure while the second one gives different initial allele frequencies to different subpop or ranges. These parameters are

- `subPop`: specifies applicable subpopulations. If `alleleFreqs` are given, `alleleFreqs` should have the same length as `subPop`. (One freq each `subPop`)
- `indRange`: range(s) of absolute index of individuals. I.e., one `([1, 2])` or more `([ [1, 4], [5, 6] ])` ranges are acceptable. 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. (Note that some earlier versions of `simuPOP` may use `[4,6]` for 4,5 and 6. I changed this to let the range specification in line with the Python convention.)
- `atLoci`: loci at which initialization will be done.
- `maleFreq`: initialize sex with this male frequency.
- `identicalInds`: if true, copy the genotype of the first randomly initialized individual to other individuals in the subpop/range.

---

**Example 25** Init by freq

---

Here is an example of using `alleleFreq`:

Please refer to `test/test_init.py` for more complicated examples.

### 7.5.2 Operator (C++) `initByValue`, function `InitByValue`

`initByValue` operator gets the one copy of chromosomes or the whole genotype (or of those corresponds to `atLoci`) of an individual and copy them to all or subset of individuals.

---

**Example 26** Init by value

---

Parameters `subPop`, `indRange`, `atLoci`, `maleFreq` are also supported. Note that

- If `value` is an array of values, it should have the same length as `subpop`, `indRange` or `proportions`.
- `proportions`: if given, assign given genotypes randomly.

### 7.5.3 Operator (C++) `spread`, function `Spread`

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

### 7.5.4 Operator (hybrid) `pyInit`, function `PyInit`

`pyInit` is a hybrid initializer. User should define a function with parameters `allele`, `ploidy` and `subpop` indices, and return an allele value.

---

**Example 27** Init by value

---

## 7.6 Migration

Mating is strictly within subpopulations in `simuPOP` so migrator is the only way to mix genotypes of several subpopulations. 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 subpop `b`.
  - In the last case, a given number of individuals will migrate.

- New subpopulation can be generated through migration. You simply need to migrate to a new subpop number.

Note that overall population size will not change. (Mating schemes can do that). If you would like to keep subpop size after migration, you can use the `newSubPopSize` or `newSubPopSizeExpr` parameter of a mating scheme.

### 7.6.1 Constants: `MigrByProbability`, `MigrByProportion`, `MigrByCount`

Possible values of parameter mode.

### 7.6.2 Operator (C++) `migrator`

`Opertor migrator` is used to migrate from `'fromSubPop'` to `'toSubPop'`. From and to subpop can be a number or an array of subpopulations. The migration probability/rate/counts from `i` to `j` is specified in the rate matrix. The `'fromSubPop'` and `'toSubPop'` are default to all subpopulations.

An detailed example can be found in 'some real examples' -> 'complex Migration Scheme' section.

### 7.6.3 Functions (Python) `migrIslandRates`, `migrStepstoneRates` (`simuUtil.py`)

Migrator is very flexible. It can accept arbitrary migration matrix, from any subset of subpops to any (even new) other subset of subpops. Several functions are defined in `simuUtil.py`, however, for easy use of popular migration models:

- `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`

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

A lot of such functions may be defined later. I guess 2-d stepstone will be the first one?

### 7.6.4 Operator (C++/Hybrid) `pyMigrator`

For evan more complicated migration schemes, you do DIY it using a `pyMigrator`. This operator is not strictly hybrid since it does not call python function. However, it takes a `carray` as subPop id for each individual. `pyMigrator` then complete migration according its content. For example:

Note that

---

**Example 28** pyMigrator

---

- the application sequence of the operators is `initByFreq`, `dumper`, `pyMigrator` and then `dumper` again since its stage is set to `PrePostMating`.
- Usually you will use a `pyEval` operator to re-assign `spID` during evolution.

### 7.6.5 Operator (C++) `splitSubPop`, function `SplitSubPop`

This operator takes parameters

- `which`: which subpopulation to split. If there is no subpopulation structure, use 0 as the first (and only) subpopulation.
- `sizes`: new subpopulation sizes. The sizes should add up to the original subpopulation (subpop `which`) size.
- `proportions`: Optionally, you can specify proportions of new subpops. (easier to use) The proportions should add up to 1.
- `subPopID`: the operator will automatically set new subpop ID to new subpops. You can also specify the IDs.

### 7.6.6 Operator (C++) `mergeSubPops`, function `MergeSubPops`

This operator merges subPopulations `subPops` (the only parameter) to a single subpopulation. If `subPops` are ignored, all subpopulations will be merged.

## 7.7 Mutation

`rate` can be a number (uniform rate) or an array of mutation rates, `atLoci` is defaulted to all loci. The only differences between the following mutators are they way they actually mutate an allele, and corresponding input parameters.

Mutators record the number of mutation events at each loci. You can retrieve this information using

```
mut.mutationCount(locus)
mut.mutationCounts()
```

where `mut` is any mutator and `locus` is locus index.

### 7.7.1 Operator (C++) `kamMutator`, function `KamMutate`

`kamMutator` (K-allele mutator) mutate an allele to another allelic state with equal probability. The specified mutation rate is actually 'probability to mutate' so the mutation rate to any other allelic state is actually  $\frac{r}{K-1}$ , where  $K$  is specified by parameter `maxAllele`. Here is an example of mutation:

---

**Example 29** kamMutator

---

You can also specify states for this mutator. If `states` parameter is given, all alleles must be one of the state and mutation will happen among them. `states` is defaulted to `1-maxAllele`.

### 7.7.2 Operator (C++) `smmMutator`, function `SmmMutate`

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

The following example demonstrate the use of `smmMutator`. Note that although the mutation rate is 1, some allele 1 is not mutated since they can not be mutated to 0. The same will hold for the upper bound `maxAllele` which is defaulted to 99 in this case.

---

**Example 30** `smmMutator`

---

### 7.7.3 Operator (C++/Hybrid) `gsmMutator`, function `GsmMutate`

*Generalized stepwise model* is an extension to stepwise mutation model. In this model, the change in the allelic state is draw 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  $\frac{p}{(1-p)^2}$ .

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

---

**Example 31** `gsmMutator`

---

### 7.7.4 Operator (Hybrid) `pyMutator`, function `PyMutate`

If you can not accomplish your task with the above normal mutator, you can always use this hybrid mutator. Mutation rate etc 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. Here is an example:

---

**Example 32** `pyMutator`

---

### 7.7.5 Operator (C++) `pointMutator`, function `PointMutate`

`pointMutator`, as its name suggest, does point mutation. It is syntax is:

```
pointMutator(atLoci, toAllele, atPloidy=[], inds=[], ...)
```

This mutator will turn alleles at `atLoci` on the first chromosome copy to `toAllele` for individual `inds`. You can specify `atPloidy` to mutate other, or all ploidy copy.

## 7.8 Recombination

Only one recombinator is provided. Recombination events between loci a/b and b/c are independent.

### 7.8.1 Operator (C++) recombinator

This operator takes similar parameters as a mutator. However, because of potentially uneven allelic distance, you should use one of the two parameters:

- `intensity`: intensity of recombination. The actually recombination rate is `intensity*loci distance`.
- `rate`: recombination rate after all `afterLoci`. It can also be an array of recombination rates. Should have length `totNumLoci()` or length of `afterLoci`. The recombination rates are independent of loci distance.
- `afterLoci`: recombine after loci `afterLoci`.
- `maleIntensity`, `maleRate`, `maleAfterLoci`: If you need to specify different recombination model for male and female, you can specify these parameters. In this case, `intensity`, `rate` and `afterLoci` will be treated as female parameters.

The following example forces recombination (with rate 1, an unrealistic value since the maximum recombination rate should be .5) at loci 2,6 and 10. Here I use a `parentsTagger` to mark the parents of each individual so you can (if you have enough patience) see exactly how recombination works.

---

**Example 33** Recombinator

---

Note that if `sexChrom()` is true, there is no recombination between the last chromosome (sex chromosomes XY) of male individuals. This may change later if the exchanges of genes between pseudoautosomal region of XY need to be modeled.

Recombinations after each locus will be recorded. You can retrieve this information through functions

```
rec.recCount(locus)
rec.recCounts()
```

where `rec` is the recombinator, `locus` is locus index.

## 7.9 Selection

### 7.9.1 Mechanism

Genetic selection is tricky to simulate since there are many difference *fitness* values and many different way to apply selection. `simuPOP` employees 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.
- During sexless mating (e.g. `binomialSelection`), 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 to be passed to the next generation.
- During `randomMating`, males and females are separated. Males and females are chosen from their respective groups in the same manner and mate.

It is not very clear that our method agrees with the traditional 'average number of offsprings' definition of fitness. (Note that this concept is very difficult to simulate since we do not know who will determine the number of offsprings if two parents are involved.) We can, instead, look at the consequence of selection in a simpler 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 number of 11 individuals times its probability to be chosen:

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

This is, however, is 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 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`.

## 7.9.2 Operator (C++) `mapSelector`, function `MapSelector`

`mapSelector` implements selection at one locus. User should supply a dictionary (map) of fitness values for each genotype and this selector will set each individual's fitness value according to its genotype.

The following example is a typical example of heterozygote superiority. When  $w_{11} < w_{12} > w_{22}$ , the genotype frequency 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 ( $s_1 = .1, s_2 = .2$ ).

---

### Example 34 map selector

---



### 7.9.3 Operator (C++) `maSelector`, function `MaSelect`

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

- For single-locus, fitness is the fitness for genotype AA, Aa, aa while A stands for wildtype alleles.
- For a two-locus model, fitness is the fitness for genotype

	BB	Bb	bb
AA	$w_{11}$	$w_{12}$	$w_{13}$
Aa	$w_{21}$	$w_{22}$	$w_{23}$
aa	$w_{31}$	$w_{32}$	$w_{33}$

in the order of  $w_{11}, w_{12}, \dots, w_{32}, w_{33}$ .

- For more than two-locus, use a table of length  $3^n$  in a order similar to the two-locus model.

### 7.9.4 Operator (C++) `mlSelector`, function `MlSelect`

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

**SEL\_Multiplicative:**

The fitness is calculated as  $f = \prod_i f_i$ .

**SEL\_Additive:**

The fitness is calculated as  $f = \max(0, 1 - \sum_i (1 - f_i)) = \max(0, 1 - \sum_i s_i)$ .  $f$  is set to 0 when  $f < 0$ . What is added are  $s_i$ , not  $f_i$  directly.

### 7.9.5 Operator (Hybrid) `pySelector`, function `PySelect`

`pySelector` accept a list of susceptibility loci and a Python function. For each individual, this operator will pass the genotypes at these loci (in the form of 0-0, 0-1, 1-0, 1-1 etc where X-Y is locus X - ploidy Y, in case of diploid population) and expect a returned fitness value. This, at least in theory, can accommodate all selection scenarios.

The following example simulate the same scenario as above, with  $s_1 = .2, s_2 = .3$  ( $sop = .6$ ) and a `pySelector`. Note that although alleles at two loci are passed, the `sel` function only uses the first one.

---

**Example 35** python selector

---

## 7.10 Penetrance

Penetrance is the probability that one will have the disease when he has certain genotype(s). Calculation of penetrance is similar to that of fitness. The parameter set is also similar. An individual will be randomly marked as affected/unaffected according to his penetrance value. For example, an individual will have .8 probability to be affected if the penetrance is .8.

Penetrance can be applied at any stage. The default stage is `DuringMating`. The penetrance will be calculated and affected status is set for each offspring during mating. You can also use penetrance as `PreMating`, `PostMating` or even `PrePostMating` operator. In these cases, affected status will be set to all individuals according to their penetrance value. It is also possible to use `exposePenetrance` parameter to set an array penetrance in these cases. This is useful to actually have a look at penetrance values and see if the values are as expected.

Affected status will be used for statistical purpose, and most importantly, ascertainment. They will be calculated along with fitness although they might not be used at every generation. You can use two operators: one for fitness/selection, active at every generation; one for affected status, active only at ascertainment, to avoid unnecessary calculation of affected status.

Penetrance values are used to set the affectedness of individuals, and are usually not saved. If you would like to know the penetrance value, you need to

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

One important note about penetrance functions is that they only apply to the current generation of a population. This is usually not a problem for operators, but if you need to set affected status for a population with ancestral populations, you should do

```
for i in range(0, pop.ancestralDepth()+1):
    pop.useAncestralPop(i)
    PyPenetrance(pop, ...)
pop.useAncestralPop(0)
```

### 7.10.1 Operator (C++) `mapPenetrance` (post, during-Mating), function `MapPenetrance`

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

```
mapPenetrance(locus=1, penetrance={'1-1':0, '1-2':0.5, '2-2':1})
```

Note that this dictionary can be more than three elements to accommodate more than one disease alleles.

### 7.10.2 Operator (C++) `maPenetrance` (post, during-Mating), function `MaPenetrance`

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

```
maPenetrance(loci=[1,5], wildtype=[1], penetrance=[0,0.5,1,0,0,1,0,1,1])
```

this operator behave the same as the mapPenetrance example but will work if there are more than one disease alleles.

### 7.10.3 Operator (C++) mlPenetrance(post, during-Mating), function MlPenetrance

mlPenetrance is the 'multiple-loci' penetrance calculator. It accepts a list of penetrances and combine them according to the mode parameter which can take the values:

**PEN\_Multiplicative:**

The penetrance is calculated as  $f = \prod f_i$ .

**PEN\_Additive**

The penetrance is calculated as  $f = \min(1, \sum f_i)$ .  $f$  is set to 1 when  $f < 0$ . What is added are  $s_i$ , not  $f_i$  directly.

**PEN\_Heterogeneity:**

The penetrance is calculated as  $f = 1 - \prod (1 - f_i)$ .

Please refer to ? for detailed information about these models.

For example, if each locus follows an additive penetrance model, we can have

```
pen = []
for loc in loci:
    pen.append( maPenetrance(locus=loc, wildtype=[1],
        penetrance=[0.0.3,0.6] ) )
# the multi-loci penetrance
penMulti = mlPenetrance(mode=PEN_Multiplicative, peneOps=pen)
```

### 7.10.4 Operator (Hybrid) pyPenetrance(post, during-Mating), function PyPenetrance

For each individual, user provide a function to calculate penetrance. This method is very flexible but will be slower than previous operators since a function will be called for each individual. This operator accept the following parameters:

- **loci**: disease susceptibility loci. The genotype *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.
- **func**: a user-defined function that takes a array of genotype and return a penetrance value. The returned value should be between 0 and 1.

For example, for the same multi-locus model before, we can define is using pyPenetrance as

```
def peneFunc(geno):
    p = 1
```

```

for l in range(len(geno)/2):
    p *= (geno[l*2]+geno[l*2+1]-2)*0.3
return p
penMulti = pyPenetrance(loci=loci, func=peneFunc)

```

As you can see, using this operator, you can define arbitrarily complex penetrance functions. Typical such penetrance functions are interaction between loci (using a multi-locus penetrance table), even random ones.

It would be useful to let peneFunc take parameters. This can be done by defining a python function that return a penetrance function. This may sound intimidating but it is really easy:

```

def peneFunc(table):
    def func(geno):
        return table[geno[0]-1][geno[1]-1]
    return func
# then, given a table, you can do
pen = pyPenetrance(loci=loci, func=peneFunc( ((0,0.5),(0.3,0.8)) ))

```

Now, for any table, you can use peneFunc to return a penetrance function that uses this table.

## 7.11 Quantitative Trait

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.

The following operators/functions calculate quantitative traits for each individual and store the values in an array QT. Because migration, mating etc will change individual order, the values in QT should be used soon after they are calculated.

### 7.11.1 Operator (C++) mapQuanTrait, function MapQuanTrait

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

### 7.11.2 Operator (C++) maQuanTrait, function MaQuanTrait

maQuanTrait is called 'multiple-alleles' quantitative trait. It separate alleles into two groups: wildtype and disease alleles. wildtype alleles are specified by parameter wildtype and any other alleles are considered as diseased allele. maQuanTrait accepts an array of fitness as described before. Quantitative trait is then set for any given genotype.  $N(0, \sigma^2)$  will be added to returned trait value.

### 7.11.3 Operator (C++) mlQuanTrait, function MlQuanTrait

mlQuanTrait is the 'multiple-loci' QT calculator. It accepts a list of QuanTraits and combine them according to the mode parameter which can take the values:

QT\_Multiplicative:

The mean of quantitative trait is calculated as  $f = \prod f_i$ .

QT\_Additive:

The mean of quantitative trait is calculated as  $f = \sum f_i$ .

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

$$f = \sum_i (f_i + N(0, \sigma_i^2)) + \sigma^2$$

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

#### 7.11.4 Operator (Hybrid) `pyQuanTrait`, function `PyQuanTrait`

For each individual, user provide a function to calculate quantitative trait.

### 7.12 Ascertainment (subset of population)

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

Individuals in sampled populations may or may not keep their original order. Please check each sampling scheme for details.

Most of the ascertainment operators support the following options:

- `times`: how many times to sample from the population.
- `name`: name of samples in local namespace. This variable is an array of populations of size `times`. Default to `sample`. If `name=""` is set, samples will not be saved in local namespace.
- `saveAs, format`: filename and format to save the samples.
- `nameExpr, saveAsExpr`: expression version of parameter `name` and `saveAs`. They will be dynamically evaluated in population's local namespace.

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

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

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

#### 7.12.1 function `population::shrinkByIndID()`

This function look at the `subPopID()` field of each individual and remove anyone with value 0.

### 7.12.2 Operator (C++) `pySubset`, function `PySubset`

This operator shrink a population according to a given array or the `subPopID()` value of each individual. Subpopulations are kept intact.

### 7.12.3 Operator (C++/hybrid) `pySample`, function `PySample`

`PySample(pop, info, name, saveAs, format)` or `Sample(pop)` if you already set info for each individual using `setSubPopID()` function. The operator version of these functions are `pySample(info, times, name, nameExpr, saveAs, saveAsExpr, format)`.

### 7.12.4 Operator (C++) `randomSample`, function `RandomSample`

`RandomSample(pop, size, times, name, saveAs, format)` will randomly choose size individuals (or sizes from subpopulations) and return a new population. The operator version is `randomSample(size, times, name, nameExpr, saveAs, saveAsExpr, format)`.

The function form returns the samples directly. The operator keeps samples in an array name in local namespace. You can access them through `dvars()` or `vars()` functions.

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

### 7.12.5 Opeartor (C++) `caseControlSample`, function `CaseControlSample`

`CaseControlSample(pop, cases, controls, times, name, saveAs, format)` will randomly choose cases affected individuals and controls unaffected individuals. The operator version of this function is `caseControlSample(case, cases, control, controls, times, name, nameExpr, saveAs, saveAsExpr, format)`. The affected status is usually set by penetrance function/operators. The sample populations will have two subpopulations: cases and controls.

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

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

The following example shows how to draw a random sample (without replacement of course) from an existing population.

---

**Example 36** random sample

---

### 7.12.6 Operator (C++) `affectedSibpairSample`, function `AffectedSibpairSample`

The use of this operator needs special preparation for the population. Obviously, to obtain affected sibpairs, we need to know the parents and the affectedness tatus of each individual. Furthermore, to get parental genotype, the population should have `ancestralDepth` at least 1. The biggest 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 offsprings with different parents. On the otherhand, it is very unlikely that two offsprings will have the same parents. The probability

of having a sibling for an offspring is  $\frac{1}{N^2}$  (do not consider selection). Therefore, we will have to allow multiple offsprings per mating at the cost of smaller effective population size.

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

```
endGen = 1000
# having two offsprings only at the last three generations
def numOffsprings(gen):
    if gen >= endGen - 3:
        return 2
    else:
        return 1
# evolve ...
simu = simulator(pop, randomMating(numOffspringsFunc = numOffsprings))
simu.evolve( ...
    parentsTagger(begin = endGen - 3),
    mapPenetrance(..., begin = endGen - 2),
    setAncestralDepth(1, at = endGen - 2 )
...)
```

to let your population evolve *normally* and start to store ancestral generations and allow multiple offsprings at the last several generations.

Briefly, you should

- set ancestral depth to at least 1 to allow analyzing of parental generation,
- use parentsTagger to track parents for each individual, with the usual limit of no post-mating migration, and
- allow multiple offsprings at least at the last generation. (You do not have to use fixed number of offsprings. Other mating mode like MATE\_GeometricDistribution can also be used.)
- use a penetrance operator to set affected status of each individual

and finally use this operator (or function)

```
affectedSibpairSample(size, times, name, saveAs, format)
```

to get samples accessible from `dvars().name[i]`. Each sample will

- have  $2 \times \text{size}$  of paired individuals. (e.g. `individual(2n)` and `individual(2n+1)`,  $n=0,1,\dots,\text{size}-1$  are siblings.
- have an ancestral generation of the same size, with parents to the sibpairs.
- if `size` is an array, get `size[sp]` sibpairs from subpop `sp`.

Other than samples name, variable `numSibpairs` will be set to indicate the total number of affected sibpairs in the population. Subpopulation structure will be kept in the samples so you will know how many individuals are drawn from each subpopulation. (This info is also saved in variable `numSibpairs` of each sample.

## 7.13 Statistics Calculation

### 7.13.1 Operator (C++) `stat`, function `Stat`

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

For each statistics, I will list corresponding parameter (of `stat`), variables and mathematics formula if applicable. Note that these statistics are dependent to each other. For example, heterotype and allele frequency of related loci will be automatically calculated if linkage disequilibrium is requested.

#### Population size

- parameter: `popSize=True/False`
- variable:
  - `numSubPop` number of subpopulation
  - `popSize, subPop[sp]['popSize']`
  - `subPopSize`, an array of subpopulation size. Not available for subpopulations.

#### Number of male/female

- parameter: `numOfMale=True/False`
- variable:
  - `numOfMale, subPop[sp]['numOfMale']`
  - `numOfFemale, subPop[sp]['numOfFemale']`

#### Number/proportion of affected/unaffected individuals

- parameter: `numOfAffected=True/False`
- variable:
  - `numOfAffected, subPop[sp]['numOfAffected']`
  - `numOfUnaffected, subPop[sp]['numOfUnaffected']`
  - `propOfAffected, subPop[sp]['propOfAffected']`
  - `propOfUnaffected, subPop[sp]['propOfUnaffected']`

#### Number of distinct alleles at a locus

This is done through the calculation of allele frequency. Therefore, allele frequency will also be calculated if this statistics is requested.

- parameter: `numOfAlleles=[loc1, loc2, ...]` where `loc1` etc are absolute locus indices.
- variable: a carryay of number of alleles for **all loci**. Unrequested loci will have 0 distinct alleles.
  - `numOfAlleles, subPop[sp]['numOfAlleles']`, number of distinct alles at each loci. (Calculated only at requested loci.)



### Allele frequency/count

- parameter: **alleleFreq**=[loc1, loc2, ...] where loc1 etc are loci where allele frequencies will be counted.
- variable: the following carray objects will be set. 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]

### heterozygote frequency/count

- parameter: **heteroFreq**=[loc1,loc2,...]:  
an array of loci to calculate observed heterozygosity and expected heterozygosity.
- variables: array of observed heterozygosity. **heteroNum**[loc][1] is the number of heterozygote 1x,  $x \neq 1$ . Number and frequency (proportion) of heterozygotes are calculated for each allele.

**HeteroNum**[loc] and **HeterFreq**[loc] is the overall heterozygosity number and frequency. I.e., number/frequency of genotype  $xy$   $x \neq y$ . From this number, we can easily derive number of homozygosity.

Variables are:

- **HeteroNum**[loc], **subPop**[sp]['HeteroNum'][loc], overall heterozygote number
- **HeteroFreq**[loc], **subPop**[sp]['HeteroFreq'][loc], overall heterozygote frequency
- **heteroNum**[loc][allele], **subPop**[sp]['heteroNum'][loc][allele]
- **heteroFreq**[loc][allele], **subPop**[sp]['heteroFreq'][loc][allele]

### expected heterozygosity

- parameter: **expHetero**=[loc1, loc2,...]
- Expected heterozygosity
$$h_{exp} = 1 - p_i^2$$
- variable: **expHetero**[loc], **subPop**[sp]['expHetero'][loc]

### homozygosity frequency/count

- parameter: **homoFreq**=[loc1, loc2, ...]
- Number and frequency of homozygotes  $xx$ .
- variable: **homoNum**[loc], **homoFreq**[loc], **subPop**[sp]['homoNum'][loc], **subPop**[sp]['homoFreq'][loc]

## genotype frequency/count

- parameter:
  - **genoFreq**=[**loc1**,**loc2**,...]: an array of loci to calculate genotype frequency. All genotypes in the population will be counted.
  - **hasPhase**: if a/b and b/a are the same genotype. default is True.
- variables: Dictionary variables **genoNum**, **genoFreq**, **subPop**[**sp**]['**genoNum**'], **subPop**[**sp**]['**genoFreq**'] will be set. Note that the index **a**, **b** of **genoFreq**[**a**][**b**] are dictionary keys (unlike list used for **alleleFreq** etc) so you will get **KeyError** when you use a wrong key. **genoNum.setdefault(a, {})** is preferred.
  - **genoNum**[**a**][**geno**], **subPop**[**sp**]['**genoNum**'] [**a**][**geno**]
  - **genoFreq**[**a**][**geno**], **subPop**[**sp**]['**genoFreq**'] [**a**][**geno**], number/frequency of genotype **geno** at allele **a**. **geno** has the form **x-y**.

## haplotype frequency

- parameter: **haploFreq**: a matrix of haplotypes (allele sequence on the 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.
- variable: Dictionary variables **haploNum**, **haploFreq**, 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**], **subPop**[**sp**]['**haploNum**'] [**haplo**]
  - **haploFreq**[**haplo**], **subPop**[**sp**]['**haploFreq**'] [**haplo**], number/frequency of allele sequences on loci **haplo**.

## Linkage disequilibrium

- parameter:  

```
LD: LD = [ [1,2], [ 0,1,1,2],[1,2,1,2]]
```

For each item [**loc1**, **loc2**, **allele1**, **allele2**], **D**, **D'** and **r<sup>2</sup>** 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,

$$\begin{aligned} D &= P_{AB} - P_A P_B \\ D' &= D / D_{max} \\ D_{max} &= \begin{cases} \min(P_A(1 - P_B), (1 - P_A)P_B) & \text{if } D > 0 \\ \min(P_A P_B, (1 - P_A)(1 - P_B)) & \text{if } D < 0 \end{cases} \\ r^2 &= \frac{D^2}{P_A(1 - P_A)P_B(1 - P_B)} \end{aligned}$$

If  $A$  and  $B$  are not specified,  $D$ ,  $D'$  and  $r^2$  will be the averaged value: (basically  $\sum \sum P_A P_B ||$ )

$$D = \sum_i \sum_j P_i P_j |D_{ij}|$$

$$D' = \sum_i \sum_j P_i P_j |D'_{ij}|$$

$$r^2 = \sum_i \sum_j P_i P_j r_{ij}^2 = \sum_i \sum_j \frac{D_{ij}^2}{(1 - P_i)(1 - P_j)}$$

where  $p_i$  and  $q_j$  are the population allele frequencies of the  $i$ th allele on loc1 and the  $j$ th allele on loc2. Please note that some other authors uses

$$r^2 = \sum_i \sum_j \frac{D_{ij}^2}{P_i P_j}$$

If you are sure the later is correct, please send me an email (with reference).

- variables:

if loc1 and loc2 are specified. The values are LD measures averaged over all possible allele pairs. If al1 and al2 are specified, these values are calculated using these two alleles.

```
- ld['loc1-loc2']['al1-al2'], subPop[sp]['ld']['loc1-loc2']['al1-al2']
- ld_prime['loc1-loc2']['al1-al2'], subPop[sp]['ld_prime']['loc1-loc2']['al1-al2']
- r2['loc1-loc2']['al1-al2'], subPop[sp]['r2']['loc1-loc2']['al1-al2']
- 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]
```

Please note the difference between the datastructure used for ld and LD. The names are potentially very confusing but I have no better idea.

$F_{st}$

- parameter: **Fst**: **Fst** = [0,1,2], calculate  $F_{st}$ ,  $F_{is}$ ,  $F_{it}$  based on alleles at locu 0, 1, 2 respectively. The locus-specific values will be used to calculate AvgFst etc. Terms and values that match ?.

- $F$  ( $F_{IT}$ ): 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 population as a whole)
- $f$  ( $F_{IS}$ ): the correlation of genes within individuals within populations. Populations refers to subpopulations in simuPOP term.

- variables:

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

## Relatedness

The relatedness values between two individuals, or two groups of individuals are calculated according to ? and ?. The first one is referred to as `method=REL_Queller` and the second one is `method=REL_Lynch`. The parameters are

- `relGroups`: can be in the form of either `[[1,2,3],[5,6,7],[8,9]]` or `[2,3,4]`. The first form specifies groups of individuals, the second form specifies subpopulations. By default, relatedness between subpopulations are calculated.
- `relLocs`: calculate relatedness values based on `relLocs` loci.
- `relMethod`: either `REL_Queller` or `REL_Lynch`

The results are pairwise relatedness values, in the form of a matrix. Original group or subpopulations numbers are discarded.

- `relatedness[grp1][grp2]` is the relatedness value between `grp1` and `grp2`. There is no subpop level relatedness values.

## 7.14 Expression and Statements

### 7.14.1 Operator (C++) `output`

This operator output a simple string. For example,

```
output(r'\n', rep=REP_LAST)
```

output a newline at the last replicate.

### 7.14.2 Operator (Python) `tab` (defined in `simuUtli.py`)

Output a tab. (Wrapper of output operator)

### 7.14.3 Operator (Python) `endl` (defined in `simuUtli.py`)

Output a new line. (Wrapper of output operator)

### 7.14.4 Operator (hybrid) `pyEval`, function `PyEval`

We have seen the `expr` and `stmts` parameter of `pyEval`. These are python expression/statements that will be executed when `pyEval` is applied to a population. Statements can also be executed when `pyEval` is created and destroyed. The corresponding parameters are `preStmts` and `postStmts`. For example, operator `varPlotter` uses this feature to initialize R plot and save plot to a file when finished.

### 7.14.5 Operator (hybrid) `pyExec`, function `PyExec`

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

### 7.14.6 Function (Python) `ListVars` (defined in `simuUtil.py`)

`ListVars(variable)`

This function list any variable in an indented text format. You can use `listVar(simuVars)` to have a look at all replicates or `listVar(simuVars[0]['subPop'][0])` to see variables for the first subpoulation in replicate one.

## 7.15 Visualization

There is no special visualizer (there was indeed a `matlabPlotter` before ver 0.5.9 but I decide to remove it since matlab is not universally available.) Since everything is exposed dynamically, all you need to do is plotting variables in whatever way you prefer. The basic steps are:

- find an appropriate tool. I prefer R/Rpy to any other tools since I am familiar with R. You can make your own choice.
- write a function to plot variable. If you would like to plot history of a variable, you can use the `Aggregator` object defined in `simuUtil.py`.
- wrap this function as an operator.

`simuRPy.py` provides a pure Python operator `varPlotter`. It is defined in `simuSciPy` and `simuMatPlt.py` as well but they are lack of subplot capacity (so the usages are different) due to the limit of SciPy/gplt and Matplotlib's plotting capacity. Also note as of Apr, 2006, the development of gplt in scipy is stopped so support of `simuPOP/simuSciPy` is stopped as well.

### 7.15.1 Operator (Python) `varPlotter` (`simuRPy.py`)

The use of `varPlotter` is easy, if you would like to

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 of 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 paramter `mfrow` to change the layout.

- if you would like to plot each item of your array variable in a subplot, use

```
varPlotter(var='expr', varDim=len, byVal=1)
```

in case of a single replicate or

```
varPlotter(var='expr', varDim=len, byVal=1, numRep=nr)
```

There will be numRep lines in each subplot

### Plotting without history

- use option `history=False`. Parameters `byVal`, `varDim` etc will be ignored.

Other options are

1. `title`, `xtitle`, `ytitle`: title of your figure(s). title is defaulted to your expression, xtitle is defaulted to generation.
2. `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.
3. `update`: update figure after `update` calls. This is used when you do not want to update the figure too often, maybe for efficiency purpose.
4. `saveAs`: save figures in files `saveAs#gen.eps`. For example, if `saveAs='demo'`, you will get files `demo1.eps`, `demo2.eps` etc.
5. `separate`: plot data lines in separate panel.
6. `image`: use R image function to plot image, instead of lines.
7. `level`: level of image colors. default to 20
8. `leaveOpen`: whether or not leave the plot open when plotting is done. Default to true.

Here is an example:

## 7.15.2 plot through python/SciPy/Matplotlib

`varPlotter` is also available for SciPy/Matplotlib but there is no subplots (so no `byVal` etc) and the usage is different. The `__init__` function of `varPlotter` takes the following parameters:

- `win` window size. Actually the number of generations to display. default to 0 (no limit). If this is set to be a positive number, only the last win data will be displayed.
- `update` generations between successive re-draw of figure. We can not use 'step' parameter of `pyEval` operator since we need to collect data at each generation.
- `title`, `xtitle`, `ytitle` titles/labels to be displayed
- `legend` an array of strings, legend of the lines. If ignored, "var0", "var1" etc will be used. If gives only one string (e.g, str), "str", "str1",... etc will be used. Otherwise, the length of legend has to be the same as data size.

### 7.15.3 Object (Python) `freqPlotter` (defined in `simuRPy.py`)

The plotting function used for Reich's simulation, using R as plotting engine. It is put in `simuRPy.py` mainly for demonstration purposes.

## 7.16 Tagging (used for pedigree tracking)

### 7.16.1 Operator (C++) `inheritTagger`, `duringMating`

This during-mating operator will copy the tag info from his/her parents. Depending on

- `mode = TAG_Paternal`
- `mode = TAG_Maternal`
- `mode = TAG_Both`

this tagger will obtain tag from his/her father (two tag fields), mother (two tag fields) or both (first tag field from both). You can check the tagger test under `test` directory for an example.

An example may be tagging one or a few parents and see, at the last generation, how many offspring they have.

### 7.16.2 Operator (C++) `parentsTagger`, `duringMating`

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

## 7.17 Data collector

Sometimes, instead of output data directly, we may want to collect history data on some expression. Data collector is designed for this purpose.

### 7.17.1 operator (Python) `collector`, in `simuUtil.py`

This operator accepts the following parameters:

- `name`: name by which the collected data will be displayed. Variable name will be list of stored values. (generation is not stored. You can always put it in `expr` though.)
- `expr`: an expression that will be evaluated. The result will be converted to a list (if needed) and stored in `name[gen]`.

When this operator is called, it will evaluate `expr` and store its result in `name[gen]`. After evolution, you will get a dictionary of values indexed by generation number.

## 7.18 Output

7.18.1 operator (C++) `savePopulation`

7.18.2 function (Python) `SaveFstat` (in `simuUtil.py`)

7.18.3 operator (Python) `saveFstat` (in `simuUtil.py`)

7.18.4 function (Python) `loadFstat` (in `simuUtil.py`)

## 7.19 Terminator

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

7.19.1 Operator (C++) `terminateIf`

This operator terminates the evolution under certain conditions. For example,

```
terminateIf(condition='alleleFreq[0][1]<0.05', begin=100)
```

terminate 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 an `stat` operator before it so that variable `alleleFreq` exists in the local namespace.

7.19.2 Operator (C++) `continueIf`

The same as `terminateIf` but continue if the condition is true.

## 7.20 Conditional operator

7.20.1 Operator (C++) `ifElse`

`ifElse` is an interesting operator. It accepts:

- an expression that will be evaluated when `ifElse` is called.
- 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 depend on its value, apply the supplied operators. Note that the `begin`, `at`, `step`, `at` parameters of if/else operators will be ignored. For example, you can mimic the `at` parameter of an operator by

```
ifElse('rep in [2,5,9]', operator)
```

Anyway, the real use of this mechanism is monitoring the population statistics and act accordingly. The following example uses some advanced operators of `simuPOP`:



- set affected status using `maPenetrance` as a `DuringMating` operator. (`penetrance` can be used at other stages)
- count the number of affected individuals. Note that this has to be done after the `penetrance` operator is applied.
- If no one is effected, inject some mutations into the population. Note the use of `ifElse` operator.
- expose individual affectedness to local namespaces. Note the use of `exposePop` option. With this, you can call any population member function.
- plot affectedness, use `image`.
- Use `dryrun` to exam simulator first.

---

**Example 37** Conditional operator
 

---

## 7.21 Miscellaneous

### 7.21.1 Operator: (C++) `noneOp`

This operator does nothing. It is used like follows:

```
if savePop :
    saveOp = savePopulation(output='a.txt')
else:
    saveOp = noneOp()
simu.evolve( [ ... saveOp ])
```

### 7.21.2 Operator: (C++) `pause`

This operator will pause the simulation and wait for user response. User can use 'q' to stop evolution, 's' to escape to a python shell, or any other key to continue.

There are two ways to use this operator, the first one is to pause the simulation at specified generations, using the usual operator parameters like `at`. Another way is to pause a simulation with any key stroke, using the `stopOnKeyStroke` parameter. This feature is useful for presentation and 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 controled by parameter `exposePop` and `popName`. This feature is useful when you want to examine the properties of a population during evolution.

### 7.21.3 Operator: (C++) `ticToc`, function `TicToc`

This operator, when called, output the difference between current and 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 measuing duration between several generations (set `step` parameter.)

### 7.21.4 Operator: (C++) `setAncestralDepth`, function `pop.setAncestralDepth`

`setAncestralDepth` set the number of ancestral generations to keep in a population. This is useful when constructing pedigree trees from a population.

## 7.22 Random Number Generator

Random number generator is a tricky business. Reliable and fast RNGs are hard to find and everyone seems to trust/distrust certain RNGs. To avoid such arguments, I have included all RNGs from GSL (The GNU Scientific Library <http://sources.redhat.com/gsl/>) and you can choose any of the 61 RNGs, if you really know what the differences between them. (I do not, except that some of them are really bad but fast.) Note that RNG that can not generate a full range of integers are removed.

---

### Example 38 Random number generator

---

If you need to use a random number generator in your `pyEval` operator, you can either use python random module (`import random`) or use `rng()` function to get the random number generator of `simuPOP`. Note that `rng()` does not have many member functions and it might be tricky to use them correctly. (This object is not designed to be used at the Python level. For a full list of member functions, check `src/utility.h`)

---

### Example 39 Random number generator

---

Since `simuPOP` 0.7.1, RNGs are seeded in the following order:

- use random number from `/dev/urandom` if it is available
- use random number from `/dev/random` if it is available
- use python expression `(random.randint(0, sys.maxint) + int(time.time())) % sys.maxint`. This method is used only when `simuPOP` is first loaded so if you are going to set random number generator by yourself, the relevant code in `simuPOP.py` is recommended.

The seed can also be retrieved using `rng().seed()` function, which should be saved for serious simulations.

## 7.23 Debug-related operators/functions

Standard `simuPOP` library can print out lots of debug information upon request. These are mostly for internal debugging use 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 info:

```
>>> 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 create a persistent population object:

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

If the output is overwhelming after you turn on all debug info, you can turn on certain part of the info by using the following functions:

- `ListDebugCode()` list all debug code.
- `turnOnDebug()`, `TurnOnDebug(code)` turn on a debug code
- `turnOffDebug()`, `TurnOffDebug(code)` turn off debug code

`turnOnDebug()` and `turnOffDebug()` are operators and accept all operator parameters `begin`, `step` etc. Usually, you can `turnOnDebug` before `simuPOP` starts to misbehave to output more info about a potential bug.

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 when `DBG_PROFILE` is suitable for measuring individual operator performance. If you would like to measure execution time of all operators in several generations, `ticToc` operator is better.



# Extending simuPOP

simuPOP can be extended easily using Python programming language. Because almost all data are exposed to the python interface, your ability of extending simuPOP is unlimited. However, because Python is slower than C++ and the exchange of data between internal C++ data structure and python interface may be costly, it is not recommended to write frequently used operators in python. Appropriate pure python operators are visualizers, statistics calculator, file outputers etc.

To write smuPOP extension, you will have to know more data structure and member functions of population. Note that for efficiency and implementation reasons, many of the following functions do not provide keyword parameters.

## 8.1 Genotypic structure

The genotypes of an individual are organized as a single array. For example, if you have an diploid individual with two chromosomes, having 2 and 3 loci respectively. The genotypes should be in the order of

0-0-0, 1-0-0, 0-1-0, 1-1-0, 2-1-0, 0-0-1, 1-0-1, 0-1-1, 1-1-1, 2-1-1

where X-X-X are locus-chromosome-ploidy indices. An important consequence of this arrangement is that 'locus location' + 'total number of loci' is the location of the locus on the other set of chromosomes.

Several functions are provided to retrieve genotypic info:

- `ploidy()`
- `numChrom()`
- `numLoci(chrom)`, number of loci on chromosome `chrom`
- `totNumLoci()`
- `genoSize()`, size of genotype. Equals to `totNumLoci()*ploidy()`
- `alleleName()`, if not specified by `alleleNames` parameter when creating a population, return allele number
- `locusPos(loc)`, locus position on chromosome (Distance to the beginning of chromosome)
- `arrlociPos()`, return an `carray` of the loci distance.

The last function is very interesting. It actually return the reference of the internal loci distance array. If you change the value of the returned array, the internal loci distance will be changed! All functions with this property will be named `arrFunc()`.

The following example shows how to change locus distance through this function.

## 8.2 Accessing genotype and other info

Genotype of an individual can be retrieved through the following functions

- `ind.allele(index, p=0)`
- `ind.setAllele(value, index, p=0)`
- `ind.arrGenotype(p=0, ch=0)`

`p` means ploidy. I.e., the index of copies of chromosomes. `ch` means chromosome. For example

```
pop.individual(1).arrGenotype(1, 2)
```

returns an array of alleles on the third chromosome of the second copy of chromosomes, of the second individual in the population `pop`.

---

**Example 41** genotype

---

Sex, affected status can be accessed through `sex`, `setSex`, `affected`, `setAffected` functions.

---

**Example 42** genotype

---

### 8.2.1 Direct populaiton manipulation

FIXME

## 8.3 Writing Pure Python Operator

Now we know how to access information for individuals in a population, but how can we use them in reality? Namely, how can you write an pure Python operator?

### 8.3.1 Use `pyOperator`

There are two kinds of pure python operators. The first one is easy: define a function and wrap it with a `pyOperator` operator. This method is highly recommended because of its simplicity. Many user scripts will use this kind of pure python operator. You can find such examples in `scripts` directory. A good one may be `simuCDCV.py` where a pure python operator is used to calculate and visualize special statistics.

For example, if you would like to record a silly statistics, namely the genotype of the  $m$  individual at locu  $n$ , you can do:

```

def sillyStat(pop, para):
    # para can be used to pass any number of parameters
    (filename, m, n) = para # unpack parameter
    f = open(filename)
    f.write('%d ' % pop.individual(m).allele(n) )
    f.close()
# then in the evolve function
evolve(...)
    ops=[ # other operators
        pyOperator(func=sillyStat, param=('file.txt', 2, 1) )
    ]
)

```

`pyOperator` is by default a post-mating operator, you can redefine its stage by stage parameter.

### 8.3.2 Use Python eval function

This kind of pure python operator acts more like an ordinary operator. They are usually `pyEval` or `pyExec` operators returned by a wrapper function. For example, the following function defines a `tab` operator:

---

#### Example 43 Tab operator

---

This function actually returns an operator

```
output(r"\t", rep=REP_LAST, begin=500)
```

This kind of operators have some advantages, namely

- it acts more like ordinary operator.
- it is more efficient since it is handled (at least the first layer) by a C/C++ operator.

However, because of its complexity, such operators can only be found in system libraries. You can ignore the rest of this section if `pyOperator` is enough to you.

To define a pure python operator, here is what you will generally do:

- Write a function that act on a population. This function should be able to be called like `func(simu.population(0))` .
- Wrap this function as an operator.

For example, function `saveInFstatFormat(pop, output, outputExpr, dict)` saves a population in FSTAT format. Its definition is (first 15 lines)

---

#### Example 44 genotype

---

Note that

- You can use this function independently like

```
saveInFstatFormat(simu.population(1), 'a.txt')
```

- `pop.vars()` is used to evaluate `outputExpr`

Then you can wrap this function by an operator, actually a function that returns a `pyEval` operator:

---

**Example 45** save fstat

---

This function takes all parameters of an ordinary operator:

```
saveFstat(at=[-1], outputExpr=r"'a'+str(rep)+'.txt'")
```

and generate a `pyEval` operator (use above example)

```
pyEval(exposePop=1, at=[-1],
        stmts=r""saveInFSTATFormat(pop,
        output="", outputExpr=r"'a'+str(rep)+'.txt'""
    )
```

In this example,

- `pyEval` works in the local namespace of each replicate. To access that replicate of population, you should use the magic paramter `exposePop` of `pyEval`. When set true, `pyEval` will automatically set a variable `pop` in the current local namespace before any statement is executed. This is why we can call `saveInFSTATFormat(pop...)`
- `"'a'"` quotes are used to avoid conflict with quotes in `outputExpr` etc.

.

## 8.4 Ultimate extension: working in C++

It is sometimes desired to write `simuPOP` extension in C++. For example,

- when you need some other mating scheme
- when you need certain operator that a pure Python implementation would be too slow.
- If some aspect of `simuPOP` is too limited (like the number of maximum alleles)

It is not difficult to write `simuPOP` extension in C++, once you know how `simuPOP` is organized. The general procedure is

- install the latest version of SWIG (>1.3.28)
- check out `simuPOP` source using subversion
- build from source and see if your programming environment works well
- to add an operator, make changes in appropriate `.h` file, check `simuPOP_common.i` if your operator can not be used.

The source code is reasonably well commented with full doxygen based documentation. Please post to the `simuPOP` forum if you encounter any problem while writing operators in C++.



## 8.5 Debugging

### 8.5.1 test scripts

There are many test scripts under the `test` directory. It is recommended that you run the test scripts after you install simuPOP. 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
```

Please report any failed test.

### 8.5.2 Memory leak detection

Python extensions tend to have memory leak problem, caused by the refcount mechanism. If your simuPOP script uses more and more RAM without population size increase, you may have this problem. You may try to disable individual operators and see find out the offending operator if the problem persist.

Potential simuPOP developers can make use of simuPOP's built-in refcount detection mechanism. To use it,

- Compile python with configure option `--with-pydebug` . This will enable `sys.totalrefcount()` etc
- Compile simuPOP with `-DPy_REF_DEBUG`. This can be done in `setup.py`, or better in `SConstruct`.

`simulator.evolve` will check reference count at the end of each generation and report any increased reference count. Some operators may create python object (like ascertainment operators) but if you see repeated warning at each generation, there is definitely a memory leak.



# BIBLIOGRAPHY



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