
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.

simuPOP is written in C++ and is provided as Python modules. It 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/Spplus or Matlab-like environment where users can interactively create, manipulate and evolve populations, monitor and visualize population statistics and apply gene mapping methods. Please refer to the *simuPOP user's guide* for a detailed introduction to simuPOP concepts, and a number of examples on how to use simuPOP to perform various simulations.

This reference manual lists all variables, functions, classes and utility modules of simuPOP. Please report any error to the simuPOP mailing list `simupop-list@lists.sourceforge.net`.

How to cite simuPOP:

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

Bo Peng and Christopher Amos (2008) Forward-time simulations of nonrandom mating populations using simuPOP. *bioinformatics*, **24** (11): 1408-1409.

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Chapter 1

simuPOP Components

1.1 Individual, population and simulator

1.1.1 Class `GenoStruTrait`

All individuals in a population share the same genotypic properties such as number of chromosomes, number and position of loci, names of markers, chromosomes, and information fields. These properties are stored in this `GenoStruTrait` class and are accessible from `individual`, `population`, and `simulator` classes. Currently, a genotypic structure consists of

- Ploidy, namely the number of homologous sets of chromosomes, of a population. Haplodiploid population is also supported.
- Number of chromosomes and number of loci on each chromosome.
- Positions of loci, which determine the relative distance between loci on the same chromosome. No unit is assumed so these positions can be ordinal (1, 2, 3, ..., the default), in physical distance (bp, kb or mb), or in map distance (e.g. centiMorgan) depending on applications.
- Names of alleles. Although alleles at different loci usually have different names, simuPOP uses the same names for alleles across loci for simplicity.
- Names of loci and chromosomes.
- Names of information fields attached to each individual.

In addition to basic property access functions, this class also provides some utility functions such as `locusByName`, which looks up a locus by its name.

class `GenoStruTrait` ()

A `GenoStruTrait` object is created with the creation of a `population` so it cannot be initialized directly.

`ploidy` ()

Return the number of homologous sets of chromosomes, specified by the *ploidy* parameter of the `population` function. Return 2 for a haplodiploid population because two sets of chromosomes are stored for both males and females in such a population.

`ploidyName` ()

Return the ploidy name of this population, can be one of `haploid`, `diploid`, `haplodiploid`, `triploid`, `tetraploid` or `#-ploidy` where # is the ploidy number.

chromBegin (*chrom*)
Return the index of the first locus on chromosome *chrom*.

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

chromEnd (*chrom*)
Return the index of the last locus on chromosome *chrom* plus 1.

chromName (*chrom*)
Return the name of a chromosome *chrom*. Default to `chrom#` where # is the 1-based index of the chromosome.

chromNames ()
Return a list of the names of all chromosomes.

chromType (*chrom*)
Return the type of a chromosome *chrom* (Customized, Autosome, ChromosomeX, or ChromosomeY).

chromTypes ()
Return the type of all chromosomes (Customized, Autosome, ChromosomeX or ChromosomeY).

numChrom ()
Return the number of chromosomes.

absLocusIndex (*chrom*, *locus*)
Return the absolute index of locus *locus* on chromosome *chrom*. An `IndexError` will be raised if *chrom* or *locus* is out of range. c.f. `chromLocusPair`.

chromLocusPair (*locus*)
Return the chromosome and relative index of a locus using its absolute index *locus*. c.f. `absLocusIndex`.

lociByNames (*names*)
Return the indexes of loci with names *names*. Raise a `ValueError` if any of the loci cannot be found.

lociDist (*locus1*, *locus2*)
Return the distance between loci *locus1* and *locus2* on the same chromosome. A negative value will be returned if *locus1* is after *locus2*.

lociNames ()
Return the names of all loci specified by the *lociNames* parameter of the `population` function. An empty list will be returned if *lociNames* was not specified.

lociPos ()
Return the positions of all loci, specified by the *lociPos* parameter of the `population` function. The default positions are 1, 2, 3, 4, ... on each chromosome.

locusByName (*name*)
Return the index of a locus with name *name*. Raise a `ValueError` if no locus is found. Note that empty strings are used for loci without name but you cannot lookup such loci using this function.

locusName (*locus*)
Return the name of locus *locus* specified by the *lociNames* parameter of the `population` function. An empty string will be returned if no name has been given to locus *locus*.

locusPos (*locus*)
Return the position of locus *locus* specified by the *lociPos* parameter of the `population` function. An `IndexError` will be raised if the absolute index *locus* is greater than or equal to the total number of loci.

numLoci (*chrom*)
Return the number of loci on chromosome *chrom*, equivalent to `numLoci () [chrom]`.

numLoci ()
Return the number of loci on all chromosomes.

totNumLoci()

Return the total number of loci on all chromosomes.

alleleName(allele, locus=0)

Return the name of allele *allele* at *locus* specified by the *alleleNames* parameter of the *population* function. *locus* could be ignored if alleles at all loci share the same names. If the name of an allele is unspecified, its index ('0', '1', '2', etc) is returned. An *IndexError* will be raised if *allele* is larger than the maximum allowed allele state of this module (*ModuleMaxAllele*).

alleleNames(locus=0)

Return a list of allele names at given by the *alleleNames* parameter of the *population* function. *locus* could be ignored if alleles at all loci share the same names. This list does not have to cover all possible allele states of a population so *alleleNames()[allele]* might fail (use *alleleNames(allele)* instead).

infoField(idx)

Return the name of information field *idx*.

infoFields()

Return a list of the names of all information fields of the population.

infoIdx(name)

Return the index of information field *name*. Raise an *IndexError* if *name* is not one of the information fields.

1.1.2 Class individual

A population consists of individuals with the same genotypic structure. An individual object cannot be created independently, but references to individuals can be retrieved using member functions of a *population* object. In addition to structural information shared by all individuals in a population (provided by class *genoStruTrait*), the *individual* class provides member functions to get and set *genotype*, *sex*, *affection status* and *information fields* of an individual.

Genotypes of an individual are stored sequentially and can be accessed locus by locus, or in batch. The alleles are arranged by position, chromosome and ploidy. That is to say, the first allele on the first chromosome of the first homologous set is followed by alleles at other loci on the same chromosome, then markers on the second and later chromosomes, followed by alleles on the second homologous set of the chromosomes for a diploid individual. A consequence of this memory layout is that alleles at the same locus of a non-haploid individual are separated by *individual::totNumLoci()* loci. It is worth noting that access to invalid chromosomes, such as the Y chromosomes of female individuals, are not restricted.

class individual()

An individual object cannot be created directly. It has to be accessed from a *population* object using functions such as *population::individual(idx)*.

allele(idx, ploidy=-1, chrom=-1)

Return the current allele at a locus, using its absolute index *idx*. If a ploidy *ploidy* and/or a chromosome indexes are given, *idx* is relative to the beginning of specified homologous copy of chromosomes (if *chrom=-1*) or the beginning of the specified homologous copy of specified chromosome (if *chrom >= 0*).

setAllele(allele, idx, ploidy=-1, chrom=-1)

Set allele *allele* to a locus, using its absolute index *idx*. If a ploidy *ploidy* and/or a chromosome indexes are given, *idx* is relative to the beginning of specified homologous copy of chromosomes (if *chrom=-1*) or the beginning of the specified homologous copy of specified chromosome (if *chrom >= 0*).

genotype(ploidy=-1, chrom=-1)

Return an editable array (a *carray* of length *totNumLoci()*) that represents all alleles on the *p*-th

homologous set of chromosomes. If *ploidy* or *chrom* is given, only alleles on the *chrom-th* chromosome (or all chromosomes if *chrom* = -1) of *ploidy-th* homologous copy of chromosomes will be returned.

setGenotype (*geno*, *ploidy*=-1, *chrom*=-1)

Fill the genotype of an individual using a list of alleles *geno*. If parameters *ploidy* and/or *chrom* are specified, alleles will be copied to only all or specified chromosome on selected homologous copy of chromosomes. *geno* will be reused if its length is less than number of alleles to be filled.

setSex (*sex*)

Set individual sex to Male or Female.

sex ()

Return the sex of an individual, 1 for male and 2 for female.

sexChar ()

Return the sex of an individual, M for male or F for female.

affected ()

Return True if this individual is affected.

affectedChar ()

Return A if this individual is affected, or U otherwise.

setAffected (*affected*)

Set affection status to *affected* (True or False).

info (*field*)

Return the value of an information field *field* (by index or name).

intInfo (*field*)

Return the value of an information field *field* (by index or name) as an integer number.

setInfo (*value*, *field*)

Set the value of an information field *field* (by index or name) to *value*.

1.1.3 Class population

A simuPOP population consists of individuals of the same genotypic structure, organized by generations, subpopulations and virtual subpopulations. It also contains a Python dictionary that is used to store arbitrary population variables.

In addition to genotypic structured related functions provided by the `GenoStruTrait` class, the population class provides a large number of member functions that can be used to

- Create, copy and compare populations.
- Manipulate subpopulations. A population can be divided into several subpopulations. Because individuals only mate with individuals within the same subpopulation, exchange of genetic information across subpopulations can only be done through migration. A number of functions are provided to access subpopulation structure information, and to merge and split subpopulations.
- Define and access virtual subpopulations. A *virtual subpopulation splitter* can be assigned to a population, which defines groups of individuals called *virtual subpopulations* (VSP) within each subpopulation.
- Access individuals individually, or through iterators that iterate through individuals in (virtual) subpopulations.
- Access genotype and information fields of individuals at the population level. From a population point of view, all genotypes are arranged sequentially individual by individual. Please refer to class `individual` for an introduction to genotype arrangement of each individual.

- Store and access *ancestral generations*. A population can save arbitrary number of ancestral generations. It is possible to directly access an ancestor, or make an ancestral generation the current generation for more efficient access.
- Insert or remove loci, resize (shrink or expand) a population, sample from a population, or merge with other populations.
- Manipulate population variables and evaluate expressions in this *local namespace*.
- Save and load a population.

class population (*size*=[], *ploidy*=2, *loci*=[], *chromTypes*=[], *lociPos*=[], *ancGen*=0, *chromNames*=[], *alleleNames*=[], *lociNames*=[], *subPopNames*=[], *infoFields*=[])

The following parameters are used to create a population object:

size: A list of subpopulation sizes. The length of this list determines the number of subpopulations of this population. If there is no subpopulation, *size*=[*popSize*] can be written as *size*=*popSize*.

ploidy: Number of homologous sets of chromosomes. Default to 2 (diploid). For efficiency considerations, all chromosomes have the same number of homologous sets, even if some customized chromosomes or some individuals (e.g. males in a haplodiploid population) have different numbers of homologous sets. The first case is handled by setting *chromTypes* of each chromosome. Only the haplodiploid populations are handled for the second case, for which *ploidy*=Haplodiploid should be used.

loci: A list of numbers of loci on each chromosome. The length of this parameter determines the number of chromosomes. Default to [1], meaning one chromosome with a single locus.

chromTypes: A list that specifies the type of each chromosome, which can be Autosome, ChromosomeX, ChromosomeY, or Customized. All chromosomes are assumed to be autosomes if this parameter is ignored. Sex chromosome can only be specified in a diploid population where the sex of an individual is determined by the existence of these chromosomes using the XX (Female) and XY (Male) convention. Both sex chromosomes have to be available and be specified only once. Because chromosomes X and Y are treated as two chromosomes, recombination on the pseudo-autosomal regions of the sex chromosomes is not supported. Customized chromosomes are special chromosomes whose inheritance patterns are undefined. They rely on user-defined functions and operators to be passed from parents to offspring. Multiple customized chromosomes have to be arranged consecutively.

lociPos: Positions of all loci on all chromosome, as a list of float numbers. Default to 1, 2, ... etc on each chromosome. *lociPos* should be arranged chromosome by chromosome. If *lociPos* are not in order within a chromosome, they will be re-arranged along with corresponding *lociNames* (if specified).

ancGen: Number of the most recent ancestral generations to keep during evolution. Default to 0, which means only the current generation will be kept. If it is set to -1, all ancestral generations will be kept in this population (and exhaust your computer RAM quickly).

chromNames: A list of chromosome names. Default to "" for all chromosomes.

alleleNames: A list or a nested list of allele names. If a list of alleles is given, it will be used for all loci in this population. For example, *alleleNames*=('A', 'C', 'T', 'G') gives names A, C, T, and G to alleles 0, 1, 2, and 3 respectively. If a nested list of names is given, it should specify alleles names for all loci.

lociNames: A list of names for each locus. It can be empty or a list of unique names for each locus. If loci are not specified in order, loci names will be rearranged according to their position on the chromosome.

subPopNames: A list of subpopulation names. All subpopulations will have name "" if this parameter is not specified.

infoFields: Names of information fields (named float number) that will be attached to each individual.

absIndIndex (*idx*, *subPop*)

Return the absolute index of an individual *idx* in subpopulation *subPop*.

numSubPop ()

Return the number of subpopulations in a population. Return 1 if there is no subpopulation structure.

subPopBegin (*subPop*)

Return the index of the first individual in subpopulation *subPop*. An `IndexError` will be raised if *subPop* is out of range.

subPopEnd (*subPop*)

Return the index of the last individual in subpopulation *subPop* plus 1, so that `range(subPopBegin(subPop), subPopEnd(subPop))` can iterate through the index of all individuals in subpopulation *subPop*.

subPopIndPair (*idx*)

Return the subpopulation ID and relative index of an individual, given its absolute index *idx*.

setSubPopName (*name*, *subPop*)

Assign a name *name* to subpopulation *subPop*. *does* not have to be unique.

subPopByName (*name*)

Return the index of the first subpopulation with name *name*. An `IndexError` will be raised if subpopulations are not named, or if no subpopulation with name *name* is found. Virtual subpopulation name is not supported.

subPopName (*subPop*)

Return the "spName - vspName" (virtual named subpopulation), "" (unnamed non-virtual subpopulation), "spName" (named subpopulation) or "vspName" (unnamed virtual subpopulation), depending on whether subPopulation is named or if *subPop* is virtual.

subPopNames ()

Return the names of all subpopulations (excluding virtual subpopulations). An empty string will be returned for unnamed subpopulations.

popSize ()

Return the total number of individuals in all subpopulations.

subPopSize (*subPop*=[])

Return the size of a subpopulation (`subPopSize(sp)`) or a virtual subpopulation (`subPopSize([sp, vsp])`). If no *subpop* is given, it is the same as `popSize()`.

subPopSizes ()

Return the sizes of all subpopulations in a list. Virtual subpopulations are not considered.

numVirtualSubPop ()

Return the number of virtual subpopulations (VSP) defined by a VSP splitter. Return 0 if no VSP is defined.

setVirtualSplitter (*splitter*)

Set a VSP *splitter* to the population, which defines the same VSPs for all subpopulations. If different VSPs are needed for different subpopulations, a `combinedSplitter` can be used to make these VSPs available to all subpopulations.

indByID (*id*, *ancGen*=-1, *idField*="ind_id")

Return a reference to individual with *id* stored in information field *idField* (default to `ind_id`). This function by default search the present and all ancestral generations (`ancGen=-1`), but you can specify a specific generation if you know which generation to search (`ancGen=0` for present generation, `ancGen=1` for parental generation, and so on). If no individual with *id* is found, an `IndexError` will be raised.

individual (*idx*, *subPop*=[])

Return a reference to individual *idx* in the population (if *subPop*=[], default) or a subpopulation (if *subPop*=*sp*). Virtual subpopulation is not supported.

individuals (*subPop*=[])

Return an iterator that can be used to iterate through all individuals in a population (if *subPop*=[], default), or a (virtual) subpopulation (*subPop*=*spID* or (*spID*, *vspID*)).

genotype (*subPop*=[])

Return an editable array of the genotype of all individuals in a population (if *subPop*=[], default), or individuals in a subpopulation *subPop*. Virtual subpopulation is unsupported.

setGenotype (*geno*, *subPop*=[])

Fill the genotype of all individuals in a population (if *subPop*=[]) or in a (virtual) subpopulation *subPop* (if *subPop*=*sp* or (*sp*, *vsp*)) using a list of alleles *geno*. *geno* will be reused if its length is less than *subPopSize*(*subPop*)**totNumLoci*()**ploidy*() .

ancestor (*idx*, *gen*, *subPop*=[])

Return a reference to individual *idx* in ancestral generation *gen*. The correct individual will be returned even if the current generation is not the present one (see also *useAncestralGen*). If a valid *subPop* is specified, *index* is relative to that *subPop*. Virtual subpopulation is not supported.

ancestralGens ()

Return the actual number of ancestral generations stored in a population, which does not necessarily equal to the number set by *setAncestralDepth*() .

push (*pop*)

Push population *pop* into the current population. Both populations should have the same genotypic structure. The current population is discarded if *ancestralDepth* (maximum number of ancestral generations to hold) is zero so no ancestral generation can be kept. Otherwise, the current population will become the parental generation of *pop*, a the greatness level of all existing ancestral generations by one. If *ancestralDepth* is positive and there are already *ancestralDepth* ancestral generations (see also: *ancestralGens*()), the greatest ancestral generation will be discarded. In any case, population *pop* becomes invalid as all its individuals are absorbed by the current population.

setAncestralDepth (*depth*)

Set the intended ancestral depth of a population to *depth*, which can be 0 (does not store any ancestral generation), -1 (store all ancestral generations), and a positive number (store *depth* ancestral generations. If there exists more than *depth* ancestral generations (if *depth* > 0), extra ancestral generations are removed.

useAncestralGen (*idx*)

Making ancestral generation *idx* (0 for current generation, 1 for parental generation, 2 for grand-parental generation, etc) the current generation. This is an efficient way to access population properties of an ancestral generation. *useAncestralGen*(0) should always be called afterward to restore the correct order of ancestral generations.

addChrom (*lociPos*, *lociNames*=[], *chromName*="", *alleleNames*=[], *chromType*=Autosome)

Add chromosome *chromName* with given type *chromType* to a population, with loci *lociNames* inserted at position *lociPos*. *lociPos* should be ordered. *lociNames* and *chromName* should not exist in the current population. Allele names could be specified for all loci (a list of names) or differently for each locus (a nested list of names), using parameter *alleleNames*. Empty loci names will be used if *lociNames* is not specified.

addChromFrom (*pop*)

Add chromosomes in population *pop* to the current population. Population *pop* should have the same number of individuals as the current population in the current and all ancestral generations. This function merges genotypes on the new chromosomes from population *pop* individual by individual.

addIndFrom (*pop*)

Add all individuals, including ancestors, in *pop* to the current population. Two populations should have the same genotypic structures and number of ancestral generations. Subpopulations in population *pop* are kept.

addLoci (*chrom*, *pos*, *lociNames*=[], *alleleNames*=[])

Insert loci *lociNames* at positions *pos* on chromosome *chrom*. These parameters should be lists of the same length, although *names* may be ignored, in which case empty strings will be assumed. Single-value input is allowed for parameter *chrom* and *pos* if only one locus is added. Alleles at inserted loci are initialized with zero alleles. Note that loci have to be added to existing chromosomes. If loci on a new chromosome need to be added, function `addChrom` should be used. Optionally, allele names could be specified either for all loci (a single list) or each loci (a nested list). This function returns indexes of the inserted loci.

addLociFrom (*pop*)

Add loci from population *pop*, chromosome by chromosome. Added loci will be inserted according to their position. Their position and names should not overlap with any locus in the current population. Population *pop* should have the same number of individuals as the current population in the current and all ancestral generations.

extract (*field*="", *loci*=AllAvail, *infoFields*=AllAvail, *ancGen*=-1, *ped*=None, *pedFields*=[])

Extract subsets of individuals, loci and/or information fields from the current population and create a new population. By default, all genotypes and information fields for all individuals in all ancestral generations are extracted. If an valid (non-empty) information field (*field*) is given, individuals with negative values at this field will be removed and others are put into subpopulations specified by this field. The extracted population will keep the original subpopulation names if two populations have the same number of subpopulations. If a list of loci is specified, only genotypes at specified loci are extracted. If a list of *infoFields* is specified, only these information fields are extracted. If *ancGen* is not -1 (default, meaning all ancestral generations), only *ancGen* ancestral generations will be extracted. As an advanced feature, *field* can be information field of a pedigree object *ped*. This allows extraction of individuals according to pedigrees identified in a pedigree object. Additional information fields from *pedFields* can be copied to the extracted population. This pedigree should have the same number of individuals in all generations.

mergeSubPops (*subPops*=[], *name*="")

Merge subpopulations *subPops*. If *subPops* is empty (default), all subpopulations will be merged. *subPops* do not have to be adjacent to each other. They will all be merged to the subpopulation with the smallest subpopulation ID. Indexes of the rest of the subpopulation may be changed. A new name can be assigned to the merged subpopulation through parameter *name* (an empty *name* will be ignored). This function returns the ID of the merged subpopulation.

recodeAlleles (*alleles*, *loci*=AllAvail, *alleleNames*=[])

Recode alleles at *loci* (default to all loci in a population) to other values according to parameter *alleles*. This parameter can a list of new allele numbers for alleles 0, 1, 2, ... (allele *x* will be recoded to `newAlleles[x]`) or a Python function. In the latter case, each allele and the index of the locus it resides are passed to this function. The return value will become the new allele. A new list of allele names could be specified for these *loci*. Different sets of names could be specified for each locus if a nested list of names are given. This function recode alleles for all subpopulations in all ancestral generations.

removeIndividuals (*inds*)

Remove individual(s) *inds* (absolute indexes) from the current population. A subpopulation will be kept even if all individuals from it are removed. This function only affects the current generation.

removeLoci (*loci*=[], *keep*=[])

Remove *loci* (absolute indexes) and genotypes at these loci from the current population. Alternatively, a parameter *keep* can be used to specify loci that will not be removed.

removeSubPops (*subPops*)

Remove subpopulation(s) *subPop* and all their individuals. Indexes of subpopulations after removed subpopulations will be shifted.

resize (*sizes*, *propagate*=False)

Resize population by giving new subpopulation sizes *sizes*. Individuals at the end of some subpopulations will be removed if the new subpopulation size is smaller than the old one. New individuals will be appended to a subpopulation if the new size is larger. Their genotypes will be set to zero (default), or be copied from existing individuals if *propagate* is set to `True`. More specifically, if a subpopulation with

3 individuals is expanded to 7, the added individuals will copy genotypes from individual 1, 2, 3, and 1 respectively. Note that this function only resizes the current generation.

setSubPopByIndInfo (*field*)

Rearrange individuals to their new subpopulations according to their integer values at information field *field* (value returned by `individual::indInfo(field)`). Individuals with negative values at this *field* will be removed. Existing subpopulation names are kept. New subpopulations will have empty names.

splitSubPop (*subPop*, *sizes*, *names*=[])

Split subpopulation *subPop* into subpopulations of given *sizes*, which should add up to the size of subpopulation *subPop*. If *subPop* is not the last subpopulation, indexes of subpopulations after *subPop* are shifted. If *subPop* is named, the same name will be given to all new subpopulations unless a new set of *names* are specified for these subpopulations. This function returns the IDs of split subpopulations.

addInfoFields (*fields*, *init*=0)

Add a list of information fields *fields* to a population and initialize their values to *init*. If an information field already exists, it will be re-initialized.

indInfo (*field*, *subPop*=[])

Return the values (as a list) of information field *field* (by index or name) of all individuals (if *subPop*=[], default), or individuals in a (virtual) subpopulation (if *subPop*=*sp* or (*sp*, *vsp*)).

setIndInfo (*values*, *field*, *subPop*=[])

Set information field *field* (specified by index or name) of all individuals (if *subPop*=[], default), or individuals in a (virtual) subpopulation (*subPop*=*sp* or (*sp*, *vsp*)) to *values*. *values* will be reused if its length is smaller than the size of the population or (virtual) subpopulation.

setInfoFields (*fields*, *init*=0)

Set information fields *fields* to a population and initialize them with value *init*. All existing information fields will be removed.

updateInfoFieldsFrom (*fields*, *pop*, *fromFields*=[], *ancGen*=-1)

Update information fields *fields* from *fromFields* of another population (or pedigree) *pop*. Two populations should have the same number of individuals. If *fromFields* is not specified, it is assumed to be the same as *fields*. If *ancGen* is not -1, only the most recent *ancGen* generations are updated.

clone ()

Create a cloned copy of a population. Note that Python statement `pop1 = pop` only creates a reference to an existing population *pop*.

save (*filename*)

Save population to a file *filename*, which can be loaded by a global function `LoadPopulation(filename)`.

vars (*subPop*=[])

Return variables of a population as a Python dictionary. If a valid subpopulation *subPop* is specified, a dictionary `vars()["subPop"][subPop]` is returned. A `ValueError` will be raised if key *subPop* does not exist in `vars()`, or if key *subPop* does not exist in `vars()["subPop"]`.

dvars (*subPop*=[])

Return a wrapper of Python dictionary returned by `vars(subPop)` so that dictionary keys can be accessed as attributes.

1.1.4 Class simulator

A *simuPOP* simulator is responsible for evolving one or more replicates of a *population* forward in time, subject to various *operators*. Populations in a simulator are created as identical copies of a population and will become different

after evolution. A *mating scheme* needs to be specified, which will be used to generate offspring generations during evolution. A number of functions are provided to access simulator properties, access populations and their variables, copy, save and load a simulator.

The most important member function of a simulator is `evolve`, which evolves populations forward in time, subject to various *operators*. For convenience, member functions are provided to set virtual splitter, add information field and set ancestral depth to all populations in a simulator.

class `simulator` (*pop*, *matingScheme*, *rep*=1)

Create a simulator with *rep* replicates of population *pop*. Population *pop* will be copied *rep* times (default to 1), while keeping the passed population intact. A mating scheme *matingScheme* will be used to evolve these populations.

Note Population *pop* is copied to a simulator so the input population will be kept untouched.

`clone()`

Clone a simulator, along with all its populations. Note that Python assign statement `simul = simu` only creates a symbolic link to an existing simulator.

`save(filename)`

Save a simulator to file *filename*, which can be loaded by a global function `LoadSimulator`.

`gen()`

Return the current generation number, which is the initial generation number (0, or some value set by `setGen(gen)`) plus the total number of generations evolved.

`setGen(gen)`

Set the current generation number of a simulator to *gen*.

`evolve(ops=[], preOps=[], postOps=[], gen=-1, dryrun=False)`

Evolve all populations *gen* generations, subject to operators *ops*, *preOps* and *postOps*. Operators *preOps* are applied to all populations (subject to applicability restrictions of the operators, imposed by the *rep* parameter of these operators) before evolution. They are usually used to initialize populations. Operators *postOps* are applied to all populations after the evolution.

Operators *ops* are applied during the life cycle of each generation. Depending on the stage of these operators, they can be applied before-, during-, and/or post-mating. These operators can be applied at all or some of the generations, depending the *begin*, *end*, *step*, and *at* parameters of these operators. Populations in a simulator are evolved one by one. At each generation, the applicability of these operators are determined. Pre-mating operators are applied to a population first. A mating scheme is then used to populate an offspring generation. For each offspring, his or her sex is determined before during-mating operators of the mating scheme are used to transmit parental genotypes. During-mating operators specified in this function will be applied afterwards. An offspring will be discarded if any of the during-mating operator fails (return `False`). After an offspring generation is successfully generated and becomes the current generation, applicable post-mating operators are applied to it. Because the order at which operators are applied can be important, and the stage(s) at which operators are applied are not always clear, a parameter *dryRun* can be used. If set to `True`, this function will print out the order at which all operators are applied, without actually evolving the populations.

Parameter *gen* can be set to a positive number, which is the number of generations to evolve. If *gen* is negative (default), the evolution will continue indefinitely, until all replicates are stopped by a special kind of operators called *terminators*. At the end of the evolution, the generations that each replicates have evolved are returned. If not all replicates are stopped at the same generation, the negative replicate numbers are calculated according to *active* replicates, meaning replicate -1 will refer to the last active replicate even if the last replicate has stopped. In addition, *postOps* are applied to all replicates, including those that stopped before other replicates.

Note: Operators *ops*, *preOps* and *postOps* are copied before they are applied during evolution. Input operators will therefore not be changed.

extract (*rep*)
 Extract the *rep-th* population from a simulator. This will reduce the number of populations in this simulator by one.

numRep ()
 Return the number of replicates.

population (*rep*)
 Return a reference to the *rep-th* population of a simulator. The reference will become invalid once the simulator starts evolving or becomes invalid (removed). Modifying the returned object is discouraged because it will change the population within the simulator. If an independent copy of the population is needed, use `simu.population(rep).clone()`.

add (*pop*)
 Add a population *pop* to the end of an existing simulator. This creates an cloned copy of *pop* in the simulator so the evolution of the simulator will not change *pop*.

populations ()
 Return a Python iterator that can be used to iterate through all populations in a simulator.

setMatingScheme (*matingScheme*)
 Set a new mating scheme *matingScheme* to a simulator.

vars (*rep*, *subPop*=[])
 Return the local namespace of the *rep-th* population, equivalent to `x.population(rep).vars(subPop)`.

dvars (*rep*, *subPop*=[])
 Return a wrapper of Python dictionary returned by `vars(rep, subPop)` so that dictionary keys can be accessed as attributes.

1.1.5 Class pedigree

The pedigree class is derived from the population class. Unlike a population class that emphasizes on individual properties, the pedigree class emphasizes on relationship between individuals.

A pedigree class can be created from a population, or loaded from a disk file, which is usually saved by an operator during a previous evolutionary process. Depending on how a pedigree is saved, sex and affection status information may be missing.

class pedigree (*pop*, *loci*=[], *infoFields*=[], *ancGen*=-1, *fatherField*="father_idx", *motherField*="mother_idx")
 Create a pedigree object from a population, using a subset of loci (parameter *loci*, default to no loci), information fields (parameter *infoFields*, default to no information field except for *parentFields*), and ancestral generations (parameter *ancGen*, default to all ancestral generations). By default, information field *father_idx* and *mother_idx* are used to locate parents. If individuals in a pedigree has only one parent, the information field that stores parental indexes should be specified in parameter *fatherField* or *motherField*. The other field should be set to an empty string.

clone ()
 Create a cloned copy of a pedigree.

numParents ()
 Return the number of parents each individual has. This function returns the number of information fields used to store parental indexes, even if one of the fields are unused.

father (*idx*, *subPop*)

Return the index of the father of individual *idx* in subpopulation *subPop* in the parental generation. Return -1 if this individual has no father (*fatherField* is empty or the value of information field is negative).

mother (*idx*, *subPop*)

Return the index of the mother of individual *idx* in subpopulation *subPop* in the parental generation. Return -1 if this individual has no mother (*motherField* is empty or the value of information field is negative).

locateRelatives (*relType*=[], *relFields*=[], *ancGen*=-1)

This function locates relatives (of type *relType*) of each individual and store their indexes in specified information fields *relFields*. The length of *relFields* determines how many relatives an individual can have.

Parameter *relType* specifies what type of relative to locate. It can be *Self*, *Spouse* (having at least one common offspring), *Offspring*, *FullSibling* (having common father and mother), *Sibling* (having at least one common parent) or *SpouseAndOffspring* (One spouse and their common offspring). Optionally, you can specify the sex of relatives you would like to locate, in the form of *relType*=(*type*, *sexChoice*). *sexChoice* can be *AnySex* (default), *MaleOnly*, *FemaleOnly*, *SameSex* or *OppositeSex*. *sexChoice* for *SpouseAndOffspring* only refer to sex of offspring.

This function will by default go through all ancestral generations and locate relatives for all individuals. This can be changed by setting parameter *ancGen* to the greatest ancestral generation you would like to process.

traceRelatives (*pathGen*, *pathFields*, *pathSex*=[], *resultFields*=[])

Trace a relative path in a population and record the result in the given information fields *resultFields*. This function is used to locate more distant relatives based on the relatives located by function *locateRelatives*. For example, after siblings and offspring of all individuals are located, you can locate mother's sibling's offspring using a *relative path*, and save their indexes in each individuals information fields *resultFields*.

A *relative path* consists of three pieces of information specified by three parameters. Parameter *pathGen* specifies starting, intermediate and ending generations. *pathFields* specifies which information fields to look for at each step, and *pathSex* specifies sex choices at each generation, which should be a list of *AnySex*, *MaleOnly*, *FemaleOnly*, *SameSex* and *OppositeSex*. The default value for this parameter is *AnySex* at all steps. The length of *pathGen* should be one more than *pathFields*, and *pathSex* if *pathSex* is given.

For example, if *pathGen*=[0, 1, 1, 0], *pathFields* = [['father_idx', 'mother_idx'], ['sib1', 'sib2'], ['off1', 'off2']], and *pathSex* = [*AnySex*, *MaleOnly*, *FemaleOnly*], this function will locate *father_idx* and *mother_idx* for each individual at generation 0, find all individuals referred by *father_idx* and *mother_idx* at generation 1, find information fields *sib1* and *sib2* from these parents and locate male individuals referred by these two information fields. Finally, the information fields *off1* and *off2* from these siblings are located and are used to locate their female offspring at the present generation. The results are father or mother's brother's daughters. Their indexes will be saved in each individuals information fields *resultFields*. Note that this function will locate and set relatives for individuals only at the starting generation specified at *pathGen*[0].

1.1.6 Class **vspSplitter**

This class is the base class of all virtual subpopulation (VSP) splitters, which provide ways to define groups of individuals in a subpopulation who share certain properties. A splitter defines a fixed number of named VSPs. They do not have to add up to the whole subpopulation, nor do they have to be distinct. After a splitter is assigned to a population, many functions and operators can be applied to individuals within specified VSPs.

Only one VSP splitter can be assigned to a population, which defined VSPs for all its subpopulations. If different splitters are needed for different subpopulations, a *combinedSplitter* should be used.

class vspSplitter ()

This is a virtual class that cannot be instantiated.

clone ()

All VSP splitter defines a `clone ()` function to create an identical copy of itself.

name (vsp)

Return the name of VSP *vsp* (an index between 0 and `numVirtualSubPop ()`).

numVirtualSubPop ()

Return the number of VSPs defined by this splitter.

1.1.7 Class sexSplitter

This splitter defines two VSPs by individual sex. The first VSP consists of all male individuals and the second VSP consists of all females in a subpopulation.

class sexSplitter ()

Create a sex splitter that defines male and female VSPs.

name (vsp)

Return "Male" if *vsp*=0 and "Female" otherwise.

numVirtualSubPop ()

Return 2.

1.1.8 Class affectionSplitter

This class defines two VSPs according individual affection status. The first VSP consists of unaffected individuals and the second VSP consists of affected ones.

class affectionSplitter ()

Create a splitter that defined two VSPs by affection status.

name (vsp)

Return "Unaffected" if *vsp*=0 and "Affected" if *vsp*=1.

numVirtualSubPop ()

Return 2.

1.1.9 Class infoSplitter

This splitter defines VSPs according to the value of an information field of each individual. A VSP is defined either by a value or a range of values.

class infoSplitter (field, values=[], cutoff=[])

Create an information splitter using information field *field*. If parameter *values* is specified, each item in this list defines a VSP in which all individuals have this value at information field *field*. If a set of cutoff values are defined in parameter *cutoff*, individuals are grouped by intervals defined by these cutoff values. For example, `cutoff=[1, 2]` defines three VSPs with $v < 1$, $1 \leq v < 2$ and $v \geq 2$ where *v* is the value of an individual at information field *field*. Of course, only one of the parameters *values* and *cutoff* should be defined, values in *cutoff* should be distinct, and in an increasing order.

name (vsp)

Return the name of a VSP *vsp*, which is `field = value` if VSPs are defined by values in parameter *values*, or `field < value` (the first VSP), `v1 <= field < v2` and `field >= v` (the last VSP) if VSPs are defined by cutoff values.

numVirtualSubPop()

Return the number of VSPs defined by this splitter, which is the length parameter *values* or the length of *cutoff* plus one, depending on which parameter is specified.

1.1.10 Class **proportionSplitter**

This splitter divides subpopulations into several VSPs by proportion.

class proportionSplitter (*proportions=[]*)

Create a splitter that divides subpopulations by *proportions*, which should be a list of float numbers (between 0 and 1) that add up to 1.

name (*vsp*)

Return the name of VSP *vsp*, which is "Prop p" where p=proportions[*vsp*].

numVirtualSubPop()

Return the number of VSPs defined by this splitter, which is the length of parameter *proportions*.

1.1.11 Class **rangeSplitter**

This class defines a splitter that groups individuals in certain ranges into VSPs.

class rangeSplitter (*ranges*)

Create a splitter according to a number of individual ranges defined in *ranges*. For example, `rangeSplitter(ranges=[[0, 20], [40, 50]])` defines two VSPs. The first VSP consists of individuals 0, 1, ..., 19, and the second VSP consists of individuals 40, 41, ..., 49. Note that a nested list has to be used even if only one range is defined.

name (*vsp*)

Return the name of VSP *vsp*, which is "Range [a, b]" where [a, b] is range ranges[*vsp*].

numVirtualSubPop()

Return the number of VSPs, which is the number of ranges defined in parameter *ranges*.

1.1.12 Class **genotypeSplitter**

This class defines a VSP splitter that defines VSPs according to individual genotype at specified loci.

class genotypeSplitter (*loci, alleles, phase=False*)

Create a splitter that defines VSPs by individual genotype at *loci* (a locus index or a list of loci indexes). Each list in a list *allele* defines a VSP, which is a list of allowed alleles at these *loci*. If only one VSP is defined, the outer list of the nested list can be ignored. If *phase* is true, the order of alleles in each list is significant. If more than one set of alleles are given, individuals having either of them is qualified.

For example, in a haploid population, `loci=1, alleles=[0, 1]` defines a VSP with individuals having allele 0 or 1 at locus 1, `alleles=[[0, 1], [2]]` defines two VSPs with individuals in the second VSP having allele 2 at locus 1. If multiple loci are involved, alleles at each locus need to be defined. For example, VSP defined by `loci=[0, 1], alleles=[0, 1, 1, 1]` consists of individuals having alleles [0, 1] or [1, 1] at loci [0, 1].

In a haploid population, `loci=1, alleles=[0, 1]` defines a VSP with individuals having genotype [0, 1] or [1, 0] at locus 1. `alleles=[[0, 1], [2, 2]]` defines two VSPs with individuals in the second VSP having genotype [2, 2] at locus 1. If *phase* is set to True, the first VSP will only have individuals with genotype [0, 1]. In the multiple loci case, alleles should be arranged by haplotypes, for example, `loci=[0, 1], alleles=[0, 0, 1, 1], phase=True` defines a VSP with individuals having genotype -0-0-,

-1-1- at loci 0 and 1. If `phase=False` (default), genotypes -1-1-, -0-0-, -0-1- and -1-0- are all allowed.

name (*vsp*)

Return name of VSP *vsp*, which is "Genotype loc1,loc2:genotype" as defined by parameters *loci* and *alleles*.

numVirtualSubPop ()

Number of virtual subpops of subpopulation *sp*

1.1.13 Class `combinedSplitter`

This splitter takes several splitters and stacks their VSPs together. For example, if the first splitter defines 3 VSPs and the second splitter defines 2, the two VSPs from the second splitter become the fourth (index 3) and the fifth (index 4) VSPs of the combined splitter. This splitter is usually used to define different types of VSPs to a population.

class combinedSplitter (*splitters=[]*)

Create a combined splitter using a list of *splitters*. For example, `combinedSplitter([sexSplitter(), affectionSplitter()])` defines a combined splitter with four VSPs.

name (*vsp*)

Return the name of a VSP *vsp*, which is the name a VSP defined by one of the combined splitters.

numVirtualSubPop ()

Return the number of VSPs defined by this splitter, which is the sum of the number of VSPs of all combined splitters.

1.2 Mating Schemes

1.2.1 Class `homoMating`

A homogeneous mating scheme that uses a parent chooser to choose parents from a prenatal generation, and an offspring generator to generate offspring from chosen parents. It can be either used directly, or within a heterogeneous mating scheme. In the latter case, it can be applied to a (virtual) subpopulation.

class homoMating (*chooser, generator, subPopSize=[], subPop=[], weight=0*)

Create a homogeneous mating scheme using a parent chooser *chooser* and an offspring generator *generator*.

If this mating scheme is used directly in a simulator, it will be responsible for creating an offspring population according to parameter *subPopSize*. This parameter can be a list of subpopulation sizes (or a number if there is only one subpopulation) or a Python function. The function should take two parameters, a generation number and a list of subpopulation sizes before mating, and return a list of subpopulation sizes for the offspring generation. A single number can be returned if there is only one subpopulation. If latter form is used, the specified function will be called at each generation to determine the size of the offspring generation. Parameters *subPop* and *weight* are ignored in this case.

If this mating scheme is used within a heterogeneous mating scheme. Parameters *subPop* and *weight* are used to determine which (virtual) subpopulation this mating scheme will be applied to, and how many offspring this mating scheme will produce. Please refer to mating scheme `heteroMating` for the use of these two parameters.

clone ()

Deep copy of a homogeneous mating scheme.

1.2.2 Class `heteroMating`

A heterogeneous mating scheme that applies a list of mating schemes to different (virtual) subpopulations.

class `heteroMating` (*matingSchemes*, *subPopSize*=[], *shuffleOffspring*=True)

Create a heterogeneous mating scheme that will apply a list of homogeneous mating schemes *matingSchemes* to different (virtual) subpopulations. The size of the offspring generation is determined by parameter *subPopSize*, which can be a list of subpopulation sizes or a Python function that returns a list of subpopulation sizes at each generation. Please refer to `homoMating` for a detailed explanation of this parameter.

Each mating scheme defined in *matingSchemes* can be applied to one or more (virtual) subpopulation. If parameter *subPop* is not specified, a mating scheme will be applied to all subpopulations. If a (virtual) subpopulation is specified, a mating scheme will be applied to a specific (virtual) subpopulation. A special case is when *subPop* is given as `(-1, vsp)`. In this case, the mating scheme will be applied to virtual subpopulation *vsp* in all subpopulations.

If multiple mating schemes are applied to the same subpopulation, a weight (parameter *weight*) can be given to each mating scheme to determine how many offspring it will produce. The default for all mating schemes are 0. In this case, the number of offspring each mating scheme produces is proportional to the size of its parental (virtual) subpopulation. If all weights are negative, the numbers of offspring are determined by the multiplication of the absolute values of the weights and their respective parental (virtual) subpopulation sizes. If all weights are positive, the number of offspring produced by each mating scheme is proportional to these weights. Mating schemes with zero weight in this case will produce no offspring. If both negative and positive weights are present, negative weights are processed before positive ones.

If multiple mating schemes are applied to the same subpopulation, offspring produced by these mating schemes are shuffled randomly. If this is not desired, you can turn off offspring shuffling by setting parameter *shuffleOffspring* to `False`.

`clone()`

Deep copy of a heterogeneous mating scheme

1.2.3 Class `pedigreeMating`

A pedigree mating scheme that evolves a population following a pedigree object.

class `pedigreeMating` (*ped*, *generator*, *setSex*=False, *setAffection*=False, *copyFields*=[])

Creates a mating scheme that evolve a population following a pedigree object *ped*. Considering this pedigree as a population with *N* ancestral generations, the starting population is the greatest ancestral generation of *ped*. The mating scheme creates an offspring generation that match the size of generation *N-1* and chooses parents according to the parents of individuals at this generation. Depending on the *gen* parameter of the simulator, the process continues generation by generation for *N* generations if *gen* >= *N*, or *gen* generations if *gen* < *N*. During the evolution, an offspring generator *generator* is used to produce one offspring at a time, regardless of the *numOffspring* setting of this offspring generator. If individuals in pedigree *ped* has only one parent, the offspring generator should be compatible.

By default, the pedigree mating scheme does not set offspring sex and affection status using sex and affection status of corresponding individuals in the pedigree. However, if such information is valid in the pedigree object *ped*, you can set parameters *setSex* and/or *setAffection* to `True` to set sex and/of affection status to offspring during the evolutionary process. Similarly, you can specify some information fields in *copyFields* to copy some information fields from pedigree to the evolving population. Note that these information will be copied also to the starting population (from the greatest ancestral generation in *ped*).

`clone()`

Deep copy of a Python mating scheme

1.2.4 Class `sequentialParentChooser`

This parent chooser chooses a parent from a parental (virtual) subpopulation sequentially. Sex and selection is not considered. If the last parent is reached, this parent chooser will restart from the beginning of the (virtual) subpopulation.

class `sequentialParentChooser` ()

Create a parent chooser that chooses a parent from a parental (virtual) subpopulation sequentially.

`clone` ()

Deep copy of a sequential parent chooser.

1.2.5 Class `sequentialParentsChooser`

This parent chooser chooses two parents (a father and a mother) sequentially from their respective sex groups. Selection is not considered. If all fathers (or mothers) are exhausted, this parent chooser will choose fathers (or mothers) from the beginning of the (virtual) subpopulation again.

class `sequentialParentsChooser` ()

Create a parent chooser that chooses two parents sequentially from a parental (virtual) subpopulation.

`clone` ()

Deep copy of a sequential parents chooser.

1.2.6 Class `randomParentChooser`

This parent chooser chooses a parent randomly from a (virtual) parental subpopulation. Parents are chosen with or without replacement. If parents are chosen with replacement, a parent can be selected multiple times. If natural selection is enabled, the probability that an individual is chosen is proportional to his/her fitness value stored in an information field *selectionField* (default to "fitness"). If parents are chosen without replacement, a parent can be chosen only once. An `RuntimeError` will be raised if all parents are exhausted. Selection is disabled in the without-replacement case.

class `randomParentChooser` (*replacement=True, selectionField="fitness"*)

Create a random parent chooser that choose parents with or without replacement (parameter *replacement*, default to `True`). If selection is enabled and information field *selectionField* exists in the passed population, the probability that a parent is chosen is proportional to his/her fitness value stored in *selectionField*.

`clone` ()

Deep copy of a random parent chooser.

1.2.7 Class `randomParentsChooser`

This parent chooser chooses two parents, a male and a female, randomly from a (virtual) parental subpopulation. Parents are chosen with or without replacement from their respective sex group. If parents are chosen with replacement, a parent can be selected multiple times. If natural selection is enabled, the probability that an individual is chosen is proportional to his/her fitness value among all individuals with the same sex. Selection will be disabled if specified information field *selectionField* (default to "fitness") does not exist. If parents are chosen without replacement, a parent can be chosen only once. An `RuntimeError` will be raised if all males or females are exhausted. Selection is disabled in the without-replacement case.

class `randomParentsChooser` (*replacement=True, selectionField="fitness"*)

Create a random parents chooser that choose two parents with or without replacement (parameter *replacement*,

default to `True`). If selection is enabled and information field *selectionField* exists in the passed population, the probability that a parent is chosen is proportional to his/her fitness value stored in *selectionField*.

clone ()

Deep copy of a random parents chooser.

1.2.8 Class `polyParentsChooser`

This parent chooser is similar to random parents chooser but instead of selecting a new pair of parents each time, one of the parents in this parent chooser will mate with several spouses before he/she is replaced. This mimicks multi-spouse mating schemes such as polygyny or polyandry in some populations. Natural selection is supported for both sexes.

class `polyParentsChooser` (*polySex=Male, polyNum=1, selectionField="fitness"*)

Create a multi-spouse parents chooser where each father (if *polySex* is Male) or mother (if *polySex* is Female) has *polyNum* spouses. The parents are chosen with replacement. If natural selection is enabled, the probability that an individual is chosen is proportional to his/her fitness value among all individuals with the same sex. Selection will be disabled if specified information field *selectionField* (default to "fitness") does not exist.

clone ()

Deep copy of a parent chooser.

1.2.9 Class `alphaParentsChooser`

This parent chooser mimicks some animal populations where only certain individuals (usually males) can mate. Alpha individuals can be chosen either randomly (with natural selection) or according to an information field. After the alpha individuals are selected, the parent chooser works identical to a random mating scheme, except that one of the parents are chosen from these alpha individuals.

class `alphaParentsChooser` (*alphaSex=Male, alphaNum=0, alphaField="", selectionField="fitness"*)

Create a parent chooser that chooses father (if *alphaSex* is Male) or mother (if *alphaSex* is Female) from a selected group of alpha individuals. If *alphaNum* is given, alpha individuals are chosen randomly or according to individual fitness if natural selection is enabled. If *alphaField* is given, individuals with non-zero values at this information field are considered as alpha individuals. After alpha individuals are selected, *alphaSex* parent will be chosen from the alpha individuals randomly or according to individual fitness. The other parents are chosen randomly.

clone ()

Deep copy of an alpha parents chooser.

1.2.10 Class `infoParentsChooser`

This parent chooser chooses an individual randomly, and then his/her spouse his/her spouse from a given set of information fields, which stores indexes of individuals in the same generation. An information field will be ignored if its value is negative, or if sex is incompatible.

Depending on what indexes are stored in these information fields, this parent chooser can be used to implement different types of mating schemes where selection of spouse is limited. For example, a consanguineous mating scheme can be implemented using this mating scheme if certain type of relatives are located for each individual, and are used for mating.

This parent chooser uses `randomParentChooser` to choose one parent and randomly choose another one from the information fields. Natural selection is supported during the selection of the first parent. Because of potentially uneven distribution of valid information fields, the overall process may not be as random as expected.

class infoParentsChooser (*infoFields=[]*, *func=None*, *param=None*, *selectionField="fitness"*)

Create a information parent chooser a parent randomly (with replacement, and with selection if natural selection is enabled), and then his/her spouse from indexes stored in *infoFields*. If a Python function *func* is specified, it will be called before parents are chosen. This function accepts the parental population and an optional parameter *param* and is usually used to locate qualified spouse for each parent. The return value of this function is ignored.

clone ()

Deep copy of a infomation parent chooser.

1.2.11 Class pyParentsChooser

This parents chooser accept a Python generator function that repeatedly yields one or two parents, which can be references to individual objects or indexes relative to each subpopulation. The parent chooser calls the generator function with parental population and a subpopulation index for each subpopulation and retrieves parents repeatedly using the iterator interface of the generator function.

This parent chooser does not support virtual subpopulation directly. A `ValueError` will be raised if this parent chooser is applied to a virtual subpopulation. However, because virtual subpopulations are defined in the passed parental population, it is easy to return parents from a particular virtual subpopulation using virtual subpopulation related functions.

class pyParentsChooser (*parentsGenerator*)

Create a Python parent chooser using a Python generator function *parentsGenerator*. This function should accept a population object (the parental population) and a subpopulation number and return the reference or index (relative to subpopulation) of a parent or a pair of parents repeatedly using the iterator interface of the generator function.

clone ()

Deep copy of a python parent chooser.

1.2.12 Class offspringGenerator

An *offspring generator* generates offspring from parents chosen by a parent chooser. It is responsible for creating a certain number of offspring, determining their sex, and transmitting genotypes from parents to offspring.

class offspringGenerator (*ops*, *numOffspring=1*, *sexMode=RandomSex*)

Create a basic offspring generator. This offspring generator uses *ops* genotype transmitters to transmit genotypes from parents to offspring. It expects *numParents* from an upstream parents chooser and raises an `RuntimeError` if incorrect number of parents are passed. If both one and two parents can be handled, 0 should be specified for this parameter.

A number of *during-mating operators* (parameter *ops*) can be used to, among other possible duties such as setting information fields of offspring, transmit genotype from parents to offspring. Additional during-mating operators passed from the `simulator.evolve()` function will be applied afterwards. This general offspring generator does not have any default during-mating operator but all stock mating schemes use an offspring generator with a default operator. For example, a `mendelianOffspringGenerator` is used by `randomMating` to trasmit genotypes.

Parameter *numOffspring* is used to control the number of offspring per mating event, or in another word the number of offspring in each family. It can be a number, a function, or a mode parameter followed by some optional arguments. If a number is given, given number of offspring will be generated at each mating event. If a Python function is given, it will be called each time when a mating event happens. Current generation number will be passed to this function, and its return value will be considered the number of offspring. In the last case, a tuple (or a list) in one of the following forms: (`GeometricDistribution`, *p*), (`PoissonDistribution`, *p*), (`BinomialDistribution`, *p*, *N*), or (`UniformDistribution`, *a*, *b*) can be given. The

number of offspring will be determined randomly following these statistical distributions. Please refer to the simuPOP user's guide for a detailed description of these distributions and their parameters.

Parameter *sexMode* is used to control the sex of each offspring. Its default value is usually *RandomSex* which assign Male or Female to each individual randomly, with equal probabilities. If *NoSex* is given, all individuals will be Male. *sexMode* can also be one of (*ProbOfMale*, *p*), (*NumOfMale*, *n*), and (*NumOfFemale*, *n*). The first case specifies the probability of male for each offspring. The next two cases specifies the number of male or female individuals in each family, respectively. If *n* is greater than or equal to the number of offspring in this family, all offspring in this family will be Male or Female.

clone()

Make a deep copy of this offspring generator.

1.2.13 Class **controlledOffspringGenerator**

This offspring generator populates an offspring population and controls allele frequencies at specified loci. At each generation, expected allele frequencies at these loci are passed from a user defined allele frequency *trajectory* function. The offspring population is populated in two steps. At the first step, only families with disease alleles are accepted until until the expected number of disease alleles are met. At the second step, only families with wide type alleles are accepted to populate the rest of the offspring generation. This method is described in detail in "Peng et al, (2007) *Forward-time simulations of populations with complex human diseases*, PLoS Genetics".

class controlledOffspringGenerator (*loci*, *alleles*, *freqFunc*, *ops*=[], *numOffspring*=1, *sexMode*=*RandomSex*)

Create an offspring generator that selects offspring so that allele frequency at specified loci in the offspring generation reaches specified allele frequency. At the beginning of each generation, expected allele frequency of *alleles* at *loci* is returned from a user-defined trajectory function *freqFunc*. If there is no subpopulation, this function should return a list of frequencies for each locus. If there are multiple subpopulations, *freqFunc* can return a list of allele frequencies for all subpopulations or combined frequencies that ignore population structure. In the former case, allele frequencies should be arranged by *loc0_sp0*, *loc1_sp0*, ... *loc0_sp1*, *loc1_sp1*, ..., and so on. In the latter case, overall expected number of alleles are scattered to each subpopulation in proportion to existing number of alleles in each subpopulation, using a multinomial distribution.

After the expected alleles are calculated, this offspring generator accept and reject families according to their genotype at *loci* until allele frequencies reach their expected values. The rest of the offspring generation is then filled with families without only wild type alleles at these *loci*.

This offspring generator is derived from class *offspringGenerator*. Please refer to class *offspringGenerator* for a detailed description of parameters *ops*, *numOffspring* and *sexMode*.

clone()

Deep copy of a controlled random mating scheme.

1.2.14 Pre-defined mating schemes

cloneMating (*numOffspring*=1, *sexMode*=None, *ops*=<*simuPOP.simuPOP.cloneGenoTransmitter*>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*=None)

A homogeneous mating scheme that uses a sequential parent chooser and a clone offspring generator. Please refer to class *offspringGenerator* for parameters *ops* and *numOffspring*, and to class *homoMating* for parameters *subPopSize*, *subPop* and *weight*. Parameters *sexMode* and *selectionField* are ignored because this mating scheme does not support natural selection, and *cloneOffspringGenerator* copies sex from parents to offspring.

randomSelection (*numOffspring*=1, *sexMode*=None, *ops*=<*simuPOP.simuPOP.cloneGenoTransmitter*>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a random single-parent parent chooser with replacement, and a clone offspring generator. This mating scheme is usually used to simulate the basic haploid Wright-Fisher

model but it can also be applied to diploid populations. Please refer to class `randomParentChooser` for parameter *selectionField*, to class `offspringGenerator` for parameters *ops* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*. Parameter *sexMode* is ignored because `cloneOffspringGenerator` copies sex from parents to offspring.

randomMating (*numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a random parents chooser with replacement and a Mendelian offspring generator. This mating scheme is widely used to simulate diploid sexual Wright-Fisher random mating. Please refer to class `randomParentsChooser` for parameter *selectionField*, to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*.

monogamousMating (*numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*=None)

A homogeneous mating scheme that uses a random parents chooser without replacement and a Mendelian offspring generator. It differs from the basic random mating scheme in that each parent can mate only once so there is no half-sibling in the population. Please refer to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*. Parameter *selectionField* is ignored because this mating scheme does not support natural selection.

polygamousMating (*polySex*=1, *polyNum*=1, *numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a multi-spouse parents chooser and a Mendelian offspring generator. It differs from the basic random mating scheme in that each parent of sex *polySex* will have *polyNum* spouses. Please refer to class `polyParentsChooser` for parameters *polySex*, *polyNum* and *selectionField*, to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*.

alphaMating (*alphaSex*=1, *alphaNum*=0, *alphaField*="", *numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses an alpha-individual parents chooser and a Mendelian offspring generator. It differs from the basic random mating scheme in that selection of parents of sex *alphaSex* is limited to certain alpha individuals, which are chosen either randomly (parameter *alphaNum*) or from an information field (parameter *alphaField*). This mating scheme is usually used to simulate animal population where only a few alpha individuals have the right to mate. Please refer to class `alphaParentsChooser` for parameters *alphaSex*, *alphaNum*, *alphaField* and *selectionField*, to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*.

haplodiploidMating (*numOffspring*=1.0, *sexMode*=31, *ops*=<simuPOP.simuPOP.haplodiploidGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a random parents chooser with replacement and a haplodiploid offspring generator. It should be used in a haplodiploid population where male individuals only have one set of homologous chromosomes. Please refer to class `randomParentsChooser` for parameter *selectionField*, to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*.

selfMating (*replacement*=True, *numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.selfingGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a random single-parent parent chooser with or without replacement (parameter *replacement*) and a selfing offspring generator. It is used to mimic self-fertilization in certain plant populations. Please refer to class `randomParentChooser` for parameter *replacement* and *selectionField*, to class `offspringGenerator` for parameters *ops*, *sexMode* and *numOffspring*, and to class `homoMating` for parameters *subPopSize*, *subPop* and *weight*.

consanguineousMating (*infoFields*=[], *func*=None, *param*=None, *replacement*=False, *numOffspring*=1.0, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses an information parents chooser and a Mendelian offspring generator. A function *func* should be defined to locate certain types of relative to each individual and save their indexes to information fields *infoFields*. This mating scheme will then choose a parent randomly and then another parent from his/her relatives using their saved indexes. Please refer to class *infoParentsChooser* for parameters *infoFields*, *func*, *param* and *selectionField*, to class *offspringGenerator* for parameters *ops*, *sexMode* and *numOffspring*, and to class *homoMating* for parameters *subPopSize*, *subPop* and *weight*.

controlledRandomMating (*loci*=[], *alleles*=[], *freqFunc*=None, *numOffspring*=1, *sexMode*=31, *ops*=<simuPOP.simuPOP.mendelianGenoTransmitter>, *subPopSize*=[], *subPop*=[], *weight*=0, *selectionField*='fitness')

A homogeneous mating scheme that uses a random sexual parents chooser with replacement and a controlled offspring generator using Mendelian genotype transmitter. At each generation, function *freqFunc* will be called to obtain intended frequencies of alleles *alleles* at loci *loci*. The controlled offspring generator will control the acceptance of offspring so that the generation reaches desired allele frequencies at these loci. Rationals and applications of this mating scheme is described in details in a paper Peng *et al*, 2007 (*PLoS Genetics*). Please refer to class *randomParentsChooser* for parameters *selectionField*, to class *controlledOffspringGenerator* for parameters *loci*, *alleles*, *freqFunc*, to class *offspringGenerator* for parameters *ops*, *sexMode* and *numOffspring*, and to class *homoMating* for parameters *subPopSize*, *subPop* and *weight*.

1.3 Utility Classes

1.3.1 Class RNG

This random number generator class wraps around a number of random number generators from GNU Scientific Library. You can obtain and change the RNG used by the current simuPOP module through the *GetRNG()* function, or create a separate random number generator and use it in your script.

class RNG (*name*=None, *seed*=0)

Create a RNG object using specified name and seed. If *rng* is not given, environmental variable *GSL_RNG_TYPE* will be used if it is available. Otherwise, *RNGmt19937* will be used. If *seed* is not given, */dev/urandom*, */dev/random*, or other system random number source will be used to guarantee that random seeds are used even if more than one simuPOP sessions are started simultaneously.

max()

Maximum value of this RNG

maxSeed()

Return the maximum allowed seed value

name()

Return the name of the current random number generator.

randBinomial (*n*, *p*)

Generate a random number following a binomial distribution with parameters *n* and *p*. Please check the documentation of *gsl_ran_binomial* for details.

randBit()

Return a random bit.

randExponential (*v*)

Generate a random number following an exponential distribution with parameter *v*. Please check the documentation of *gsl_ran_exponential* for details.

randGeometric (*p*)
Generate a random number following a geometric distribution with parameter *p*. Please check the documentation of `gsl_ran_geometric` for details.

randGet ()
Return a random number in the range of `[0, 2, ... max()-1]`

randInt (*n*)
Return a random number in the range of `[0, 1, 2, ... n-1]`

randMultinomialVal (*N, p*)
Generate a random number following a multinomial distribution with parameters *N* and *p* (a list of probabilities). Please check the documentation of `gsl_ran_multinomial` for details.

randNormal (*m, v*)
Generate a random number following a normal distribution with mean *m* and standard deviation *v*. Please check the documentation of `gsl_ran_gaussian` for details.

randPoisson (*p*)
Generate a random number following a Poisson distribution with parameter *p*. Please check the documentation of `gsl_ran_poisson` for details.

randUniform01 ()
Generate a random number following a uniform distribution between 0 and 1. Please check the documentation of `gsl_ran_uniform` for details.

seed ()
Return the seed used to initialize the RNG. This can be used to repeat a previous session.

setRNG (*name=None, seed=0*)
Use another underlying RNG for the current RNG object. The handling of parameters *rng* and *seed* is the same as `RNG::RNG(name, seed)`.

setSeed (*seed=0*)
Set random seed for this random number generator. If *seed* is 0, method described in `setRNG` is used.

1.4 Global functions

AvailableRNGs ()
List the names of all available random number generators

CloseOutput (*output=""*)
Output files specified by '`>`' are closed immediately after they are written. Those specified by '`>>`' and '`>>>`' are closed by a simulator after `simulator.evolve()`. However, these files will be kept open if the operators are applied directly to a population using the operators' function form. In this case, function `closeOutput` can be used to close a specific file *output*, and close all unclosed files if *output* is unspecified. An exception will be raised if *output* does not exist or it has already been closed.

DebugCodes ()
Return names of all debug codes

LoadPopulation (*file*)
Load a population from a file.

LoadSimulator (*file, matingScheme*)
Load a simulator from a file with the specified mating scheme. The file format is by default determined by file extension (`format="auto"`). Otherwise, *format* can be one of `txt`, `bin`, or `xml`.

ModuleInfo ()
Return a dictionary with information regarding the currently loaded `simuPOP` module. This dictionary has the following keys:

- revision**: revision number.
- version**: simuPOP version string.
- optimized**: Is this module optimized (True or False).
- alleleType**: Allele type of the module (short, long or binary).
- maxAllele**: the maximum allowed allele state, which is 1 for binary modules, 255 for short modules and 65535 for long modules.
- compiler**: the compiler that compiles this module.
- date**: date on which this module is compiled.
- python**: version of python.
- platform**: platform of the module.
- maxNumSubPop**: maximum number of subpopulations.
- maxIndex**: maximum index size (limits population size * total number of marker).
- debug**: A list of effective debugging codes.

SetRNG (*rng=""*, *seed=0*)

Set random number generator. If *seed=0* (default), a random seed will be given. If *rng=""*, seed will be set to the current random number generator.

TurnOnDebug (*code=""*)

Set debug code *code*. More than one code could be specified using a comma separated string. Name of available codes are available from `DebugCodes`.

TurnOffDebug (*code="DBG_ALL"*)

Turn off debug code *code*. More than one code could be specified using a comma separated string. Default to turn off all debug codes.

GetRNG ()

Return the currently used random number generator

Chapter 2

Operator References (under revision)

2.1 Base class for all operators

2.1.1 Class `baseOperator`

Operators are objects that act on populations. They can be applied to populations directly using their function forms, but they are usually managed and applied by a simulator. In the latter case, operators are passed to the `evolve` function of a simulator, and are applied repeatedly during the evolution of the simulator.

The *baseOperator* class is the base class for all operators. It defines a common user interface that specifies at which generations, at which stage of a life cycle, to which populations and subpopulations an operator is applied. These are achieved by a common set of parameters such as `begin`, `end`, `step`, `at`, `stage` for all operators. Note that a specific operator does not have to honor all these parameters. For example, a recombinator can only be applied during mating so it ignores the `stage` parameter.

An operator can be applied to all or part of the generations during the evolution of a simulator. At the beginning of an evolution, a simulator is usually at the beginning of generation 0. If it evolves 10 generations, it evolves generations 0, 1, ..., and 9 (10 generations) and stops at the beginning of generation 10. A negative generation number `a` has generation number `10 + a`, with -1 referring to the last evolved generation 9. Note that the starting generation number of a simulator can be changed by its `setGen()` member function.

Output from an operator is usually directed to the standard output (`sys.stdout`). This can be configured using an output specification string, which can be `"` for no output, `'>'` standard terminal output (default), a filename prefixed by one or more `'>'` characters or a Python expression indicated by a leading exclamation mark (`'!expr'`). In the case of `'>filename'` (or equivalently `'filename'`), the output from an operator is written to this file. However, if two operators write to the same file `filename`, or if an operator writes to this file more than once, only the last write operation will succeed. In the case of `'>>filename'`, file `filename` will be opened at the beginning of the evolution and closed at the end. Outputs from multiple operators are appended. `>>>filename` works similar to `>>filename` but `filename`, if it already exists at the beginning of an evolutionary process, will not be cleared. If the output specification is prefixed by an exclamation mark, the string after the mark is considered as a Python expression. When an operator is applied to a population, this expression will be evaluated within the population's local namespace to obtain a population specific output specification. As an advanced feature, a Python function can be assigned to this parameter. Output strings will be sent to this function for processing.

class `baseOperator` (*output, stage, begin, end, step, at, rep, subPops, infoFields*)

The following parameters can be specified by all operators. However, an operator can ignore some parameters and the exact meaning of a parameter can vary.

output: A string that specifies how output from an operator is written, which can be `"` (no output), `'>'` (standard output), `'filename'` prefixed by one or more `'>'`, or a Python expression prefixed by an exclamation

`mark (' !expr')`. Alternatively, a Python function can be given to handle outputs.

stage: Stage(s) of a life cycle at which an operator will be applied. It can be `PreMating`, `DuringMating`, `PostMating` or any of their combined stages `PrePostMating`, `PreDuringMating`, `DuringPostMating` and `PreDuringPostMating`. Note that all operators have their default stage parameter and some of them ignore this parameter because they can only be applied at certain stage(s) of a life cycle.

begin: The starting generation at which an operator will be applied. Default to 0. A negative number is interpreted as a generation counted from the end of an evolution (-1 being the last evolved generation).

end: The last generation at which an operator will be applied. Default to -1, namely the last generation.

step: The number of generations between applicable generations. Default to 1.

at: A list of applicable generations. Parameters *begin*, *end*, and *step* will be ignored if this parameter is specified. A single generation number is also acceptable.

reps: A list of applicable replicates. A common default value `AllAvail` is interpreted as all replicates in a simulator. Negative indexes such as -1 (last replicate) is acceptable. `rep=idx` can be used as a shortcut for `rep=[idx]`.

subPops: A list of applicable (virtual) subpopulations, such as `subPops=[sp1, sp2, (sp2, vsp1)]`. `subPops=[sp1]` can be simplified as `subPops=sp1`. Negative indexes are not supported. A common default value (`AllAvail`) of this parameter represents all subpopulations of the population being applied. Support for this parameter vary from operator to operator and some operators do not support virtual subpopulations at all. Please refer to the reference manual of individual operators for their support for this parameter.

infoFields: A list of information fields that will be used by an operator. You usually do not need to specify this parameter because operators that use information fields usually have default values for this parameter.

apply (*pop*)
Apply an operator to population *pop* directly, without checking its applicability.

clone ()
Return a cloned copy of an operator. This function is available to all operators.

2.2 Initialization

2.2.1 Class `initSex` (Function `InitSex`)

This operator initialize sex of individuals, either randomly or use a list of sexes. For convenience, the function of this operator is included in other *initializers* such as `initByFreq` and `initByValue` so that you do not have to initialize sexes separately from genotype.

class `initSex` (*maleFreq*=0.5, *sex*=[], *stage*=`PreMating`, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=`AllAvail`, *subPops*=`AllAvail`, *infoFields*=[])
Create an operator that initialize individual sex to `Male` or `Female`. By default, it assign sex to individuals randomly, with equal probability of having a male or a female. This probability can be adjusted through parameter *maleFreq*. Alternatively, a fixed sequence of sexes can be assigned. For example, if *sex*=`[Male, Female]`, individuals will be assigned `Male` and `Female` successively. Parameter *maleFreq* is ignored if *sex* is given. If a list of (virtual) subpopulation is specified in parameter *subPop*, only individuals in these subpopulations will be initialized. Note that the *sex* sequence, if used, is assigned repeatedly regardless of subpopulation boundaries.

apply (*pop*)
Apply this operator to population *pop*

clone ()
Deep copy of an `initSex` operator.

2.2.2 Class `initByFreq` (Function `InitByFreq`)

This operator assigns alleles at all or part of loci with given allele frequencies. Alternatively, an individual can be initialized and be copied to all individuals in the same (virtual) subpopulations.

class `initByFreq` (*alleleFreq*=[], *loci*=AllAvail, *ploidy*=AllAvail, *identicalInds*=False, *stage*=PreMating, *begin*=0, *end*=1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *infoFields*=[])

This function creates an initializer that initializes individual genotypes randomly, using allele frequencies specified in parameter *alleleFreq*. Elements in *alleleFreq* specifies the allele frequencies of allele 0, 1, ... respectively. These frequencies should add up to 1. If *loci*, *ploidy* and/or *subPop* are specified, only specified loci, ploidy, and individuals in these (virtual) subpopulations will be initialized. If *identicalInds* is `True`, the first individual in each (virtual) subpopulation will be initialized randomly, and be copied to all other individuals in this (virtual) subpopulation. If a list of frequencies are given, they will be used for each (virtual) subpopulation. This operator initializes all chromosomes, including unused genotype locations and customized chromosomes.

`apply` (*pop*)

Apply this operator to population *pop*

`clone` ()

Deep copy of the operator `initByFreq`

2.2.3 Class `initByValue` (Function `InitByValue`)

This operator initialize individuals by given values.

class `initByValue` (*value*=[], *loci*=AllAvail, *ploidy*=AllAvail, *proportions*=[], *stage*=PreMating, *begin*=0, *end*=1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *infoFields*=[])

This function creates an initializer that initializes individual genotypes with given genotype *value*. If *loci*, *ploidy* and/or *subPop* are specified, only specified loci, ploidy, and individuals in these (virtual) subpopulations will be initialized. *value* can be used to initialize given *loci*, all loci, and all homologous copies of these loci. If *proportions* (a list of positive numbers that add up to 1) is given, *value* should be a list of values that will be assigned randomly according to their respective proportion. If a list of values are given without *proportions*, they will be used for each (virtual) subpopulations. This operator initializes all chromosomes, including unused genotype locations and customized chromosomes.

`apply` (*pop*)

Apply this operator to population *pop*

`clone` ()

Deep copy of the operator `initByValue`

2.2.4 Class `initInfo` (Function `InitInfo`)

This operator initializes given information fields with a sequence of values, or a user-provided function such as `random.random`.

class `initInfo` (*values*, *stage*=PreMating, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *infoFields*=[])

Create an operator that initialize individual information fields *infoFields* using a sequence of values or a user-defined function. If a list of values are given, it will be used sequentially for all individuals. The values will be reused if its length is less than the number of individuals. The values will be assigned repeatedly regardless of subpopulation boundaries. If a Python function is given, it will be called, without any argument, whenever a value is needed. If a list of (virtual) subpopulation is specified in parameter *subPop*, only individuals in these subpopulations will be initialized.

apply (*pop*)
 Apply this operator to population *pop*

clone ()
 Deep copy of an `initInfo` operator.

2.3 Expression and Statements

2.3.1 Class `pyOutput`

This operator outputs a given string when it is applied to a population.

class `pyOutput` (*msg=""*, *output=">"*, *stage=PostMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)
 Creates a `pyOutput` operator that outputs a string *msg* to *output* (default to standard terminal output) when it is applied to a population. Please refer to class `baseOperator` for a detailed description of common operator parameters such as *stage*, *begin* and *output*.

apply (*pop*)
 Simply output some info

clone ()
 Deep copy of a `pyOutput` operator.

2.3.2 Class `pyEval` (Function `PyEval`)

A `pyEval` operator evaluates a Python expression in a population's local namespace when it is applied to this population. The result is written to an output specified by parameter *output*.

class `pyEval` (*expr=""*, *stmts=""*, *exposePop=""*, *output=">"*, *stage=PostMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)
 Create a `pyEval` operator that evaluates a Python expression *expr* in a population's local namespace when it is applied to this population. If Python statements *stmts* is given (a single or multi-line string), the statement will be executed before *expr*. If *exposePop* is set to a non-empty string, the current population will be exposed in its own local namespace as a variable with this name. This allows the execution of expressions such as '`pop.individual(0).allele(0)`'. The result of *expr* will be sent to an output stream specified by parameter *output*. The exposed population variable will be removed after *expr* is evaluated. Please refer to class `baseOperator` for other parameters.

Note Although the statements and expressions are evaluated in a population's local namespace, they have access to a `**global**` namespace which is the module global namespace. It is therefore possible to refer to any module variable in these expressions. Such mixed use of local and global variables is, however, strongly discouraged.

apply (*pop*)
 Apply the `pyEval` operator to population *pop*.

clone ()
 Deep copy of a `pyEval` operator

evaluate (*pop*)
 Evaluate the expression and optional statements in the local namespace of population *pop* and return its result as a string.

2.3.3 Class **pyExec** (Function `PyExec`)

This operator executes given Python statements in a population's local namespace when it is applied to this population.

```
class pyExec (stmts="", exposePop="", output=">", stage=PostMating, begin=0, end=-1, step=1, at=[],  
              reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a `pyExec` operator that executes statements *stmts* in a population's local namespace when it is applied to this population. If *exposePop* is given, current population will be exposed in its local namespace as a variable named by *exposePop*. Although multiple statements can be executed, it is recommended that you use this operator to execute short statements and use `pyOperator` for more complex ones. Note that exposed population variable will be removed after the statements are executed.

```
clone ()
```

Deep copy of a `pyExec` operator

2.3.4 Class **infoEval** (Function `InfoEval`)

Unlike operator `pyEval` and `pyExec` that work at the population level, in a population's local namespace, operator `infoEval` works at the individual level, working with individual information fields. When this operator is applied to a population, information fields of eligible individuals are put into either a temporary dictionary or in the local namespace of the population. A Python expression is then evaluated for each individual. The result is written to an output.

Note:

Unlike operator “`infoExec`“, individual information fields are not updated after this operator is applied to a population. This operator tends to generate a large amount of output so use it with caution.

```
class infoEval (expr="", stmts="", usePopVars=False, exposeInd="", output=">", stage=PostMating, begin=0,  
                end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create an operator that evaluate a Python expression *expr* using individual information fields as variables. For each eligible individual (individuals in (virtual) subpopulations specified by parameter *subPops*, default to all individuals), its information fields are copied either to a temporary namespace (default) or the population's local namespace (if *usePopVars* is `True`). If *exposeInd* is not empty, the individual itself will be exposed in this namespace as a variable with name specified by *exposeInd*. In the *usePopVars=True* case, any population variable whose name matches an information field or *exposeInd* will be silently overridden.

A Python expression (*expr*) is evaluated for each individual. The results are converted to strings and are written to an output specified by parameter *output*. Optionally, a statement (or several statements separated by newline) can be executed before *expr* is evaluated.

This operator is by default applied post-mating. If its stage is set to `DuringMating`, it will be applied to all offspring, regardless of *subPops* settings.

Note Although *expr* is evaluated in individual or population level local namespaces, it can also access a global namespace which is the module namespace of your script. However, using module level variables and functions in this operator is discouraged.

```
apply (pop)
```

Apply the `infoEval` operator

```
clone ()
```

Deep copy of a `infoEval` operator

2.3.5 Class **infoExec** (Function `InfoExec`)

Operator `infoExec` is similar to `infoEval` in that it works at the individual level, using individual information

fields as variables. The difference is that instead of evaluating an expression and outputting its result, this operator execute one or more statements and **update individual information fields** from the namespace after the specified statements are executed.

```
class infoExec (stmts="", usePopVars=False, exposeInd="", output="", stage=PostMating, begin=0, end=-1,
                step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create an operator that executes Python statements *stmts* using individual information fields as variables. For each eligible individual (individuals in (virtual) subpopulations specified by parameter *subPops*, default to all individuals), its information fields are copied either to a temporary namespace (default) or the population's local namespace (if *usePopVars* is True). If *exposeInd* is not empty, the individual itself will be exposed in this namespace as a variable with name specified by *exposeInd*. In the *usePopVars*=True case, any population variable whose name matches an information field or *exposeInd* will be silently overridden.

One or more python statements (*stmts*) are executed for each individual. Information fields of these individuals are then updated from the corresponding variables. For example, *a=1* will set information field *a* of all individuals to 1, *a=b* will set information field *a* of all individuals to information field *b* or a population variable *b* if *b* is not an information field but a population variable (needs *usePopVars*=True), and *a=ind.sex()* will set information field *a* of all individuals to its sex (needs *exposeInd*='ind').

This operator is by default applied post-mating. If its stage is set to *DuringMating*, it will be applied to all offspring, regardless of *subPops* settings.

Note Although *stmts* are executed in individual or population level local namespaces, they also have access to a global namespace which is the module namespace of your script. However, using module level variables and functions in *stmts* is discouraged.

apply (*pop*)

Apply the *infoExec* operator

clone ()

Deep copy of a *infoExec* operator

2.4 Demographic models

2.4.1 Class *migrator*

This operator migrates individuals from (virtual) subpopulations to other subpopulations, according to either pre-specified destination subpopulation stored in an information field, or randomly according to a migration matrix.

In the former case, values in a specified information field (default to *migrate_to*) are considered as destination subpopulation for each individual. If *subPops* is given, only individuals in specified (virtual) subpopulations will be migrated where others will stay in their original subpopulation. Negative values are not allowed in this information field because they do not represent a valid destination subpopulation ID.

In the latter case, a migration matrix is used to randomly assign destination subpoulations to each individual. The elements in this matrix can be probabilities to migrate, proportions of individuals to migrate, or exact number of individuals to migrate.

By default, the migration matrix should have *m* by *m* elements if there are *m* subpopulations. Element (*i*, *j*) in this matrix represents migration probability, rate or count from subpopulation *i* to *j*. If *subPops* (length *m*) and/or *toSubPops* (length *n*) are given, the matrix should have *m* by *n* elements, corresponding to specified source and destination subpopulations. Subpopulations in *subPops* can be virtual subpopulations, which makes it possible to migrate, for example, males and females at different rates from a subpopulation. If a subpopulation in *toSubPops* does not exist, it will be created. In case that all individuals from a subpopulation are migrated, the empty subpopulation will be kept.

If migration is applied by probability, the row of the migration matrix corresponding to a source subpopulation is interpreted as probabilities to migrate to each destination subpopulation. Each individual's detination subpopulation is

assigned randomly according to these probabilities. Note that the probability of staying at the present subpopulation is automatically calculated so the corresponding matrix elements are ignored.

If migration is applied by proportion, the row of the migration matrix corresponding to a source subpopulation is interpreted as proportions to migrate to each destination subpopulation. The number of migrants to each destination subpopulation is determined before random individuals are chosen to migrate.

If migration is applied by counts, the row of the migration matrix corresponding to a source subpopulation is interpreted as number of individuals to migrate to each destination subpopulation. The migrants are chosen randomly.

This operator goes through all source (virtual) subpopulations and assign destination subpopulation of each individual to an information field. An `RuntimeError` will be raised if an individual is assigned to migrate more than once. This might happen if you are migrating from two overlapping virtual subpopulations.

class migrator (*rate=[]*, *mode=ByProbability*, *toSubPops=AllAvail*, *stage=PreMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields="migrate_to"*)

Create a migrator that moves individuals from source (virtual) subpopulations *subPops* (default to migrate from all subpopulations) to destination subpopulations *toSubPops* (default to all subpopulations), according to existing values in an information field *infoFields*[0], or randomly according to a migration matrix *rate*. In the latter case, the size of the matrix should match the number of source and destination subpopulations.

Depending on the value of parameter *mode*, elements in the migration matrix (*rate*) are interpreted as either the probabilities to migrate from source to destination subpopulations (*mode = ByProbability*), proportions of individuals in the source (virtual) subpopulations to the destination subpopulations (*mode = ByProportion*), numbers of migrants in the source (virtual) subpopulations (*mode = ByCounts*), or ignored completely (*mode = ByIndInfo*). In the last case, parameter *subPops* is respected (only individuals in specified (virtual) subpopulations will migrate) but *toSubPops* is ignored.

This operator is by default applied pre-mating (parameter *stage*). Please refer to operator `baseOperator` for a detailed explanation for all parameters.

apply (*pop*)

Apply the migrator to population *pop*.

clone ()

Deep copy of a migrator

rate ()

Return migration rate

2.4.2 Class `splitSubPops` (Function `SplitSubPops`)

Split a given list of subpopulations according to either sizes of the resulting subpopulations, proportion of individuals, or an information field. The resulting subpopulations will have the same name as the original subpopulation.

class splitSubPops (*subPops=AllAvail*, *sizes=[]*, *proportions=[]*, *names=[]*, *randomize=True*, *stage=PreMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *infoFields=[]*)

Split a list of subpopulations *subPops* into finer subpopulations. A single subpopulation is acceptable but virtual subpopulations are not allowed. All subpopulations will be split if *subPops* is not specified.

The subpopulations can be split in three ways:

- If parameter *sizes* is given, each subpopulation will be split into subpopulations with given size. The *sizes* should add up to the size of all original subpopulations.
- If parameter *proportions* is given, each subpopulation will be split into subpopulations with corresponding proportion of individuals. *proportions* should add up to 1.
- If an information field is given (parameter *infoFields*), individuals having the same value at this information field will be grouped into a subpopulation. The number of resulting subpopulations is determined by the number of distinct values at this information field.

If parameter `randomize` is `True` (default), individuals will be randomized before a subpopulation is split. This is designed to remove artificial order of individuals introduced by, for example, some non-random mating schemes. Note that, however, the original individual order is not guaranteed even if this parameter is set to `False`.

Unless the last subpopulation is split, the indexes of existing subpopulations will be changed. If a subpopulation has a name, this name will become the name for all subpopulations separated from this subpopulation. Optionally, you can assign names to the new subpopulations using a list of names specified in parameter `names`. Because the same set of names will be used for all subpopulations, this parameter is not recommended when multiple subpopulations are split.

This operator is by default applied pre-mating (parameter `stage`). Please refer to operator `baseOperator` for a detailed explanation for all parameters.

Note Unlike operator `migrator`, this operator does not require an information field such as `migrate_to`.

apply (*pop*)

Apply a `splitSubPops` operator

clone ()

Deep copy of a `splitSubPops` operator

2.4.3 Class `mergeSubPops` (Function `MergeSubPops`)

This operator merges subpopulations *subPops* to a single subpopulation. If *subPops* is ignored, all subpopulations will be merged. Virtual subpopulations are not allowed in *subPops*.

class mergeSubPops (*subPops=AllAvail, name="", stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, infoFields=[]*)

Create an operator that merges subpopulations *subPops* to a single subpopulation. If *subPops* is not given, all subpopulations will be merged. The merged subpopulation will take the name of the first subpopulation being merged unless a new *name* is given.

This operator is by default applied pre-mating (parameter `stage`). Please refer to operator `baseOperator` for a detailed explanation for all parameters.

apply (*pop*)

Apply a `mergeSubPops` operator

clone ()

Deep copy of a `mergeSubPops` operator

2.4.4 Class `resizeSubPops` (Function `ResizeSubPops`)

This operator resizes subpopulations to specified sizes. Individuals are added or removed depending on the new subpopulation sizes.

class resizeSubPops (*subPops=AllAvail, sizes=[], proportions=[], propagate=True, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, infoFields=[]*)

Resize given subpopulations *subPops* to new sizes *size*, or sizes proportional to original sizes (parameter *proportions*). All subpopulations will be resized if *subPops* is not specified. If the new size of a subpopulation is smaller than its original size, extra individuals will be removed. If the new size is larger, new individuals with empty genotype will be inserted, unless parameter *propagate* is set to `True` (default). In this case, existing individuals will be copied sequentially, and repeatedly if needed.

This operator is by default applied pre-mating (parameter `stage`). Please refer to operator `baseOperator` for a detailed explanation for all parameters.

apply (*pop*)

Apply a `resizeSubPops` operator

clone()
Deep copy of a `resizeSubPops` operator

2.5 Genotype transmitters

2.5.1 Class `genoTransmitter`

This during mating operator is the base class of all genotype transmitters. It is made available to users because it provides a few member functions that can be used by derived transmitters, and by customized Python during mating operators.

```
class genoTransmitter (output="", begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
    Create a base genotype transmitter.

clearChromosome (ind, ploidy, chrom)
    Clear (set alleles to zero) chromosome chrom on the ploidy-th homologous set of chromosomes of individual ind. It is equivalent to ind.setGenotype([0], ploidy, chrom).

clone()
    Deep copy of a base genotype transmitter.

copyChromosome (parent, parPloidy, offspring, ploidy, chrom)
    Transmit chromosome chrom on the parPloidy set of homologous chromosomes from parent to the ploidy set of homologous chromosomes of offspring. It is equivalent to offspring.setGenotype(parent.genotype(parPloidy, chrom), ploidy, chrom).

copyChromosomes (parent, parPloidy, offspring, ploidy)
    Transmit the parPloidy set of homologous chromosomes from parent to the ploidy set of homologous chromosomes of offspring. Customized chromosomes are not copied. It is equivalent to offspring.setGenotype(parent.genotype(parPloidy), ploidy).

initialize (pop)
    Initialize a base genotype operator for a population. This function should be called before any other functions are used to transmit genotype.
```

2.5.2 Class `cloneGenoTransmitter`

This during mating operator copies parental genotype directly to offspring. This operator works for all mating schemes when one or two parents are involved. If both parents are passed, maternal genotype are copied. This genotype transmitter does not copy genotype on customized chromosomes.

```
class cloneGenoTransmitter (output="", begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
    Create a clone genotype transmitter (a during-mating operator) that copies genotypes from parents to offspring. If two parents are specified, genotypes are copied maternally. Parameters subPops, and infoFields are ignored.

clone()
    Deep copy of a clone genotype transmitter.
```

2.5.3 Class `mendelianGenoTransmitter`

This Mendelian offspring generator accepts two parents and pass their genotypes to an offspring following Mendel's

laws. Sex chromosomes are handled according to the sex of the offspring, which is usually determined in advance by an offspring generator. Customized chromosomes are not handled.

```
class mendelianGenoTransmitter (output="", begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-  
                                Pops=AllAvail, infoFields=[])
```

Create a Mendelian genotype transmitter (a during-mating operator) that transmits genotypes from parents to offspring following Mendel's laws. Autosomes and sex chromosomes are handled but customized chromosomes are ignored. Parameters *subPops* and *infoFields* are ignored.

```
clone ()
```

Deep copy of a Mendelian genotype transmitter.

```
initialize (pop)
```

Initialize a base genotype operator for a population. This function should be called before function `transmitGenotype` is used to transmit genotype.

```
transmitGenotype (parent, offspring, ploidy)
```

Transmit genotype from parent to offspring, and fill the *ploidy* homologous set of chromosomes. This function does not set genotypes of customized chromosomes and handles sex chromosomes properly, according to offspring sex and *ploidy*.

2.5.4 Class `selfingGenoTransmitter`

A genotype transmitter (during-mating operator) that transmits parental genotype of a parent through self-fertilization. That is to say, the offspring genotype is formed according to Mendel's laws, only that a parent serves as both maternal and paternal parents.

```
class selfingGenoTransmitter (output="", begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-  
                                Pops=AllAvail, infoFields=[])
```

Create a self-fertilization genotype transmitter that transmits genotypes of a parent to an offspring through self-fertilization. Customized chromosomes are not handled. Parameters *subPops* and *infoFields* are ignored.

```
clone ()
```

Deep copy of a selfing genotype transmitter.

2.5.5 Class `haplodiploidGenoTransmitter`

A genotype transmitter (during-mating operator) for haplodiploid populations. The female parent is considered as diploid and the male parent is considered as haploid (only the first homologous copy is valid). If the offspring is `Female`, she will get a random copy of two homologous chromosomes of her mother, and get the only paternal copy from her father. If the offspring is `Male`, he will only get a set of chromosomes from his mother.

```
class haplodiploidGenoTransmitter (output="", begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-  
                                Pops=AllAvail, infoFields=[])
```

Create a haplodiploid genotype transmitter (during-mating operator) that transmit parental genotypes from parents to offspring in a haplodiploid population. Parameters *subPops* and *infoFields* are ignored.

```
clone ()
```

Deep copy of a haplodiploid transmitter.

2.5.6 Class `mitochondrialGenoTransmitter`

This geno transmitter assumes that the first homologous copy of several (or all) `Customized` chromosomes are copies of mitochondrial chromosomes. It transmits these chromosomes randomly from the female parent to offspring.

If this transmitter is applied to populations with more than one homologous copies of chromosomes, it transmits the first homologous copy of chromosomes and clears alleles (set to zero) on other homologous copies.

```
class mitochondrialGenoTransmitter (output="", chroms=[], begin=0, end=-1, step=1, at=[],
                                     reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a mitochondrial genotype transmitter that treats all Customized chromosomes, or a list of chromosomes specified by *chroms*, as human mitochondrial chromosomes. These chromosomes should have the same length and the same number of loci. This operator transmits these chromosomes randomly from the female parent to offspring of both sexes.

```
clone ()
```

Deep copy of a mitochondrial genotype transmitter.

2.5.7 Class recombinator

A genotype transmitter (during-mating operator) that transmits parental chromosomes to offspring, subject to recombination and gene conversion. This can be used to replace *mendelianGenoTransmitter* and *selfingGenoTransmitter*. It does not work in haplodiploid populations, although a customized genotype transmitter that makes use of this operator could be defined. Please refer to the *simuPOP* user's guide or online cookbook for details.

Recombination could be applied to all adjacent markers or after specified loci. Recombination rate between two adjacent markers could be specified directly, or calculated using physical distance between them. In the latter case, a recombination intensity is multiplied by physical distance between markers.

Gene conversion is interpreted as double-recombination events. That is to say, if a recombination event happens, it has a certain probability (can be 1) to become a conversion event, namely triggering another recombination event down the chromosome. The length of the converted chromosome can be controlled in a number of ways.

Note:

simuPOP does not assume any unit to loci positions so recombination intensity could be explained differently (e.g. cM/Mb, Morgan/Mb) depending on your interpretation of loci positions. For example, if basepair is used for loci position, *intensity*= 10^{-8} indicates 10^{-8} per basepair, which is equivalent to 10^{-2} per Mb or 1 cM/Mb. If Mb is used for physical positions, the same recombination intensity could be achieved by *intensity*=0.01.

```
class recombinator (rates=[], intensity=-1, loci=AllAvail, convMode=NoConversion, output="", begin=0, end=-1,
                    step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a recombinator (a mendelian genotype transmitter with recombination and gene conversion) that passes genotypes from parents (or a parent in case of self-fertilization) to offspring.

Recombination happens by default between all adjacent markers but can be limited to a given set of *loci*. Each locus in this list specifies a recombination point between the locus and the locus immediately **before** it. Loci that are the first locus on each chromosome are ignored.

If a single recombination rate (parameter *rates*) is specified, it will be used for all loci (all loci or loci specified by parameter *loci*), regardless of physical distances between adjacent loci.

If a list of recombination rates are specified in *rates*, a parameter *loci* with the same length should also be specified. Different recombination rates can then be used after these loci (between specified loci and their immediate neighbor to the right).

A recombination intensity (*intensity*) can be used to specify recombination rates that are proportional to physical distances between adjacent markers. If the physical distance between two markers is *d*, the recombination rate between them will be *intensity* * *d*. No unit is assumed for loci position and recombination intensity.

Gene conversion is controlled using parameter *convMode*, which can be

- **NoConversion**: no gene conversion (default).

- (`NumMarkers`, `prob`, `n`): With probability *prob*, convert a fixed number (*n*) of markers if a recombination event happens.
- (`GeometricDistribution`, `prob`, `p`): With probability *prob*, convert a random number of markers if a recombination event happens. The number of markers converted follows a geometric distribution with probability *p*.
- (`TractLength`, `prob`, `n`): With probability *prob*, convert a region of fixed tract length (*n*) if a recombination event happens. The actual number of markers converted depends on loci positions of surrounding loci. The starting position of this tract is the middle of two adjacent markers. For example, if four loci are located at 0, 1, 2, 3 respectively, a conversion event happens between 0 and 1, with a tract length 2 will start at 0.5 and end at 2.5, covering the second and third loci.
- (`ExponentialDistribution`, `prob`, `p`): With probability *prob*, convert a region of random tract length if a recombination event happens. The distribution of tract length follows an exponential distribution with probability *p*. The actual number of markers converted depends on loci positions of surrounding loci.

`simuPOP` uses this probabilistic model of gene conversion because when a recombination event happens, it may become a recombination event if the Holliday junction is resolved/repared successfully, or a conversion event if the junction is not resolved/repared. The probability, however, is more commonly denoted by the ratio of conversion to recombination events in the literature. This ratio varies greatly from study to study, ranging from 0.1 to 15 (Chen et al, Nature Review Genetics, 2007). This translates to 0.1/0.9 to 15/16 of the gene conversion probability.

A recombinator usually does not send any output. However, if an information field is given (parameter *infoFields*), this operator will treat this information field as a unique ID of parents and offspring and output all recombination events in the format of `offspring_id parent_id starting_ploidy loc1 loc2 ...` where *starting_ploidy* indicates which homologous copy genotype replication starts from (0 or 1), *loc1*, *loc2* etc are loci after which recombination events happen. If there are multiple chromosomes on the genome, you will see a lot of (fake) recombination events because of independent segregation of chromosomes. Such a record will be generated for each set of homologous chromosomes so a diploid offspring will have two lines of output. Note that individual IDs need to be set (using a `idTagger` operator) before this recombinator is applied.

Note conversion tract length is usually short, and is estimated to be between 337 and 456 bp, with overall range between maybe 50 - 2500 bp. This is usually not enough to convert, for example, two adjacent markers from the HapMap dataset. There is no recombination between sex chromosomes (Chromosomes X and Y), although recombination is possible between pseudoautosomal regions on these chromosomes. If such a feature is required, you will have to simulate the pseudoautosomal regions as separate chromosomes.

clone()

Deep copy of a recombinator

initialize(*pop*)

Initialize a recombinator for the genotypic structure of population *pop*. This function should be called before a recombinator is explicitly applied to a population.

transmitGenotype(*parent*, *offspring*, *ploidy*)

This function transmits genotypes from a *parent* to the *ploidy*-th homologous set of chromosomes of an *offspring*. It can be used, for example, by a customized genotype transmitter to use sex-specific recombination rates to transmit parental genotypes to offspring.

2.6 Mutation

2.6.1 Class `mutator`

Class `mutator` is the base class of all mutators. It handles all the work of picking an allele at specified loci from

certain (virtual) subpopulation with certain probability, and calling a derived mutator to mutate the allele. Alleles can be changed before and after mutation if existing allele numbers do not match those of a mutation model.

class mutator (*rates=[]*, *loci=AllAvail*, *mapIn=[]*, *mapOut=[]*, *context=0*, *output=">"*, *stage=PostMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)

A mutator mutates alleles from one state to another with given probability. This base mutator does not perform any mutation but it defines common behaviors of all mutators.

By default, a mutator mutates all alleles in all populations of a simulator at all generations. A number of parameters can be used to restrict mutations to certain generations (parameters *begin*, *end*, *step* and *at*), replicate populations (parameter *rep*), (virtual) subpopulations (parameter *subPops*) and loci (parameter *loci*). Please refer to class `baseOperator` for a detailed explanation of these parameters.

Parameter *rate* or its equivalence specifies the probability that a mutation event happens. The exact form and meaning of *rate* is mutator-specific. If a single rate is specified, it will be applied to all *loci*. If a list of mutation rates are given, they will be applied to each locus specified in parameter *loci*. Note that not all mutators allow specification of multiple mutation rate, especially when the mutation rate itself is a list or matrix.

Alleles at a locus are non-negative numbers 0, 1, ... up to the maximum allowed allele for the loaded module (1 for binary, 255 for short and 65535 for long modules). Whereas some general mutation models treat alleles as numbers, other models assume specific interpretation of alleles. For example, an `acgtMutator` assumes alleles 0, 1, 2 and 3 as nucleotides A, C, G and T. Using a mutator that is incompatible with your simulation will certainly yield erroneous results.

If your simulation assumes different alleles with a mutation model, you can map an allele to the allele used in the model and map the mutated allele back. This is achieved using a *mapIn* list with its *i*-th item being the corresponding allele of real allele *i*, and a *mapOut* list with its *i*-th item being the real allele of allele *i* assumed in the model. For example *mapIn*=[0, 0, 1] and *mapOut*=[1, 2] would allow the use of a `snpmutator` to mutate between alleles 1 and 2, instead of 0 and 1. Parameters *mapIn* and *mapOut* also accept a user-defined Python function that returns a corresponding allele for a given allele. This allows easier mapping between a large number of alleles and advanced models such as random emission of alleles.

Some mutation models are context dependent. Namely, how an allele mutates will depend on its adjacent alleles. Whereas most `simuPOP` mutators are context independent, some of them accept a parameter *context* which is the number of alleles to the left and right of the mutated allele. For example *context=1* will make the alleles to the immediate left and right to a mutated allele available to a mutator. These alleles will be mapped in if parameter *mapIn* is defined. How exactly a mutator makes use of these information is mutator dependent.

apply (*pop*)

Apply a mutator.

clone ()

Deep copy of a `mutator`

fillContext (*pop*, *ptr*, *locus*)

A rarely used feature, performance should be a secondary consideration.

2.6.2 Class `matrixMutator` (Function `MatrixMutate`)

A matrix mutator mutates alleles 0, 1, ..., *n*-1 using a *n* by *n* matrix, which specifies the probability at which each allele mutates to another. Conceptually speaking, this mutator goes through all mutable allele and mutate it to another state according to probabilities in the corresponding row of the rate matrix. Only one mutation rate matrix can be specified which will be used for all specified loci. #

class matrixMutator (*rate*, *loci=AllAvail*, *mapIn=[]*, *mapOut=[]*, *output=">"*, *stage=PostMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)

Create a mutator that mutates alleles 0, 1, ..., *n*-1 using a *n* by *n* matrix *rate*. Item (*i*, *j*) of this matrix specifies the probability at which allele *i* mutates to allele *j*. Diagonal items (*i*, *i*) are ignored because they are automatically determined by other probabilities. Only one mutation rate matrix can be specified which will be

used for all loci in the applied population, or loci specified by parameter *loci*. Please refer to classes `mutator` and `baseOperator` for detailed explanation of other parameters.

```
clone()  
    Deep copy of a matrixMutator
```

2.6.3 Class `kamMutator` (Function `KamMutate`)

This mutator implements a *k-allele* mutation model that assumes *k* allelic states (alleles 0, 1, 2, ..., *k-1*) at each locus. When a mutation event happens, it mutates an allele to any other states with equal probability.

```
class kamMutator (k, rates=[], loci=AllAvail, mapIn=[], mapOut=[], output">", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])  
    Create a k-allele mutator that mutates alleles to one of the other k-1 alleles with equal probability. This mutator by default applies to all loci unless parameter loci is specified. A single mutation rate will be used for all loci if a single value of parameter rates is given. Otherwise, a list of mutation rates can be specified for each locus in parameter loci. Please refer to classes mutator and baseOperator for descriptions of other parameters.
```

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

2.6.4 Class `smmMutator` (Function `SmmMutate`)

A stepwise mutation model treats alleles at a locus as the number of tandem repeats of microsatellite or minisatellite markers. When a mutation event happens, the number of repeats (allele) either increase or decrease. A standard stepwise mutation model increases or decreases an allele by 1 with equal probability. More complex models (generalized stepwise mutation model) are also allowed. Note that an allele cannot be mutated beyond boundaries (0 and maximum allowed allele).

```
class smmMutator (rates=[], loci=AllAvail, incProb=0.5, maxAllele=0, mutStep=[], mapIn=[], mapOut=[], output">", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])  
    Create a stepwise mutation mutator that mutates an allele by increasing or decreasing it. This mutator by default applies to all loci unless parameter loci is specified. A single mutation rate will be used for all loci if a single value of parameter rates is given. Otherwise, a list of mutation rates can be specified for each locus in parameter loci.
```

When a mutation event happens, this operator increases or decreases an allele by *mutStep* steps. Acceptable input of parameter *mutStep* include

- A number: This is the default mode with default value 1.
- (`GeometricDistribution`, *p*): The number of steps follows a geometric distribution with parameter *p*.
- A Python function: This user defined function accepts the allele being mutated and return the steps to mutate.

The mutation process is usually neutral in the sense that mutating up and down is equally likely. You can adjust parameter *incProb* to change this behavior.

If you need to use other generalized stepwise mutation models, you can implement them using a `pyMutator`. If performance becomes a concern, I may add them to this operator if provided with a reliable reference.

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


2.6.5 Class `pyMutator` (Function `PyMutate`)

This hybrid mutator accepts a Python function that determines how to mutate an allele when a mutation event happens.

```
class pyMutator (rates=[], loci=AllAvail, func=None, context=0, mapIn=[], mapOut=[], output=">",
                 stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a hybrid mutator that uses a user-provided function to mutate an allele when a mutation event happens. This function (parameter *func*) accepts the allele to be mutated and return a mutated allele. If *context* is specified, the *context* alleles to the left and to the right of the mutated alleles will be passed to this function as the second parameter. Invalid context alleles (e.g. left allele to the first locus of a chromosome) will be marked by -1. The passed, returned and context alleles might be changed if parameters *mapIn* and *mapOut* are used although allele mappings, if needed, are usually handled in *func* as well. This mutator by default applies to all loci unless parameter *loci* is specified. A single mutation rate will be used for all loci if a single value of parameter *rates* is given. Otherwise, a list of mutation rates can be specified for each locus in parameter *loci*. Please refer to classes `mutator` and `baseOperator` for descriptions of other parameters.

```
clone ()
```

Deep copy of a `pyMutator`

2.6.6 Class `mixedMutator` (Function `MixedMutate`)

This mixed mutator accepts a list of mutators and use one of them to mutate an allele when a mutation event happens.

```
class mixedMutator (rates=[], loci=AllAvail, mutators=[], prob=[], mapIn=[], mapOut=[], context=0, output=">",
                    stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a mutator that randomly chooses one of the specified *mutators* to mutate an allele when a mutation event happens. The mutators are chosen according to a list of probabilities (*prob*) that should add up to 1. The passed and returned alleles might be changed if parameters *mapIn* and *mapOut* are used. Most parameters, including *loci*, *mapIn*, *mapOut*, *rep*, and *subPops* of mutators specified in parameter *mutators* are ignored. This mutator by default applies to all loci unless parameter *loci* is specified. Please refer to classes `mutator` and `baseOperator` for descriptions of other parameters.

```
clone ()
```

Deep copy of a `mixedMutator`

2.6.7 Class `contextMutator` (Function `ContextMutate`)

This context-dependent mutator accepts a list of mutators and use one of them to mutate an allele depending on the context of the mutated allele.

```
class contextMutator (rates=[], loci=AllAvail, mutators=[], contexts=[], mapIn=[], mapOut=[], output=">",
                      stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[])
```

Create a mutator that choose one of the specified *mutators* to mutate an allele when a mutation event happens. The mutators are chosen according to the context of the mutated allele, which is specified as a list of alleles to the left and right of an allele (*contexts*). For example, `contexts=[(0,0), (0,1), (1,1)]` indicates which mutators should be used to mutate allele *x* in the context of `0x0`, `0x1`, and `1x1`. A context can include more than one alleles at both left and right sides of a mutated allele but all contexts should have the same (even) number of alleles. If an allele does not have full context (e.g. when a locus is the first locus on a chromosome),

unavailable alleles will be marked as -1. There should be a mutator for each context but an additional mutator can be specified as the default mutator for unmatched contexts. If parameters *mapIn* is specified, both mutated allele and its context alleles will be mapped. Most parameters, including *loci*, *mapIn*, *mapOut*, *rep*, and *subPops* of mutators specified in parameter *mutators* are ignored. This mutator by default applies to all loci unless parameter *loci* is specified. Please refer to classes `mutator` and `baseOperator` for descriptions of other parameters.

clone()
Deep copy of a `context-dependentMutator`

2.6.8 Class `pointMutator` (Function `PointMutate`)

A point mutator is different from all other mutators because mutations in this mutator do not happen randomly. Instead, it happens to specific loci and mutate an allele to a specific state, regardless of its original state. This mutator is usually used to introduce a mutant to a population.

class `pointMutator` (*loci*, *allele*, *ploidy*=0, *inds*=[], *output*=">", *stage*=`PostMating`, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=`AllAvail`, *subPops*=0, *infoFields*=[])

Create a point mutator that mutates alleles at specified *loci* to a given *allele* of individuals *inds*. If there are multiple alleles at a locus (e.g. individuals in a diploid population), only the first allele is mutated unless indexes of alleles are listed in parameter *ploidy*. This operator is by default applied to individuals in the first subpopulation but you can apply it to a different or more than one (virtual) subpopulations using parameter **subPops** ("`AllAvail`" is also accepted). Please refer to class `baseOperator` for detailed descriptions of other parameters.

apply(*pop*)
Apply a `pointMutator`

clone()
Deep copy of a `pointMutator`

2.6.9 Derived mutation operators

`snpMutator` (*u*=0, *v*=0, **args*, ***kwargs*)

Because there are only two alleles, this mutation model only needs to know the mutation rate from allele 0 to 1 (parameter *u*) and from 1 to 0 (parameter *v*).

`acgtMutator` (*rate*=[], *model*='general', **args*, ***kwargs*)

This operator assumes alleles 0, 1, 2, 3 as nucleotides A, C, G and T and use a 4 by 4 mutation rate matrix to mutate them. Although a general model needs 12 parameters, less parameters are needed for specific nucleotide mutation models (parameter *model*). The length and meaning of parameter *rate* is model dependent. Currently supported models are Jukes and Cantor 1969 model (`JC69`), Kimura's 2-parameter model (`K80`), Felsenstein 1981 model (`F81`), Hasegawa, Kishino and Yano 1985 model (`HKY85`), Tamura 1992 model (`T92`), Tamura and Nei 1993 model (`TN93`), Generalized time reversible model (`GTR`), and a general model (`general`) with 12 parameters. Please refer to the `simuPOP` user's guide for detailed information about each model.

2.7 Selection

2.7.1 Class `selector`

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

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

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

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

Note:

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

```
class selector (stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail)
    Create a selector
    apply (pop)
        Set fitness to all individuals. No selection will happen!
    clone ()
        Deep copy of a selector
```

2.7.2 Class `mapSelector` (Function `MapSelector`)

Selection according to the genotype at one or more loci This map selector implements selection according to genotype at one or more loci. A user provided dictionary (map) of genotypes will be used in this selector to set each individual's fitness value.

```
class mapSelector (loci, fitness, phase=False, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail)
    Create a map selector
    locus: The locus index. A shortcut to loci=[locus]
    loci: The locus indexes. The genotypes at these loci will be used to determine the fitness value.
    fitness: A dictionary of fitness values. The genotype must be in the form of 'a-b' for a single locus, and 'a-b|c-d|e-f' for multi-loci. In the haploid case, the genotype should be specified in the form of 'a' for single locus, and 'a|b|c' for multi-locus models.
    phase: If True, genotypes a-b and b-a will have different fitness values. Default to False.
    output: And other parameters please refer to help(baseOperator.__init__)
    clone ()
        Deep copy of a map selector
```

2.7.3 Class `maSelector` (Function `MaSelect`)

Multiple allele selector (selection according to wildtype or diseased alleles) This is called 'multiple-allele' selector. It separates alleles into two groups: wildtype and diseased alleles. Wildtype alleles are specified by parameter `wildtype` and any other alleles are considered as diseased alleles.

This selector accepts an array of fitness values:

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

class `maSelector` (*loci, fitness, wildtype=0, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail*)

Create a multiple allele selector Please refer to `baseOperator` for other parameter descriptions.

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

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

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

Note

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

`clone()`

Deep copy of a `maSelector`

`indFitness (ind, gen)`

Calculate/return the fitness value, currently assuming diploid

2.7.4 Class `mlSelector` (Function `MlSelect`)

Selection according to genotypes at multiple loci in a multiplicative model This selector is a 'multiple-locus model' selector. The selector takes a vector of selectors (can not be another `mlSelector`) and evaluate the fitness of an individual as the product or sum of individual fitness values. The mode is determined by parameter `mode`, which takes one of the following values

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

class `mlSelector` (*selectors, mode=Multiplicative, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail*)

Create a multiple-locus selector Please refer to `mapSelector` for other parameter descriptions.

selectors: A list of selectors

`clone()`

Deep copy of a `mlSelector`

2.7.5 Class `pySelector` (Function `PySelect`)

Selection using user provided function This selector assigns fitness values by calling a user provided function. It accepts a list of loci and a Python function `func`. For each individual, this operator will pass the genotypes at these loci, generation number, and optionally values at some information fields to this function. The return value is treated as the fitness value. The genotypes are arranged in the order of 0-0, 0-1, 1-0, 1-1 etc. where X-Y represents locus X - ploidy Y. More specifically, `func` can be

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

class `pySelector` (*loci, func, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-Pops=AllAvail, infoFields=AllAvail*)

Create a Python hybrid selector

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

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

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

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

`clone()`

Deep copy of a `pySelector`

2.8 Penetrance

2.8.1 Class `basePenetrance`

Base class of all penetrance operators. Penetrance is the probability that one will have the disease when he has certain genotype(s). An individual will be randomly marked as affected/unaffected according to his/her penetrance value. For example, an individual will have probability 0.8 to be affected if the penetrance is 0.8.

Penetrance can be applied at any stage (default to `DuringMating`). When a penetrance operator is applied, it calculates the penetrance value of each offspring and assigns affected status accordingly. Penetrance can also be used `PreMating` or `PostMating`. In these cases, the affected status will be set to all individuals according to their penetrance values.

Penetrance values are usually not saved. If you would like to know the penetrance value, you need to

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

Penetrance functions can be applied to the current, all, or certain number of ancestral generations. This is controlled by the `ancestralGen` parameter, which is default to -1 (all available ancestral generations). You can set it to 0 if you only need affection status for the current generation, or specify a number `n` for the number of ancestral generations

(n + 1 total generations) to process. Note that the `ancestralGen` parameter is ignored if the penetrance operator is used as a during mating operator.

class basePenetrance (*ancestralGen=-1, stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[]*)

Create a penetrance operator

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

stage: Specify the stage this operator will be applied. Default to `DuringMating`.

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

apply (*pop*)

Set penetrance to all individuals and record penetrance if requested

clone ()

Deep copy of a penetrance operator

2.8.2 Class mapPenetrance (Function MapPenetrance)

Penetrance according to the genotype at one locus Assign penetrance using a table with keys 'X-Y' where X and Y are allele numbers.

class mapPenetrance (*loci, penetrance, phase=False, ancGen=-1, stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[]*)

Create a map penetrance operator

locus: The locus index. Shortcut to `loci=[locus]`

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

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

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

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

clone ()

Deep copy of a map penetrance operator

2.8.3 Class maPenetrance (Function MaPenetrance)

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

class maPenetrance (*loci, penetrance, wildtype=AllAvail, ancGen=-1, stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[]*)

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

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

loci: The locus indexes. The genotypes of these loci will be examined.

penet: An array of penetrance values of AA, Aa, aa. A is the wild type group. In the case of multiple loci, penetrance should be in the order of AABB, AABb, AAbb, AaBB, AaBb, Aabb, aaBB, aaBb, aabb.

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

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

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

2.8.4 Class **mlPenetrance** (Function **mlPenetrance**)

Penetrance according to the genotype according to a multiple loci multiplicative model This is the 'multiple-locus' penetrance calculator. It accepts a list of penetrances and combine them according to the `mode` parameter, which takes one of the following values:

- **PEN_Multiplicative**: the penetrance is calculated as $f = \prod f_i$.
- **PEN_Additive**: the penetrance is calculated as $f = \min(1, \sum f_i)$. f will be set to 1 when $f < 0$. In this case, s_i are added, not f_i directly.
- **PEN_Heterogeneity**: the penetrance is calculated as $f = 1 - \prod (1 - f_i)$.

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

class mlPenetrance (*peneOps*, *mode=Multiplicative*, *ancGen=-1*, *stage=DuringMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)
 Create a multiple locus penetrance operator
peneOps: A list of penetrance operators
mode: Can be one of **PEN_Multiplicative**, **PEN_Additive**, and **PEN_Heterogeneity**
clone()
 Deep copy of a multi-loci penetrance operator

2.8.5 Class **pyPenetrance** (Function **pyPenetrance**)

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

More specifically, `func` can be

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

class pyPenetrance (*loci*, *func*, *ancGen=-1*, *stage=DuringMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)
 Provide locus and penetrance for 11, 12, 13 (in the form of dictionary)
loci: The genotypes at these loci will be passed to the provided Python function in the form of `loc1_1`, `loc1_2`, `loc2_1`, `loc2_2`, ... if the individuals are diploid.
func: A user-defined Python function that accepts an array of genotypes at specified loci and return a penetrance value. The return value should be between 0 and 1.
infoFields: If specified, the first field should be the information field to save calculated penetrance value. The values of the rest of the information fields (if available) will also be passed to the user defined penetrance function.
output: And other parameters please refer to `help(baseOperator.__init__)`
clone()
 Deep copy of a Python penetrance operator

2.9 Quantitative Trait

2.9.1 Class `quanTrait`

Base class of 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.

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

```
class quanTrait (ancGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-  
                Pops=AllAvail, infoFields=AllAvail)  
    Create a quantitative trait operator  
  
    apply (pop)  
        Set qtrait to all individual  
  
    clone ()  
        Deep copy of a quantitative trait operator
```

2.9.2 Class `mapQuanTrait` (Function `MapQuanTrait`)

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

```
class mapQuanTrait (loci, qtrait, sigma=0, phase=False, ancGen=-1, stage=PostMating, begin=0, end=-1,  
                    step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail)  
    Create a map quantitative trait operator  
  
    locus: The locus index. The quantitative trait is determined by genotype at this locus.  
  
    loci: An array of locus indexes. The quantitative trait is determined by genotypes at these loci.  
  
    qtrait: A dictionary of quantitative traits. The genotype must be in the form of 'a-b'. This is the mean of the  
           quantitative trait. The actual trait value will be  $N(\text{mean}, \sigma^2)$ . For multiple loci, the form is 'a-b1c-d1e-f'  
           etc.  
  
    sigma: Standard deviation of the environmental factor  $N(0, \sigma^2)$ .  
  
    phase: If True, a/b and b/a will have different quantitative trait values. Default to False.  
  
    output: And other parameters please refer to help (baseOperator.__init__)  
  
    clone ()  
        Deep copy of a map quantitative trait operator
```

2.9.3 Class `maQuanTrait` (Function `MaQuanTrait`)

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

class maQuanTrait (*loci, qtrait, wildtype, sigma=[], ancGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail*)
 Create a multiple allele quantitative trait operator Please refer to `quanTrait` for other parameter descriptions.
qtrait: An array of quantitative traits of AA, Aa, aa. A is the wildtype group
sigma: An array of standard deviations for each of the trait genotype (AA, Aa, aa)
wildtype: An array of alleles in the wildtype group. Any other alleles will be considered as diseased alleles.
 Default to [0].
output: And other parameters please refer to `help(baseOperator.__init__)`
clone()
 Deep copy of a multiple allele quantitative trait

2.9.4 Class mlQuanTrait (Function MlQuanTrait)

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

- **Multiplicative**: the mean of the quantitative trait is calculated as $f = \prod f_i$.
- **Additive**: the mean of the quantitative trait is calculated as $f = \sum f_i$.

Note that all σ_i (for f_i) and σ (for f) will be considered. I.e, the trait value should be

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

for Additive case. If this is not desired, you can set some of the σ to zero.

class mlQuanTrait (*qtraits, mode=Multiplicative, sigma=0, ancGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail*)
 Create a multiple locus quantitative trait operator Please refer to `quanTrait` for other parameter descriptions.
qtraits: A list of quantitative traits
mode: Can be one of `Multiplicative` and `Additive`
clone()
 Deep copy of a multiple loci quantitative trait operator
qtrait (*ind*)
 Currently assuming diploid

2.9.5 Class pyQuanTrait (Function PyQuanTrait)

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

class pyQuanTrait (*loci, func, ancGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=AllAvail*)
 Create a Python quantitative trait operator Please refer to `quanTrait` for other parameter descriptions.
loci: The genotypes at these loci will be passed to `func`.
func: A Python function that accepts genotypes at specified loci and returns the quantitative trait value.
output: And other parameters please refer to `help(baseOperator.__init__)`
clone()
 Deep copy of a Python quantitative trait operator

2.10 Statistics Calculation

2.10.1 Class `stat` (Function `Stat`)

Operator `stat` calculates various statistics of the population being applied and sets variables in its local namespace. Other operators or functions can retrieve results from or evaluate expressions in this local namespace after `stat` is applied.

```
class stat (popSize=False, numOfMale=False, numOfAffected=False, alleleFreq=[], heteroFreq=[], homoFreq=[],  
            genoFreq=[], haploFreq=[], sumOfInfo=AllAvail, meanOfInfo=AllAvail, varOfInfo=AllAvail, max-  
            OfInfo=AllAvail, minOfInfo=AllAvail, LD=[], association=[], neutrality=[], structure=[], HWE=[],  
            vars=AllAvail, suffix="", output="", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail,  
            subPops=AllAvail, infoFields=[])
```

Create a `stat` operator that calculates specified statistics of a population when it is applied to this population. This operator is by default applied after mating (parameter `stage`) and can be applied to specified replicates (parameter `rep`) at specified generations (parameter `begin`, `end`, `step`, and `at`). This operator does not produce any output (ignore parameter `output`) after statistics are calculated. Instead, it stores results in the local namespace of the population being applied. Other operators can retrieve these variables or evaluate expression directly in this local namespace. Please refer to operator `baseOperator` for a detailed explanation of these common operator parameters.

`stat` supports parameter `subPops`. It usually calculate the same set of statistics for all subpopulations (`subPops=subPopList()`). If a list of (virtual) subpopulations are specified, statistics for only specified subpopulations will be calculated. However, different statistics treat this parameter differently and it is very important to check its reference before you use `subPops` for any statistics.

Calculated statistics are saved as variables in a population's local namespace. These variables can be numbers, lists or dictionaries and can be retrieved using functions `population.vars()` or `population.dvars()`. A special default dictionary (`defdict`) is used for dictionaries whose keys are determined dynamically. Accessing elements of such a dictionary with an invalid key will yield value 0 instead of a `KeyError`. If the same variables are calculated for one or more (virtual) subpopulation, the variables are stored in `vars()['subPop'][sp]['var']` where `sp` is a subpopulation ID (`sp`) or a tuple of virtual subpopulation ID (`(sp, vsp)`). `population.vars(sp)` and `population.dvars(sp)` provide shortcuts to these variables.

Operator `stat` outputs a number of most useful variables for each type of statistic. For example, `alleleFreq` calculates both allele counts and allele frequencies and it by default sets variable `alleleFreq` (`dvars().alleleFreq`) for all or specified subpopulations. If this does not fit your need, you can use parameter `vars` to output additional parameters, or limit the output of existing parameters. More specifically, for this particular statistic, the available variables are `'alleleFreq'`, `'alleleNum'`, `'alleleFreq_sp'` (`'alleleFreq'` in each subpopulation), and `'alleleNum_sp'` (`'alleleNum'` in each subpopulation). You can set `vars=['alleleNum_sp']` to output only subpopulation specific allele count. An optional suffix (parameter `suffix`) can be used to append a suffix to default parameter names. This parameter can be used, for example, to calculate and store the same statistics for different subpopulations (e.g. pairwise `Fst`).

Operator `stat` supports the following statistics:

popSize: If `popSize=True`, number of individuals in all or specified subpopulations (parameter `subPops`) will be set to the following variables:

- `popSize` (default): Number of individuals in all or specified subpopulations. Because `subPops` does not have to cover all individuals, it may not be the actual population size.
- `popSize_sp`: Size of (virtual) subpopulation `sp`.
- `subPopSize` (default): A list of (virtual) subpopulation sizes. This variable is easier to use than accessing `popSize` from each (virtual) subpopulation.

numOfMale: If `numOfMale=True`, number of male individuals in all or specified (virtual) subpopulations will be set to the following variables:

- **numOfMale** (default): Total number of male individuals in all or specified (virtual) subpopulations.
- **numOfFemale** (default): Total number of female individuals in all or specified (virtual) subpopulations.
- **propOfMale**: Proportion of male individuals.
- **propOfFemale**: Proportion of female individuals.
- **numOfMale_sp**: Number of male individuals in each (virtual) subpopulation.
- **numOfFemale_sp**: Number of female individuals in each (virtual) subpopulation.
- **propOfMale_sp**: Proportion of male individuals in each (virtual) subpopulation.
- **propOfFemale_sp**: Proportion of female individuals in each (virtual) subpopulation.

numOfAffected: If *numOfAffected=True*, number of affected individuals in all or specified (virtual) subpopulations will be set to the following variables:

- **numOfAffected** (default): Total number of affected individuals in all or specified (virtual) subpopulations.
- **numOfUnaffected** (default): Total number of unaffected individuals in all or specified (virtual) subpopulations.
- **propOfAffected**: Proportion of affected individuals.
- **propOfUnaffected**: Proportion of unaffected individuals.
- **numOfAffected_sp**: Number of affected individuals in each (virtual) subpopulation.
- **numOfUnaffected_sp**: Number of unaffected individuals in each (virtual) subpopulation.
- **propOfAffected_sp**: Proportion of affected individuals in each (virtual) subpopulation.
- **propOfUnaffected_sp**: Proportion of unaffected individuals in each (virtual) subpopulation.

alleleFreq: This parameter accepts a list of loci (by indexes), at which allele frequencies will be calculated. This statistic outputs the following variables, all of which are dictionary (with loci indexes as keys) of default dictionaries (with alleles as keys). For example, `alleleFreq[loc][a]` returns 0 if allele *a* does not exist.

- **alleleFreq** (default): `alleleFreq[loc][a]` is the frequency of allele *a* at locus for all or specified (virtual) subpopulations.
- **alleleNum** (default): `alleleNum[loc][a]` is the number of allele *a* at locus for all or specified (virtual) subpopulations.
- **alleleFreq_sp**: Allele frequency in each (virtual) subpopulation.
- **alleleNum_sp**: Allele count in each (virtual) subpopulation.

heteroFreq and **homoFreq**: These parameters accept a list of loci (by indexes), at which the number and frequency of homozygotes and/or heterozygotes will be calculated. These statistics are only available for diploid populations. The following variables will be outputted:

- **heteroFreq** (default for parameter *heteroFreq*): A dictionary of proportion of heterozygotes in all or specified (virtual) subpopulations, with loci indexes as dictionary keys.
- **homoFreq** (default for parameter *homoFreq*): A dictionary of proportion of homozygotes in all or specified (virtual) subpopulations.
- **heteroNum**: A dictionary of number of heterozygotes in all or specified (virtual) subpopulations.
- **homoNum**: A dictionary of number of homozygotes in all or specified (virtual) subpopulations.
- **heteroFreq_sp**: A dictionary of proportion of heterozygotes in each (virtual) subpopulation.
- **homoFreq_sp**: A dictionary of proportion of homozygotes in each (virtual) subpopulation.
- **heteroNum_sp**: A dictionary of number of heterozygotes in each (virtual) subpopulation.
- **homoNum_sp**: A dictionary of number of homozygotes in each (virtual) subpopulation.

genoFreq: This parameter accept a list of loci (by index) at which number and frequency of all genotypes are outputted as a dictionary (indexed by loci indexes) of default dictionaries (indexed by tuples of possible indexes). This statistic is available for all population types with genotype defined as ordered alleles at a locus. The length of genotype equals the number of homologous copies of chromosomes (ploidy) of a population. Genotypes for males or females on sex chromosomes or in haplodiploid populations will have different length. Because genotypes are ordered, (1, 0) and (0, 1) (two possible genotypes in a diploid population) are considered as different genotypes. This statistic outputs the following variables:

- **genoFreq** (default): A dictionary (by loci indexes) of default dictionaries (by genotype) of genotype frequencies. For example, `genoFreq[1][(1, 0)]` is the frequency of genotype (1, 0) at locus 1.
- **genoNum** (default): A dictionary of default dictionaries of genotype counts of all or specified (virtual) subpopulations.
- **genoFreq_sp**: genotype frequency in each specified (virtual) subpopulation.
- **genoFreq_sp**: genotype count in each specified (virtual) subpopulation.

haploFreq: This parameter accepts one or more lists of loci (by index) at which number and frequency of haplotypes are outputted as default dictionaries. `[(1, 2)]` can be abbreviated to `(1, 2)`. For example, using parameter `haploFreq=(1, 2, 4)`, all haplotypes at loci 1, 2 and 4 are counted. This statistic saves results to dictionary (with loci index as keys) of default dictionaries (with haplotypes as keys) such as `haploFreq[(1, 2, 4)][(1, 1, 0)]` (frequency of haplotype (1, 1, 0) at loci (1, 2, 3)). This statistic works for all population types. Number of haplotypes for each individual equals to his/her ploidy number. Haplodiploid populations are supported in the sense that the second homologous copy of the haplotype is not counted for male individuals. This statistic outputs the following variables:

- **haploFreq** (default): A dictionary (with tuples of loci indexes as keys) of default dictionaries of haplotype frequencies. For example, `haploFreq[(0, 1)][(1, 1)]` records the frequency of haplotype (1, 1) at loci (0, 1) in all or specified (virtual) subpopulations.
- **haploNum** (default): A dictionary of default dictionaries of haplotype counts in all or specified (virtual) subpopulations.
- **haploFreq_sp**: Haptype frequencies in each (virtual) subpopulation.
- **haploNum_sp**: Haptype count in each (virtual) subpopulation.

sumOfInfo, meanOfInfo, varOfInfo, maxOfInfo and minOfInfo: Each of these five parameters accepts a list of information fields. For each information field, the sum, mean, variance, maximum or minimal (depending on the specified parameter(s)) of this information field at individuals in all or specified (virtual) subpopulations will be calculated. The results will be put into the following population variables:

- **sumOfInfo** (default for *sumOfInfo*): A dictionary of the sum of specified information fields of individuals in all or specified (virtual) subpopulations. This dictionary is indexed by names of information fields.
- **meanOfInfo** (default for *meanOfInfo*): A dictionary of the mean of information fields of all individuals.
- **varOfInfo** (default for *varOfInfo*): A dictionary of the sample variance of information fields of all individuals.
- **maxOfInfo** (default for *maxOfInfo*): A dictionary of the maximum value of information fields of all individuals.
- **minOfInfo** (default for *minOfInfo*): A dictionary of the minimal value of information fields of all individuals.
- **sumOfInfo_sp**: A dictionary of the sum of information fields of individuals in each subpopulation.
- **meanOfInfo_sp**: A dictionary of the mean of information fields of individuals in each subpopulation.
- **varOfInfo_sp**: A dictionary of the sample variance of information fields of individuals in each subpopulation.

- `maxOfInfo_sp`: A dictionary of the maximum value of information fields of individuals in each subpopulation.
- `minOfInfo_sp`: A dictionary of the minimal value of information fields of individuals in each subpopulation.

LD: Parameter `LD` accepts one or a list of loci pairs (e.g. `LD=[[0,1],[2,3]]`) with optional primary alleles at both loci (e.g. `LD=[0,1,0,0]`). For each pair of loci, this operator calculates linkage disequilibrium and optional association statistics between two loci. When primary alleles are specified, signed linkage disequilibrium values are calculated with non-primary alleles are combined. Otherwise, absolute values of diallelic measures are combined to yield positive measure of LD. Association measures are calculated from a m by n contingency of haplotype counts ($m=n=2$ if primary alleles are specified). Please refer to the `simuPOP` user's guide for detailed information. This statistic sets the following variables:

- `LD` (default) Basic LD measure for haplotypes in all or specified (virtual) subpopulations. Signed if primary alleles are specified.
- `LD_prime` (default) Lewontin's D' measure for haplotypes in all or specified (virtual) subpopulations. Signed if primary alleles are specified.
- `R2` (default) Correlation LD measure for haplotypes in all or specified (virtual) subpopulations.
- `LD_ChiSq` ChiSq statistics for a contingency table with frequencies of haplotypes in all or specified (virtual) subpopulations.
- `LD_ChiSq_p` Single side p-value for the ChiSq statistic. Degrees of freedom is determined by number of alleles at both loci and the specification of primary alleles.
- `CramerV` Normalized ChiSq statistics.
- `LD_sp` Basic LD measure for haplotypes in each (virtual) subpopulation.
- `LD_prime_sp` Lewontin's D' measure for haplotypes in each (virtual) subpopulation.
- `R2_sp` R^2 measure for haplotypes in each (virtual) subpopulation.
- `LD_ChiSq_sp` ChiSq statistics for each (virtual) subpopulation.
- `LD_ChiSq_p_sp` p value for the ChiSq statistics for each (virtual) subpopulation.
- `CramerV_sp` Cramer V statistics for each (virtual) subpopulation.

association: Parameter `association` accepts a list of loci. At each locus, one or more statistical tests will be performed to test association between this locus and individual affection status. Currently, `simuPOP` provides the following tests:

- An allele-based Chi-square test using alleles counts. This test can be applied to loci with more than two alleles, and to haploid populations.
- A genotype-based Chi-square test using genotype counts. This test can be applied to loci with more than two alleles (more than 3 genotypes) in diploid populations. aA and Aa are considered to be the same genotype.
- A genotype-based Cochran-Armitage trend test. This test can only be applied to diallelic loci in diploid populations. A codominant model is assumed.

This statistic sets the following variables:

- `Allele_ChiSq` A dictionary of allele-based Chi-Square statistics for each locus, using cases and controls in all or specified (virtual) subpopulations.
- `Allele_ChiSq_p` (default) A dictionary of *p-values* of the corresponding Chi-square statistics.
- `Geno_ChiSq` A dictionary of genotype-based Chi-Square statistics for each locus, using cases and controls in all or specified (virtual) subpopulations.
- `Geno_ChiSq_p` A dictionary of *p-values* of the corresponding genotype-based Chi-square test.

- `Armitage_p` A dictionary of *p-values* of the Cochran-Armitage tests, using cases and controls in all or specified (virtual) subpopulations.
- `Allele_ChiSq_sp` A dictionary of allele-based Chi-Square statistics for each locus, using cases and controls from each subpopulation.
- `Allele_ChiSq_p_sp` A dictionary of *p-values* of allele-based Chi-square tests, using cases and controls from each (virtual) subpopulation.
- `Geno_ChiSq_sp` A dictionary of genotype-based Chi-Square tests for each locus, using cases and controls from each subpopulation.
- `Geno_ChiSq_p_sp` A dictionary of *p-values* of genotype-based Chi-Square tests, using cases and controls from each subpopulation.
- `Armitage_p_sp` A dictionary of *p-values* of the Cochran- Armitage tests, using cases and controls from each subpopulation.

neutrality: This parameter performs neutrality tests (detection of natural selection) on specified loci. It currently only outputs *Pi*, which is the average number of pairwise difference between loci. This statistic outputs the following variables:

- `Pi` Mean pairwise difference between all sequences from all or specified (virtual) subpopulations.
- `Pi_sp` Mean pairwise difference between all sequences in each (virtual) subpopulation.

structure: Parameter `structure` accepts a list of loci at which statistics that measure population structure are calculated. This parameter currently supports the following statistics:

- Weir and Cockerham's *Fst* (1984). This is the most widely used estimator of Wright's fixation index and can be used to measure population differentiation. However, this method is designed to estimate *Fst* from samples of larger populations and might not be appropriate for the calculation of *Fst* of large populations.
- Nei's *Gst* (1973). The *Gst* estimator is another estimator for Wright's fixation index but it is extended for multi-allele (more than two alleles) and multi-loci cases. This statistics should be used if you would like to obtain a *true* *Fst* value of a large population.
- `F_st` (default) The WC84 *Fst* statistic estimated for all specified loci.
- `F_is` The WC84 *Fis* statistic estimated for all specified loci.
- `F_it` The WC84 *Fit* statistic estimated for all specified loci.
- `f_st` A dictionary of locus level WC84 *Fst* values.
- `f_is` A dictionary of locus level WC84 *Fis* values.
- `f_it` A dictionary of locus level WC84 *Fit* values.
- `G_st` Nei's *Gst* statistic estimated for all specified loci.
- `g_st` A dictionary of Nei's *Gst* statistic estimated for each locus.

HWE: Parameter `HWE` accepts a list of loci at which exact two-side tests for Hardy-Weinberg equilibrium will be performed. This statistic is only available for diallelic loci in diploid populations. It outputs the following variables:

- `HWE` (default) A dictionary of *p-values* of HWE tests using genotypes in all or specified (virtual) subpopulations.
- `HWE_sp` A dictionary of *p-values* of HWS tests using genotypes in each (virtual) subpopulation.

apply (*pop*)

Apply the `stat` operator

clone ()

Deep copy of a `stat` operator

2.11 Tagging operators

2.11.1 Class `idTagger` (Function `TagID`)

An `idTagger` gives a unique ID for each individual it is applied to. These ID can be used to uniquely identify an individual in a multi-generational population and be used to reliably reconstruct a pedigree.

To ensure uniqueness across populations, a single source of ID is used for this operator. Individual IDs are assigned consecutively starting from 0. If you would like to reset the sequence or start from a different number, you can call the `reset(startID)` function of any `idTagger`.

An `idTagger` is usually used during-mating to assign ID to each offspring. However, if it is applied directly to a population, it will assign unique IDs to all individuals in this population. This property is usually used in the `preOps` parameter of function `simulator.evolve` to assign initial ID to a population.

class `idTagger` (*begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, output="", infoFields="ind_id"*)

Create an `idTagger` that assign an unique ID for each individual it is applied to. The IDs are created sequentially and are stored in an information field specified in parameter *infoFields* (default to `ind_id`). This operator is considered a during-mating operator but it can be used to set ID for all individuals of a population when it is directly applied to the population. Because the information field is supposed to record a unique ID for the whole population, and because the IDs are increasingly assigned, this operator will raise a `RuntimeError` if parental IDs are the same, or are larger than the ID to be assigned to an offspring.

apply (*pop*)

Set an unique ID to all individuals with zero ID.

clone ()

Deep copy of an `idTagger`

reset (*startID=0*)

Reset the global individual ID number so that `idTaggers` will start from `id` (default to 0) again.

2.11.2 Class `inheritTagger`

An inheritance tagger passes values of parental information field(s) to the corresponding fields of offspring. If there are two parental values from parents of a sexual mating event, a parameter *mode* is used to specify how to assign offspring information fields.

class `inheritTagger` (*mode=Paternal, stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, output="", infoFields=[]*)

Creates an inheritance tagger that passes values of parental information fields (parameter *infoFields*) to the corresponding fields of offspring. If there is only one parent, values at the specified information fields are copied directly. If there are two parents, parameter *mode* specifies how to pass them to an offspring. More specifically,

- `mode=Maternal` Passing the value from mother.
- `mode=Paternal` Passing the value from father.
- `mode=Mean` Passing the average of two values.
- `mode=Maximum` Passing the maximum value of two values.
- `mode=Minumum` Passing the minimum value of two values.
- `mode=Summation` Passing the summation of two values.
- `mode=Multiplication` Passing the multiplication of two values.

An `RuntimeError` will be raised if any of the parents does not exist. This operator does not support parameter `subPops` and does not output any information.

clone()
Deep copy of a `inheritTagger`

2.11.3 Class `summaryTagger`

A summary tagger summarize values of one or more parental information field to another information field of an offspring. If mating is sexual, two sets of parental values will be involved.

class `summaryTagger` (*mode=Mean, stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, output="", infoFields=[]*)

Creates a summary tagger that summarize values of one or more parental information field (`infoFields[:-1]`) to an offspring information field (`infoFields[-1]`). A parameter *mode* specifies how to pass summarize parental values. More specifically,

- *mode=Mean* Passing the average of values.
- *mode=Maximum* Passing the maximum value of values.
- *mode=Minumum* Passing the minimum value of values.
- *mode=Summation* Passing the sum of values.
- *mode=Multiplication* Passing the multiplication of values.

This operator does not support parameter `subPops` and does not output any information.

clone()
Deep copy of a `summaryTagger`

2.11.4 Class `parentsTagger`

This tagging operator records the indexes of parents (relative to the parental generation) of each offspring in specified information fields (default to `father_idx` and `mother_idx`). Only one information field should be specified if an asexual mating scheme is used so there is one parent for each offspring. Information recorded by this operator is intended to be used to look up parents of each individual in multi-generational population.

class `parentsTagger` (*stage=DuringMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, output="", infoFields=["father_idx", "mother_idx"]*)

Create a parents tagger that records the indexes of parents of each offspring when it is applied to an offspring during-mating. If two information fields are specified (parameter *infoFields*, with default value `['father_idx', 'mother_idx']`), they are used to record the indexes of each individual's father and mother. Value `-1` will be assigned if any of the parent is missing. If only one information field is given, it will be used to record the index of the first valid parent (father if both parents are valid). This operator ignores parameters *stage*, *output*, and *subPops*.

clone()
Deep copy of a `parentsTagger`

2.11.5 Class `pedigreeTagger`

This tagging operator records the ID of parents of each offspring in specified information fields (default to `father_id` and `mother_id`). Only one information field should be specified if an asexual mating scheme is used so there is one parent for each offspring. Information recorded by this operator is intended to be used to record full pedigree information of an evolutionary process.

class pedigreeTagger (*idField*="ind_id", *output*="", *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *infoFields*=["father_id", "mother_id"])

Create a pedigree tagger that records the ID of parents of each offspring when it is applied to an offspring during-mating. If two information fields are specified (parameter *infoFields*, with default value ['father_id', 'mother_id']), they are used to record the ID of each individual's father and mother stored in the *idField* (default to *ind_id*) field of the parents. Value -1 will be assigned if any of the parent is missing. If only one information field is given, it will be used to record the ID of the first valid parent (father if both pedigree are valid).

This operator by default does not send any output but will output the ID of offspring, father, and mother if a valid output stream is specified. The output will be in the format of *off_id father_id mother_id*. *father_id* or *mother_id* will be ignored if only one parent is involved. This operator ignores parameter *stage*, and *subPops*.

clone()
Deep copy of a pedigreeTagger

2.11.6 Class pyTagger

A Python tagger takes some information fields from both parents, pass them to a user provided Python function and set the offspring individual fields with the return values.

class pyTagger (*func*=None, *stage*=DuringMating, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *output*="", *infoFields*=[])

Create a hybrid tagger that passes parental information fields (parameter *infoFields*) to an user provided function *func* and use its return values to assign corresponding information fields of offspring. If more than one parent are available, maternal values are passed after paternal values. For example, if *infoFields*=['A', 'B'], the user-defined function should expect an array of size 4, with paternal values at fields 'A', 'B', followed by maternal values at these fields. The return value of this function should be a list, although a single value will be accepted if only one information field is specified. This operator ignores parameters *stage*, *output* and *subPops*.

clone()
Deep copy of a pyTagger

2.12 Terminator

2.12.1 Class terminateIf

This operator evaluates an expression in a population's local namespace and terminate the evolution of this population, or the whole simulator, if the return value of this expression is *True*. Termination caused by an operator will stop the execution of all operators after it. The generation at which the population is terminated will be counted in the *evolved generations* (return value from *simulator::evolve*) if termination happens after mating.

class terminateIf (*condition*="", *stopAll*=False, *message*="", *output*="", *stage*=PostMating, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=AllAvail, *subPops*=AllAvail, *infoFields*=[])

Create a terminator with an expression *condition*, which will be evaluated in a population's local namespace when the operator is applied to this population. If the return value of *condition* is *True*, the evolution of the population will be terminated. If *stopAll* is set to *True*, the evolution of all replicates of the simulator will be terminated. If this operator is allowed to write to an *output* (default to ""), the generation number, proceeded with an optional *message*.

apply(pop)
Apply an operator to population *pop* directly, without checking its applicability.

clone()
Deep copy of a `terminateIf` terminator

2.13 The Python operator

2.13.1 Class `pyOperator`

An operator that calls a user-defined function when it is applied to a population (pre- or post-mating) or offsprings (during-mating). The function can have parameters `pop` when the operator is applied pre- or post-mating, `pop`, `off`, `dad`, `mom` when the operator is applied during-mating. An optional parameter can be passed if parameter `param` is given. In the during-mating case, parameters `pop`, `dad` and `mom` can be ignored if `offspringOnly` is set to `True`.

class `pyOperator` (*func, param=None, stage=PostMating, offspringOnly=False, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail, infoFields=[]*)

Create a pure-Python operator that calls a user-defined function when it is applied. Depending on parameters `stage`, `param`, and `offspringOnly`, the function should have one of the following forms:

- `func(pop)` if `stage=PreMating` or `PostMating`, and without `param`.
- `func(pop, param)` if `stage=PreMating` or `PostMating`, and with `param`.
- `func(pop, off, dad, mom)` if `stage=DuringMating` and without `param`.
- `func(pop, off, dad, mom, param)` if `stage=DuringMating`, and with `param`.
- `func(off)` if `stage=DuringMating`, `offspringOnly=True` and without `param`.
- `func(off, param)` if `stage=DuringMating`, `offspringOnly=True` and with `param`.

where `pop` is the population to which the operator is applied, `off` is the offspring of `dad` and `mom`, and `param` is the parameter `param` specified when the operator is created. When this operator is applied during mating, it can be used in the `ops` parameter of a mating scheme, or used in the `ops` parameter of `simulator.evolve` and be applied after an offspring has been created. Please refer to the `simuPOP` user's guide for a detailed explanation.

This operator does not support parameters `output`, `subPops` and `infoFields`. If certain output is needed, it should be handled in the user defined function `func`. Because the status of files used by other operators through parameter `output` is undetermined during evolution, they should not be open or closed in this Python operator.

apply(*pop*)

Apply the `pyOperator` operator to population `pop`. Calling this function is equivalent to call `func` with parameter `pop` and optional parameter `param`.

2.14 Ascertainment operators

2.14.1 Class `randomSample`

This operator draws random individuals from a population repeatedly and forms a number of random samples. These samples can be put in the population's local namespace, or save to disk files. The function form of this operator returns a list of samples directly.

class `randomSample` (*size, *args, **kwargs*)

Draw `size` random samples from a population `times` times. `size` can be a number or a list of numbers. In the former case, individuals are drawn from the whole population and the samples has only one subpopulation. In the latter case, a given number of individuals are drawn from each subpopulation and the result sample has the

same number of subpopulation as the population from which samples are drawn. The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

RandomSample (*pop*, **args*, ***kwargs*)

Function version of operator `randomSample`.

2.14.2 Class `caseControlSample`

This operator chooses random cases and controls from a population repeatedly. These samples can be put in the population's local namespace, or save to disk files. The function form of this operator returns a list of samples directly.

class caseControlSample (*cases*, *controls*, **args*, ***kwargs*)

Draw *cases* affected and *controls* unaffected individuals from a population repeatedly. *cases* can be a number or a list of numbers. In the former case, affected individuals are drawn from the whole population. In the latter case, a given number of individuals are drawn from each subpopulation. The same hold for *controls*. The resulting samples have two subpopulations that hold cases and controls respectively. The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

CaseControlSample (*pop*, **args*, ***kwargs*)

Function version of operator `caseControlSample` whose `__init__` function is

Draw *cases* affected and *controls* unaffected individuals from a population repeatedly. *cases* can be a number or a list of numbers. In the former case, affected individuals are drawn from the whole population. In the latter case, a given number of individuals are drawn from each subpopulation. The same hold for *controls*. The resulting samples have two subpopulations that hold cases and controls respectively. The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

2.14.3 Class `affectedSibpairSample`

This operator chooses affected sibpairs and their parents from a population repeatedly. These samples can be put in the population's local namespace, or save to disk files. The function form of this operator returns a list of samples directly.

The population to be sampled needs to have at least one ancestral generation. In addition, parents of each offspring is needed so information fields, most likely *father_idx* and *mother_idx* should be used to track parents in the parental generation. An during mating operator *parentsTagger* is designed for such a purpose. In addition, because it is very unlikely for two random offspring to share parents, affected sibpairs can only be ascertained from populations that are generated using a mating scheme that produces more than one offspring at each mating event.

class affectedSibpairSample (*size*, *infoFields*=['*father_idx*', '*mother_idx*'], **args*, ***kwargs*)

Draw *size* families, including two affected siblings and their parents from a population repeatedly. The population to be sampled must have at least one ancestral generation. It should also have two information fields specified by parameter *infoFields* (Default to ['*father_idx*', '*mother_idx*']). Parameter *size* can be a number or a list of numbers. In the former case, affected sibpairs are drawn from the whole population. In the latter case, a given number of affected sibpairs are drawn from each subpopulation. In both cases, affected sibpairs in the resulting sample form their own subpopulations (of size two). The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

AffectedSibpairSample (*pop*, *size*, **args*, ***kwargs*)

Function version of operator `affectedSibpairSample` whose `__init__` function is

Draw *size* families, including two affected siblings and their parents from a population repeatedly. The pop-

ulation to be sampled must have at least one ancestral generation. It should also have two information fields specified by parameter *infoFields* (Default to [*'father_idx'*, *'mother_idx'*]). Parameter *size* can be a number or a list of numbers. In the former case, affected sibpairs are drawn from the whole population. In the latter case, a given number of affected sibpairs are drawn from each subpopulation. In both cases, affected sibpairs in the resulting sample form their own subpopulations (of size two). The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

2.15 Miscellaneous operators

2.15.1 Class `noneOp`

This operator does nothing when it is applied to a population. It is usually used as a placeholder when an operator is needed syntactically.

```
class noneOp (output=">", stage=PostMating, begin=0, end=0, step=1, at=[], reps=AllAvail, subPops=AllAvail,
              infoFields=[])
    Create a noneOp.

apply (pop)
    Apply the noneOp operator to one population
```

2.15.2 Class `dumper`

This operator dumps the content of a population in a human readable format. Because this output format is not structured and can not be imported back to simuPOP, this operator is usually used to dump a small population to a terminal for demonstration and debugging purposes.

```
class dumper (genotype=True, structure=True, ancGen=0, width=1, max=100, loci=[], output=">",
              stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, subPops=AllAvail,
              infoFields=[])
    Create a operator that dumps the genotype structure (if structure is True) and genotype (if genotype is True)
    to an output ( default to standard terminal output). Because a population can be large, this operator will only
    output the first 100 (parameter max) individuals of the present generation (parameter ancGen). All loci will
    be outputted unless parameter loci are used to specify a subset of loci. If a list of (virtual) subpopulations are
    specified, this operator will only output individuals in these outputs. Please refer to class baseOperator for
    a detailed explanation for common parameters such as output and stage.

apply (pop)
    Apply a dumper operator to population pop.

clone ()
    Deep copy of a dumper operator.
```

2.15.3 Class `savePopulation`

An operator that save populations to specified files.

```
class savePopulation (output="", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllAvail, sub-
                      Pops=AllAvail, infoFields=[])
    Create an operator that saves a population to output when it is applied to the population. This operator sup-
    ports all output specifications ("filename", 'filename' prefixed by one or more '>' characters, and
```

'!expr') but output from different operators will always replace existing files (effectively ignore '>' specification). Parameter *subPops* is ignored. Please refer to class `baseOperator` for a detailed description about common operator parameters such as *stage* and *begin*.

apply (*pop*)

Apply operator to population *pop*.

clone ()

Deep copy of a `savePopulation` operator.

2.15.4 Class `setAncestralDepth`

This operator sets the number of ancestral generations to keep during the evolution of a population. This is usually used to start storing ancestral generations at the end of an evolutionary process. A typical usage is `setAncestralDepth(1, at=-1)` which will cause the parental generation of the present population to be stored at the last generation of an evolutionary process.

class `setAncestralDepth` (*depth*, *output*=">", *stage*=`PreMating`, *begin*=0, *end*=-1, *step*=1, *at*=[],
reps=`AllAvail`, *subPops*=`AllAvail`, *infoFields*=[])

Create a `setAncestralDepth` operator that sets the ancestral depth of a population. It basically calls the `population.setAncestralDepth` member function of a population.

apply (*pop*)

Apply the `setAncestralDepth` operator to population *pop*.

2.15.5 Class `ifElse`

This operator accepts an expression that will be evaluated when this operator is applied. A list of if-operators will be applied when the expression returns `True`. Otherwise a list of else-operators will be applied.

class `ifElse` (*cond*, *ifOps*=[], *elseOps*=[], *output*=">", *stage*=`PostMating`, *begin*=0, *end*=-1, *step*=1, *at*=[],
reps=`AllAvail`, *subPops*=`AllAvail`, *infoFields*=[])

Create a conditional operator that will apply operators *ifOps* if condition *cond* is met and *elseOps* otherwise. The replicate and generation applicability parameters (*begin*, *end*, *step*, *at* and *rep*) of the *ifOps* and *elseOps* are ignored because their applicability is determined by the `ifElse` operator.

apply (*pop*)

Apply the `ifElse` operator to population *pop*.

2.15.6 Class `pause`

This operator pauses the evolution of a simulator at given generations or at a key stroke. When a simulator is stopped, you can go to a Python shell to examine the status of an evolutionary process, resume or stop the evolution.

class `pause` (*stopOnKeyStroke*=`False`, *prompt*=`True`, *output*=">", *stage*=`PostMating`, *begin*=0, *end*=-1, *step*=1,
at=[], *reps*=`AllAvail`, *subPops*=`AllAvail`, *infoFields*=[])

Create an operator that pause the evolution of a population when it is applied to this population. If *stopOnKeyStroke* is `False` (default), it will always pause a population when it is applied, if this parameter is set to `True`, the operator will pause a population if *any* key has been pressed. If a specific character is set, the operator will stop when this key has been pressed. This allows, for example, the use of several pause operators to pause different populations.

After a population has been paused, a message will be displayed (unless *prompt* is set to `False`) and tells you how to proceed. You can press 's' to stop the evolution of this population, 'S' to stop the evolution of all populations, or 'p' to enter a Python shell. The current population will be available in this Python shell as

"pop_X_Y" when X is generation number and Y is replicate number. The evolution will continue after you exit this interactive Python shell.

Note Ctrl-C will be intercepted even if a specific character is specified in parameter *stopOnKeyStroke*.

apply (*pop*)

Apply the pause operator to one population

2.15.7 Class **turnOnDebug** (Function **TurnOnDebug**)

Turn on debug. There are several ways to turn on debug information for non-optimized modules, namely

- set environment variable `SIMUDEBUG`.
- use `simuOpt.setOptions(debug)` function.
- use function `TurnOnDebug`
- use the `turnOnDebug` operator

The advantage of using an operator is that you can turn on debug at given generations.

class turnOnDebug (*code*, *stage=PreMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)

Create a `turnOnDebug` operator that turns on debug information *code* when it is applied to a population.

2.15.8 Class **turnOffDebug** (Function **TurnOffDebug**)

Turn off certain debug information. Please refer to operator `turnOnDebug` for detailed usages.

class turnOffDebug (*code="DBG_ALL"*, *stage=PreMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)

Create a `turnOffDebug` operator that turns off debug information *code* when it is applied to a population.

2.15.9 Class **ticToc**

This operator, when called, output the difference between current and the last called clock time. This can be used to estimate execution time of each generation. Similar information can also be obtained from `turnOnDebug("DBG_PROFILE")`, but this operator has the advantage of measuring the duration between several generations by setting *step* parameter.

class ticToc (*output=">"*, *stage=PreMating*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=AllAvail*, *subPops=AllAvail*, *infoFields=[]*)

Create a `ticToc` operator that outputs the elapsed since the last time it was applied, and the overall time since it was created.

2.16 Function form of operators

Dump (*pop*, **args*, ***kwargs*)

Apply operator `dumper` to population *pop*.

InitSex (*pop*, **args*, ***kwargs*)

Apply operator `initSex` to population *pop*.

InitInfo (*pop*, *args, **kwargs)

Apply operator `initInfo` to population *pop*.

InitByFreq (*pop*, *args, **kwargs)

Apply operator `initByFreq` to population *pop*.

InitByValue (*pop*, *args, **kwargs)

Apply operator `initByValue` to population *pop*.

PyEval (*pop*, *args, **kwargs)

Evaluate statements *stmts* (optional) and expression *expr* in population *pop*'s local namespace and return the result of *expr*. If *exposePop* is given, population *pop* will be exposed in its local namespace as a variable with a name specified by *exposePop*.

Note

Unlike its operator counterpart, this function returns the result of *expr* rather than writing it to an output.

PyExec (*pop*, *args, **kwargs)

Execute *stmts* in population *pop*'s local namespace.

InfoEval (*pop*, *args, **kwargs)

Evaluate *expr* for each individual, using information fields as variables. Please refer to operator `infoEval` for details.

InfoExec (*pop*, *args, **kwargs)

Execute *stmts* for each individual, using information fields as variables. Please refer to operator `infoExec` for details.

Migrate (*pop*, *args, **kwargs)

Function form of operator `migrator`.

MatrixMutate (*pop*, *args, **kwargs)

Function form of operator `matrixMutator`

SnpMutate (*pop*, *args, **kwargs)

Function form of operator `snpMutator`

AcgtMutate (*pop*, *args, **kwargs)

Function form of operator `acgtMutator`

KamMutate (*pop*, *args, **kwargs)

Function form of operator `kamMutator`

SmmMutate (*pop*, *args, **kwargs)

Function form of operator `smmMutator`

PyMutate (*pop*, *args, **kwargs)

Function form of operator `pyMutator`

MixedMutate (*pop*, *args, **kwargs)

Function form of operator `mixedMutator`

ContextMutate (*pop*, *args, **kwargs)

Function form of operator `contextMutator`

PointMutate (*pop*, *args, **kwargs)

Function form of operator `pointMutator`

Stat (*pop*, *args, **kwargs)

Apply operator `stat` with specified parameters to population *pop*. Resulting statistics could be accessed from the local namespace of *pop* using functions `pop.vars()` or `pop.dvars()`

TagID (*pop*, **args*, ***kwargs*)

Apply operator `idTagger` to population `pop` to assign a unique ID to all individuals in the population.

Chapter 3

Utility Modules

3.1 Module `simuOpt`

Module “`simuOpt`” provides a function “`simuOpt.setOptions`” to control which `simuPOP` module to load, and how it is loaded, and a class “`simuOpt.simuOpt`” that helps users manage script options.

When `simuPOP` is loaded, it checks a few environmental variables (“`SIMUOPTIMIZED`”, “`SIMUALLELETYPE`”, and “`SIMUDEBUG`”) to determine which `simuPOP` module to load, and how to load it. More options can be set using the “`simuOpt.setOptions`” function. For example, you can suppress the banner message when `simuPOP` is loaded and require a minimal revision of `simuPOP` for your script. `simuPOP` recognize the following commandline arguments

“`-optimized`” Load the optimized version of a `simuPOP` module.

“`-gui=True|False|wxPython|Tkinter`” Whether or not use a graphical toolkit and which one to use. “`-gui=False`” is usually used to run a script in batch mode (do not start a parameter input dialog and use interactive user input if a parameter can not be determined from command line or a configuration file, and it does not use its default value (“`useDefault`” not set). Please refer to parameter “`gui`” for “`simuOpt.setOptions`” for details.

class “`params.simuParam`” provides a powerful way to handle commandline arguments. Briefly speaking, a “`simuParam`” object can be created from a list of parameter specification dictionaries. The parameters are then become attributes of this object. A number of functions are provided to determine values of these parameters using commandline arguments, a configuration file, or a parameter input dialog (using “`Tkinter`” or “`wxPython`”). Values of these parameters can be accessed as attributes, or extracted as a list or a dictionary. Note that the “`simuParam.getParam`” function automatically handles the following commandline arguments.

“`-h`” or “`-help`” Print usage message.

“`-config=configFile`” Read parameters from a configuration file `*configFile*`.

3.1.1 Function `setOptions`

`setOptions` (*alleleType=None, optimized=None, gui=None, quiet=None, debug=None, revision=None*)

Set options before `simuPOP` is loaded to control which `simuPOP` module to load, and how the module should be loaded.

alleleType: Use the standard, binary or long allele version of the `simuPOP` module if *alleleType* is set to ‘short’, ‘binary’, or ‘long’ respectively. If this parameter is not set, this function will try to get its value from environmental variable `SIMUALLELETYPE`. The standard (short) module will be used if the environmental variable is not defined.

optimized: Load the optimized version of a module if this parameter is set to `True` and the standard version if it is set to `False`. If this parameter is not set (`None`), the optimized version will be used if environmental

variable `SIMUOPTIMIZED` is defined. The standard version will be used otherwise.

gui: Whether or not use graphical user interfaces, and which graphical toolkit to use. If this parameter is `None` (default), this function will check environmental variable `SIMUGUI` for a value, and assume `True` if such an option is unavailable.

gui=True: allows `simuPOP` to use `wxPython`-based dialogs if `wxPython` is available, and use `Tkinter`-based dialogs if `Tkinter` is available.

gui='Tkinter': Use `Tkinter` based dialogs even if `wxPython` is available.

gui='wxPython': Use `wxPython` based dialogs. Usually not needed.

gui=False: Do not use any graphical toolkit. Run the script in batch mode.

This option is usually left to `None` so that the same script can be ran in both GUI and batch mode using commandline option `--gui`.

quiet: If set to `True`, suppress the banner message when a `simuPOP` module is loaded.

debug: A list of debug code (as string) that will be turned on when `simuPOP` is loaded. If this parameter is not set, a list of comma separated debug code specified in environmental variable `SIMUDEBUG`, if available, will be used. Note that setting `debug=[]` will remove any debug code that might have been by variable `SIMUDEBUG`.

revision: A number indicating the required revision number for the `simuPOP` module to be loaded. `simuPOP` will fail to load if the installed `simuPOP` is older than the required revision. Please check `simuPOP` `ChangeLog` for the revision number of distributed versions.

3.1.2 Class `simuParam`

3.1.3 Class `simuParam`

class `simuParam` provides a uniform interface for `simuPOP` scripts to handle parameters. It allows users to get parameters from command line options, a configuration file, a parameter input dialog (*tkInter* or *wxPython*) or from interactive input. This class provides parameter validation, conversion and and some utility functions to print, save and restore parameters.

A `simuParam` object accepts a parameter specification list that consists of dictionaries with pre-defined keys. Each item defines an option in terms of command line option, entry name in a configuration file, label in a parameter input dialog, acceptable types, validation rules and a default value. The following keys are currently supported:

arg: Short command line option name. For example '`c`' checks the presence of argument `-c`. If a value is expected, a comma should be appended to the option name. For example, '`p:`' matches command line option `-p=100` or `-p 100`. An options that does not expect a value is displayed in the parameter input dialog as an on/off switch.

longarg: Long command line option name. For example '`version`' checks the presence of argument `--version`. A equal character should be appended to the option name if a value is expected. For example, '`mu=`' matches command line option `--mu=0.001` or `--mu 0.001`. **This item defines the name of an option and cannot be ignored.** An options that does not expect a value is displayed in the parameter input dialog as an on/off switch.

label: The label of the input field in a parameter input dialog. It will also be used as the prompt for this option during interactive parameter input. **Options without a label will not be displayed in the parameter input dialog and will not be saved to a configuration file.** A typical example of such an option is `--version`.

default: Default value for this parameter. It is used as the default value in the parameter input dialog, and as the option value when a user presses `Enter` directly during interactive parameter input. **A default value is required for all options.**

useDefault: Use default value without asking, if the value can not be determined from GUI, command line option or config file. This is usually used for options that rarely need to be changed. Setting `useDefault` to such options simplifies user input.

description: A long description of this parameter. This description will be put into the usage information, and as parameter tooltip in the parameter input dialog. This string will be reformatted when it is written to a usage string (remove newlines and extra spaces and re-indent), with the exception that **lines with 'l' as the first non-space/tab character will be outputted as is without the leading 'l' symbol.**

allowedTypes: A list of acceptable types of this option. class `simuParam` will try to convert user input to these types. For example, if `allowedTypes` is `types.ListType` or `types.TupleType` and the user's input is a scalar, the input will be converted to a list automatically. An option will not be accepted if such conversion fails. If this item is not specified, the type of the default value will be used.

validate: A function to validate the parameter. The function will be applied to user input. The option will not be accepted if this function returns `False`. This module defines a large number of such validation functions but user defined functions are also acceptable.

chooseOneOf: If specified, a list of specified values will be displayed in the parameter input dialog and users are allowed to choose one of them.

chooseFrom: If specified, a list of specified values will be displayed in the parameter input dialog and users are allowed to choose one or more of them.

separator: This item specifies a separator (group header) in the parameter input dialog. All other fields are ignored.

Not all keys need to be specified in each option description. Missing values are handled using some internal rules. For example, items without a `label` will not be displayed on the parameter dialog. This will effectively *hide* a parameter although users who know this parameter can set it using command line options.

The `simuParam.simuParam` class defines a number of functions to collect, validate, and manipulate parameters using this parameter specification list.

As a shortcut to create a `simuParam` object with a number of attributes, a `simuParam` object can be created with additional `key=value` pairs that could be assessed as attributes. This is used to create a `simuParam` object in which *parameters* are assigned directly.

class `simuParam` (*options=[]*, *doc=""*, *details=""*, ***kwargs*)

Create a `simuParam` object using a list of parameter specification dictionaries *options*. Additional *doc* and *details* can be specified which will be displayed as script summary (on the top of a parameter input dialog) and script introduction (the first part of a help message), respectively. Additional attributes could be assigned to a `simuParam` object as keyword arguments. Note that it is customary to use module document (the first string object in a Python script) as *details*, using parameter `details=__doc__`.

addOption (*pos=-1*, ***kwargs*)

Append an entry to the parameter specification list. Dictionary entries should be specified as keyword arguments such as `longarg='option='`. More specifically, you can specify parameters `arg`, `longarg` (required), `label`, `allowedTypes`, `useDefault`, `default` (required), `description`, `validate`, `chooseOneOf`, `chooseFrom` and `separator`. This option will have a name specified by `longarg` (without optional trailing `=`) and an initial default value specified by `default`.

An optional parameter *pos* can be given to specify an index before which this option will be inserted.

asDict ()

Return parameters as a dictionary.

asList ()

Return parameters as a list.

getParam (*gui=None*, *nCol=None*, *configFile=None*, *args=None*, *checkArgs=True*)

Get parameters from commandline option, configuration file, a parameter input dialog and from interactive user input.

gui: Whether or not use a dialog and which graphical toolkit to use. Global gui setting is used by default but you can also set this parameter to `True`, `False`, `Tkinter` or `wxPython` to override the global setting.

nCol: Number of columns in the parameter input dialog. This is usual determine automatically depending on the number of options.

configFile: Configuration file from which to load values of parameters. If unspecified, it will be determined from command line option `--config`.

args: Command line arguments are obtained from `sys.argv` unless a list of options are provided in this argument.

checkArgs: This function by default checks if all commandline arguments have been processed, you can set `checkArgs` to `False` if some of the arguments are intended to be processed separately.

guiGetParam (*nCol=None, gui=None*)

Get parameter from a Tkinter or wxPython dialog. The parameter will try to arrange parameters optimally but you can also set the number of columns using parameter *nCol*. If both GUI toolkits are available, wxPython will be used unless *gui* is set to Tkinter. If none of the toolkits are available, this function will raise an `ImportError`.

Note

If `simuParam.valueValidFile` or `simuParam.valueValidDir` is used to validate a parameter, double click the text input box of this parameter will open a file or directory browse dialog.

loadConfig (*file, params=[]*)

Load configuration from a file. If a list of parameters are specified in *params*, only these parameters will be processed.

processArgs (*args=None, params=[]*)

Try to get parameters from a list of arguments *args* (default to `sys.argv`). If `-h` or `--help` is in *args*, this function prints out a usage message and returns `False`. If a list of parameters are specified in *params*, only these parameters will be processed.

saveConfig (*file, params=[]*)

Write a configuration file to *file*. This file can be later read with command line option `-c` or `--config`. All parameters with a `label` entry are saved unless a list of parameters are specified in *params*. In addition to parameter definitions, command lines options to specify the same set of parameters are saved to the configuration file.

termGetParam (*params=[]*)

Get parameters from interactive user input. By default, all parameters are processed unless one of the following conditions is met:

- 1.Parameter without a label
- 2.Parameter with `useDefault` set to `True`
- 3.Parameter that have been determined from command line options or a configuration file
- 4.Parameter that have been determined by a previous call of this function.

If a list of parameters are given in *params*, these parameters are processed regardless the mentioned conditions.

usage (*usage='usage: %prog [-opt [arg] | -opt [=arg]] ...'*)

Reutn the usage message from the option description list. '`%prog`' in parameter *usage* will be replaced by `os.path.basename(sys.argv[0])`.

valueNot (*t*)

Return a function that returns true if passed option does not passes validator *t*

valueOr (*t1, t2*)

Return a function that returns true if passed option passes validator *t1* or *t2*

valueAnd (*t1, t2*)

Return a function that returns true if passed option passes validator *t1* and *t2*

valueOneOf (*t*)
Return a function that returns true if passed option is one of the values list in *t*

valueTrueFalse ()
Return a function that returns true if passed option is True or False

valueBetween (*a*, *b*)
Return a function that returns true if passed option is between value *a* and *b* (*a* and *b* included)

valueGT (*a*)
Return a function that returns true if passed option is greater than *a*

valueGE (*a*)
Return a function that returns true if passed option is greater than or equal to *a*

valueLT (*a*)
Return a function that returns true if passed option is less than *a*

valueLE (*a*)
Return a function that returns true if passed option is less than or equal to *a*

valueEqual (*a*)
Return a function that returns true if passed option equals *a*

valueNotEqual (*a*)
Return a function that returns true if passed option does not equal *a*

valueIsNum ()
Return a function that returns true if passed option is a number (int, long or float)

valueIsList ()
Return a function that returns true if passed option is a list (or tuple)

valueValidDir ()
Return a function that returns true if passed option val if a valid directory

valueValidFile ()
Return a function that returns true if passed option val if a valid file

3.2 Module `simuPOP.utils`

This module provides some commonly used operators and format conversion utilities.

3.2.1 Allele frequency trajectory simulation

3.2.2 Class `trajectory`

A `trajectory` object contains frequencies of one or more loci in one or more subpopulations over several generations. It is usually returned by member functions of class `trajectorySimulator` or equivalent global functions `ForwardTrajectory` and `BackwardTrajectory`.

The `trajectory` object provides several member functions to facilitate the use of trajectory-simulation techniques. For example, `trajectory.func()` returns a trajectory function that can be provided directly to a `controlledOffspringGenerator`; `trajectory.mutators()` provides a list of `pointMutator` that insert mutants at the right generations to initialize a trajectory.

For more information about trajectory simulation techniques and related controlled random mating scheme, please refer to the `simuPOP` user's guide, and Peng et al (PLoS Genetics 3(3), 2007).

class trajectory (*endGen*, *nLoci*)

Create a `trajectory` object of alleles at *nLoci* loci with ending generation *endGen*. *endGen* is the generation when expected allele frequencies are reached after mating. Therefore, a trajectory for 1000 generations should have *endGen*=999.

freq (*gen*, *subPop*)

Return frequencies of all loci in subpopulation *subPop* at generation *gen* of the simulated trajectory. Allele frequencies are assumed to be zero if *gen* is out of range of the simulated trajectory.

func ()

Return a Python function that returns allele frequencies for each locus at specified loci. If there are multiple subpopulations, allele frequencies are arranged in the order of *loc0_sp0*, *loc1_sp0*, ..., *loc0_sp1*, *loc1_sp1*, ... and so on. The returned function can be supplied directly to the *freqFunc* parameter of a controlled random mating scheme (*controlledRandomMating*) or a homogeneous mating scheme that uses a controlled offspring generator (*controlledOffspringGenerator*).

mutators (*loci*, *inds=0*, *allele=1*, **args*, ***kwargs*)

Return a list of *pointMutator* operators that introduce mutants at the beginning of simulated trajectories. These mutators should be added to the *ops* parameter of *simulator.evolve* function to introduce a mutant at the beginning of a generation with zero allele frequency before mating, and a positive allele frequency after mating. A parameter *loci* is needed to specify actual loci indexes in the real forward simulation. Other than default parameters *inds=0* and *allele=1*, additional parameters could be passed to point mutator as keyword parameters.

plot (*filename=None*, ***kwargs*)

Plot simulated trajectory using R through a Python module *rpy*. The function will return silently if module *plotter* cannot be imported.

This function will use different colors to plot trajectories at different loci. The trajectories are plotted from generation 0 to *endGen* even if the trajectories are short. The y-axis ranges from 0 to 1 and is labeled Allele frequency. If a valid *filename* is given, the figure will be saved to *filename* in a format specified by file extension. Currently supported formats/extensions are *eps*, *jpg*, *bmp*, *tif*, *png* and *pdf*. The availability of formats may be limited by your version of R.

This function makes use of the derived keyword parameter feature of module *plotter*. Allowed prefixes are *par*, *plot*, *lines* and *dev_print*. Allowed repeating suffix are *loc* and *sp*. For example, you could use parameter *plot_ylim* to reset the default value of *ylim* in R function *plot*.

3.2.3 Class `trajectorySimulator`

A trajectory simulator takes basic demographic and genetic (natural selection) information of an evolutionary process of a diploid population and allow the simulation of trajectory of allele frequencies of one or more loci. Trajectories could be simulated in two ways: forward-time and backward-time. In a forward-time simulation, the simulation starts from certain allele frequency and simulate the frequency at the next generation using given demographic and genetic information. The simulation continues until an ending generation is reached. A trajectory is successfully simulated if the allele frequency at the ending generation falls into a specified range. In a backward-time simulation, the simulation starts from the ending generation with a desired allele frequency and simulate the allele frequency at previous generations one by one until the allele gets lost (allele frequency equals zero).

The result of a trajectory simulation is a trajectory object which can be used to direct the simulation of a special random mating process that controls the evolution of one or more disease alleles so that allele frequencies are consistent across replicate simulations. For more information about trajectory simulation techniques and related controlled random mating scheme, please refer to the *simuPOP* user's guide, and Peng et al (PLoS Genetics 3(3), 2007).

class trajectorySimulator (*N*, *nLoci=1*, *fitness=None*, *logger=None*)

Create a trajectory simulator using provided demographic and genetic (natural selection) parameters. Member functions *simuForward* and *simuBackward* can then be used to simulate trajectories within certain range of generations. This class accepts the following parameters

N: Parameter *N* accepts either a constant number for population size (e.g. *N*=1000), a list of subpopulation sizes (e.g. *N*=[1000, 2000]), or a demographic function that returns population or subpopulation sizes at each generation. During the evolution, multiple subpopulations can be merged into one, and one population can be split into several subpopulations. The number of subpopulation is determined by the return value of the demographic function. Note that *N* should be considered as the population size at the end of specified generation.

nLoci: Number of unlinked loci for which trajectories of allele frequencies are simulated. We assume a diploid population with diallelic loci. The trajectory represents frequencies of a

fitness: Parameter *fitness* can be *None* (no selection), a list of fitness values for genotype with 0, 1, and 2 disease alleles (*AA*, *Aa*, and *aa*) at one or more loci; or a function that returns fitness values at each generation. When multiple loci are involved (*nLoci*), *fitness* can be a list of 3 (the same fitness values for all loci), a list of 3**nLoci* (different fitness values for each locus) or a list of 3***nLoci* (fitness value for each combination of genotype). The fitness function should accept generation number and a subpopulation index. The latter parameter allows, and is the only way to specify different fitness in each subpopulation.

logger: A logging object (see Python module `logging`) that can be used to output intermediate results with debug information.

simuBackward (*endGen*, *endFreq*, *minMutAge=None*, *maxMutAge=None*, *maxAttempts=1000*)

Simulate trajectories of multiple disease susceptibility loci using a forward time approach. This function accepts allele frequencies of alleles of multiple unlinked loci (*endFreq*) at the end of generation *endGen*. Depending on the number of loci and subpopulations, parameter *beginFreq* can be a number (same frequency for all loci in all subpopulations), or a list of frequencies for each locus (same frequency in all subpopulations), or a list of frequencies for each locus in each subpopulation in the order of *loc0_sp0*, *loc1_sp0*, ..., *loc0_sp1*, *loc1_sp1*, ... and so on.

This simulator will simulate a trajectory generation by generation and restart if the disease allele got fixed (instead of lost), or if the length simulated trajectory does not fall into *minMutAge* and *maxMutAge* (ignored if *None* is given). This simulator will return *None* if no valid trajectory is found after *maxAttempts* attempts.

simuForward (*beginGen*, *endGen*, *beginFreq*, *endFreq*, *maxAttempts=10000*)

Simulate trajectories of multiple disease susceptibility loci using a forward time approach. This function accepts allele frequencies of alleles of multiple unlinked loci at the beginning generation (*freq*) at generation *beginGen*, and expected *range* of allele frequencies of these alleles (*endFreq*) at the end of generation *endGen*. Depending on the number of loci and subpopulations, these parameters accept the following inputs:

beginGen: Starting generation. The initial frequencies are considered as frequencies at the *beginning* of this generation.

endGen: Ending generation. The ending frequencies are considered as frequencies at the *end* of this generation.

beginFreq: The initial allele frequency of involved loci in all subpopulations. It can be a number (same frequency for all loci in all subpopulations), or a list of frequencies for each locus (same frequency in all subpopulations), or a list of frequencies for each locus in each subpopulation in the order of *loc0_sp0*, *loc1_sp0*, ..., *loc0_sp1*, *loc1_sp1*, ... and so on.

endFreq: The range of acceptable allele frequencies at the ending generation. The ranges can be specified for all loci in all subpopulations, for all loci (allele frequency in the whole population is considered), or for all loci in all subpopulations, in the order of *loc0_sp0*, *loc1_sp0*, ..., *loc0_sp1*, ... and so on.

This simulator will simulate a trajectory generation by generation and restart if the resulting frequencies do not fall into specified range of frequencies. This simulator will return *None* if no valid trajectory is found after *maxAttempts* attempts.

ForwardTrajectory (*N*, *beginGen*, *endGen*, *beginFreq*, *endFreq*, *nLoci=1*, *fitness=None*, *maxAttempts=10000*, *logger=None*)

Given a demographic model (*N*) and the fitness of genotype at one or more loci (*fitness*), this function simulates

a trajectory of one or more unlinked loci (*nLoci*) from allele frequency *freq* at generation *beginGen* forward in time, until it reaches generation *endGen*. A `trajectory` object will be returned if the allele frequency falls into specified ranges (*endFreq*). None will be returned if no valid trajectory is simulated after `maxAttempts` attempts. Please refer to class `trajectory`, `trajectorySimulator` and their member functions for more details about allowed input for these parameters.

BackwardTrajectory (*N*, *endGen*, *endFreq*, *nLoci*=1, *fitness*=None, *minMutAge*=None, *maxMutAge*=None, *maxAttempts*=1000, *logger*=None)

Given a demographic model (*N*) and the fitness of genotype at one or more loci (*fitness*), this function simulates a trajectory of one or more unlinked loci (*nLoci*) from allele frequency *freq* at generation *endGen* backward in time, until all alleles get lost. A `trajectory` object will be returned if the length of simulated trajectory with *minMutAge* and *maxMutAge* (if specified). None will be returned if no valid trajectory is simulated after `maxAttempts` attempts. Please refer to class `trajectory`, `trajectorySimulator` and their member functions for more details about allowed input for these parameters.

3.2.4 Migration models

MigrIslandRates (*r*, *n*)

migration rate matrix

$$\begin{array}{cccc} x & m/(n-1) & m/(n-1) & \dots \\ m/(n-1) & x & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & m/(n-1) & m/(n-1) & x \end{array}$$

where $x = 1-m$

MigrHierarchicalIslandRates (*r1*, *r2*, *n*)

Return the migration rate matrix for a hierarchical island model where there are different migration rate within and across groups of islands.

r1: Within group migration rates. It can be a number or a list of numbers for each group of the islands.

r2: Across group migration rates which is the probability that someone will migrate to a subpopulation outside of his group. A list of *r2* could be specified for each group of the islands.

n: Number of islands in each group. E.g. *n*=[5, 4] specifies two groups of islands with 5 and 4 islands each.

For individuals in an island, the probability that it remains in the same island is $1-r1-r2$ (*r1*, *r2* might vary by island groups), that it migrates to another island in the same group is *r1* and migrates to another island outside of the group is *r2*. Migrate rate to a specific island depends on the size of group.

MigrSteppingStoneRates (*r*, *n*, *circular*=False)

migration rate matrix, circular stepping stone model ($X=1-m$)

$$\begin{array}{ccccccc} X & m/2 & & & & & m/2 \\ m/2 & X & m/2 & & & & 0 \\ 0 & m/2 & x & m/2 & \dots & \dots & 0 \\ \dots & & & & & & \\ m/2 & 0 & \dots & & m/2 & X & \end{array}$$

or non-circular

$$\begin{array}{ccccccc} X & m/2 & & & & & m/2 \\ m/2 & X & m/2 & & & & 0 \\ 0 & m/2 & X & m/2 & \dots & \dots & 0 \\ \dots & & & & & & \\ \dots & & & m & X & & \end{array}$$

3.2.5 A text or GUI-based progress bar

3.2.6 Class `simuProgress`

The `simuProgress` class defines a progress bar. This class will use a text-based progress bar that outputs progressing dots (.) with intermediate numbers (e.g. 5 for 50%) under a non-GUI mode (`gui=False`). In the GUI mode, a Tkinter or wxPython progress dialog will be used (`gui=Tkinter` or `gui=wxPython`). The default mode is determined by the global gui mode of `simuPOP` (see also `simuOpt.setOptions`).

This class is usually used as follows:

```
progress = simuProgress("Start simulation", 500)
for i in range(500):
    progress.update(i+1)
# if you would like to make sure the done message is displayed.
progress.done()
```

class `simuProgress` (*message, totalCount, progressChar='.', block=2, done= 'Done.
n', gui=None*)

message: Title of the progress bar.

totalCount: Total expected steps.

progressChar: Character to be displayed for each progress. This is only used for text-based progress bars.

block: Intervals at which progresses will be displayed. Default to 2 (percent).

done: Message displayed when the job is finished.

`done()`

Finish progressbar, print 'done' message if in text-mode.

`update(count)`

Update the progreebar.

3.2.7 View population variables

`ViewVars` (*var, gui=None*)

list a variable in tree format, either in text format or in a: wxPython window.

var: A dictionary variable to be viewed. Dictionary wrapper objects returned by `population.dvars()` and `simulator.dvars()` are also acceptable.

gui: If `gui` is `False` or `'Tkinter'`, a text presentation (use the `pprint` module) of the variable will be printed to the screen. If `gui` is `'wxPython'` and `wxPython` is available, a `wxPython` windows will be used. The default mode is determined by the global gui mode (see also `simuOpt.setOptions`).

3.2.8 Export `simuPOP` population

`SaveCSV` (*pop, filename="", fields=[], loci=[], header=True, shift=1, combine=None, sexCode={1: '1', 2: '2'},
affectionCode={False: '2', True: '1'}, **kwargs*)

Save a `simuPOP` population `pop` in csv format.

pop: A `simuPOP` population object. If a string is given, it will be loaded.

filename: Output filename.

fields: Information fields to be outputted.

loci: If a list of loci is given, only genotype at these loci will be written.

header: Whether or not a header should be written. These headers will include information fields, sex (if `sexCode` is not `None`), affection status (if `affectionCode` is not `None`) and loci names. If genotype at a locus needs more than one column, `_1`, `_2` etc will be appended to locus names.

genotype: list of loci to output, default to all.

combine: how to combine the markers. Default to `None`. A function can be specified, that takes the form:

```
def func(markers):  
    return markers[0]+markers[1]
```

shift: since alleles in `simuPOP` is 0-based, `shift=1` is usually needed to output alleles starting from allele 1. This parameter is ignored if `combine` is used.

3.3 Module `simuPOP.plotter`

This module defines several utility functions and Python operators that make use of the Python `rpy` module (<http://rpy.sourceforge.net>) to plot expressions and information fields of evolving populations using a popular statistical analysis language R (<http://www.r-project.org>). Note that `rpy2`, the successor of `rpy`, is currently not supported.

Each operator calls a sequence of R functions to draw and save figures. A special parameter passing mechanism is used so that you can specify arbitrary parameters to these functions. For example, you can use parameter `"par_mfrow=[2,2]"` to pass `"mfrow=[2,2]"` to function `"par"`, and use `"lty_rep=[1,2]"` to pass `"lty=1"` and `"lty=2"` to specify different line types for different replicates. The help message of each class will describe which and in what sequence these R functions are called to help you figure out which parameters are allowed.

`newDevice()`

Create a new graphics window and return its device number in R. This function essentially calls `getOption('device')()` in R.

`saveFigure(file=None, **kwargs)`

Save current figure into `file`. File format and graphics device are determined by file extension. Supported file formats include `pdf`, `png`, `bmp`, `jpg` (`jpeg`), `tif` (`tiff`), and `eps`, which correspond to R devices `pdf`, `png`, `bmp`, `jpeg`, `tiff` and `postscript`. A `postscript` device will be used if there is no file extension or the file extension is not recognizable. Additional keyword parameters will be passed to the underlying `dev.print` function.

3.3.1 Class `derivedArgs`

This class implements the derived keyword argument handling mechanism that is used by all classes defined in this module. It is provided for users who would like to use this mechanism for their own `rpy`-related operators.

An derived keyword argument is an argument that is prefixed with a function name and/or suffixed by an iterator name. The former specifies to which underlying R function this parameter will be passed to; the latter allows the users to specify a list of values that will be passed, for example, to lines representing different replicates. For example, parameter `par_mar=[1]*4` will pass `mar=[1]*4` to R function `par`, and `lty_rep=[1, 2, 3]` will pass `lty=1`, `lty=2` and `lty=3` to different replicates.

Values provided to derived arguments are usually passed unchanged, but with one exception: string value with a leading `!` mark will be evaluated against the current population before it is returned. For example, `main='! "Allele frequency at generation %d" % gen'` will return `main="Allele frequency at generation 100"` at generation 100.

`class derivedArgs (defaultFuncs=[], allFuncs=[], suffixes=[], defaultParams={}, **kwargs)`

defaultFunc: Default functions. Parameters without a prefix will be passed to these functions.

allFuncs: Allowed functions. This should be all the R functions called in your class.

suffixes: A list of allowed suffixes.

defaultParams: Default parameters in a dictionary. E.g. `{'plot_type': 'l'}` will pass `type='l'` to the `plot` function unless users provides another value.

kwargs: User specified parameters. These parameters will override default values in `defaultParams`.

addDefault (***kwargs*)

Add keyword parameters *kwargs* if they have not been defined.

getArgs (*func, pop, **kwargs*)

Get all single format parameters from keyword parameters. Additional keyword arguments can be used to specify suffix and its index. (e.g. `rep=1` will return the second element of `par_rep`). Unrecognized keyword arguments are handled as default value that will be used if a parameter is not defined. E.g. `getArgs('line', pop, rep=1, pch=4)` will get parameters for replicate 1 and add `pch=4` if `pch` is not defined.

getLegendArgs (*func, pop, args, keys, values, **kwargs*)

Get argument values for legend drawing purposes. For example,

`getMultiArgs('lines', pop, ['lty', 'pch'], 'rep', [0,1,2])`

will get parameter for `lty` and `pch` for all `rep`. If there are more keys (e.g. `['rep', 'dim']`), values should be a list of lists (e.g., `[(0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2)]`). Default values could be passed as additional keyword arguments.

3.3.2 Class `varPlotter`

This class defines a Python operator that uses R to plot the current and historical values of a Python expression (`expr`), which are evaluated (against each population's local namespace) and saved during evolution. The return value of the expression can be a number or a sequence, but should have the same type and length across all replicates and generations. Histories of each value (or each item in the returned sequence) of each replicate form a line, with generation numbers as its x-axis. Number of lines will be the number of replicates multiplied by dimension of the expression. Although complete histories are usually saved, you can use parameter `win` to save histories only within the last `win` generations.

A figure will be draw at the end of the last replicate (except for the first generation where no line could be drawn) unless the current generation is less than `update` generations away from the last generation at which a figure has been drawn. Lines for multiple replicates or dimensions could be plotted in the same figure (by default), or be separated to subplots by replicates (`byRep`), by each dimension of the results (`byDim`), or by both. These figure could be saved to files in various formats if parameter `saveAs` is specified. File format is determined by file extension. After the evolution, the graphic device could be left open (`leaveOpen`).

Besides parameters mentioned above, arbitrary keyword parameters could be specified and be passed to the underlying R drawing functions `plot` and `lines`. These parameters could be used to specify line type (`lty`), color (`col`), title (`main`), limit of x and y axes (`xlim` and `ylim`) and many other options (see R manual for details). As a special case, multiple values can be passed to each replicate and/or dimension if the name of a parameter ends with `_rep`, `_dim`, or `_repdim`. For example, `lty_rep=range(1, 5)` will pass parameters `lty=1, ... lty=4` to four replicates. You can also pass parameters to specific R functions such as `par`, `plot`, `lines`, `legend`, `dev_print` by prefixing parameter names with a function name. For example, `dev_print_width=300` will pass `width=300` to function `dev.print()` when you save your figures using this function. In addition, if the value of a parameter is a string starting with `!`, the evaluated result of the remaining string will be used as parameter value. Further customization of your figures could be achieved by writing your own hook functions that will be called before and after a figure is drawn, and after each plot call.

This operator calls R functions `par`, `plot`, `lines`, `legend`, and `dev.print`. Functions `plot` and `lines` are the default destination for keyword arguments and the ones that accept list parameters to customize lines by replicate and/or dimension.

class varPlotter (*expr*, *win*=0, *update*=1, *byRep*=False, *byDim*=False, *saveAs*=", *leaveOpen*=False, *legend*=[], *preHook*=None, *postHook*=None, *plotHook*=None, *stage*=4, *begin*=0, *end*=-1, *step*=1, *at*=[], *reps*=True, ***kwargs*)

expr: expression that will be evaluated at each replicate's local namespace when the operator is applied. Its value can be a number or a list (or tuple) but the type and length of the return value should be consistent for all replicates and at all generations.

win: Window of generations. If given, only values from generation -win to -1 will be plotted.

update: Update the figure after specified generations. For example, you can evaluate an expression and save its values at every 10 generations (parameter *step*=10) but only draw a figure after every 50 generations (parameter *update*=50).

byRep: Separate values at different replicates to different subplots.

byDim: Separate items from sequence results of *expr* to different subplots. If both *byRep* and *byDim* are True, the subplots will be arranged by variable and then replicates.

saveAs: Save figures in files *saveAs_gen.ext* (e.g. *figure_10.eps* if *saveAs*='figure.eps'). If *ext* is given, a corresponding device will be used. Otherwise, a default postscript driver will be used. Currently supported formats include .pdf, .png, .bmp, .jpg, and .tif. The default filename could be overridden by derived argument *dev_print_file*.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to False functions. If this option is set to True, you will have to close the graphic device explicitly using function *r.dev_off()*. Note that leaving the device open allows further manipulation of the figures outside of this operator.

legend: labels of the lines. This operator will look for keyword parameters such as *col*, *lty*, *lwd*, and *pch* and call the *legend* function to draw a legend. If figure has multiple lines for both replicates and dimensions, legends should be given to each dimension, and then each replicate.

preHook: A function that, if given, will be called before the figure is draw. The *r* object from the *plotter* module will be passed to this function.

postHook: A function that, if given, will be called after the figure is drawn. The *r* object from the *plotter* module will be passed to this function.

plotHook: A function that, if given, will be called after each *plot* function. The *r* object from the *plotter* module, generation list, data being plotted, replicate number (if applicable) and dimension index (if applicable) will be passed as keyword arguments *r*, *gen*, *data*, *rep* (optional) and *dim* (optional).

kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) *plot_*, *lines_*, *par_*, *legend_* and *dev_print_*, and suffixes (list parameters) *_rep*, *_dim*, and *_repdim*. Arguments without prefixes are sent to functions *plot* and *lines*. String values with a leading ! will be replaced by its evaluated result against the current population.

3.3.3 Class **scatterPlotter**

This class defines a Python operator that uses R to plot individuals in a population, using values at two information fields as their x- and y-axis.

Arbitrary keyword parameters could be specified and be passed to the underlying R drawing functions *plot* and *points*. These parameters could be used to specify point type (*pch*), color (*col*), title (*main*), limit of x and y axes (*xlim* and *ylim*) and many other options (see R manual for details). You can also pass parameters to specific R functions such as *par*, *plot*, *points*, *legend*, *pdf* by prefixing parameter names with a function name. For example, *par_mar*=[1]*4 will pass *par*=[1]*4 to function *par()* which is called before a figure is drawn. (Note that the function to save a figure is *dev.print* so parameters such as *dev_print_width* should be used.) Further customization of your figures could be achieved by writing your own hook functions that will be called before and after a figure is drawn.

The power of this operator lies in its ability to differentiate individuals from different (virtual) subpopulations. If you specify IDs of (virtual) subpopulations (VSPs) in parameter `subPops`, only individuals from these VSPs will be displayed. Points from these subpopulations will be drawn with different shapes and colors. You can also customize these points using list parameters with suffix `_sp`. For example, if you have defined two VSPs by sex and set `subPops=[(0, 0), (0, 1)]`, `col_sp=['blue', 'red']` will color male individuals with blue and female individuals with red. In addition, if the value of a parameter is a string starting with `!`, the evaluated result of the remaining string will be used as parameter value.

This operator calls R functions `par`, `plot`, `points`, `legend`, and `dev.print`. Functions `plot` and `points` are the default destination for keyword arguments and the ones that accept list parameters to customize lines by (virtual) subpopulation.

```
class scatterPlotter (infoFields=[], saveAs="", leaveOpen=False, legend=[], preHook=None,
                      postHook=None, stage=4, begin=0, end=-1, step=1, at=[], reps=True, sub-
                      Pops=<simuPOP.simuPOP.subPopList>, **kwargs)
```

infoFields: Two information fields whose values will be the x- and y-axis of each point (individual) in the plot.

subPops: A list of subpopulations and virtual subpopulations. Only individuals from these subpopulations will be plotted. Default to subpopulation indexes.

saveAs: Save figures in files `saveAs_gen_rep.ext` (e.g. `figure_10_0.eps` if `saveAs='figure.eps'`). If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used. Currently supported formats include `.pdf`, `.png`, `.bmp`, `.jpg`, and `.tif`. The default filename could be overridden by derived argument `dev_print_file`.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to `False` functions. If this option is set to `True`, you will have to close the graphic device explicitly using function `r.dev_off()`. Note that leaving the device open allows further manipulation of the figures outside of this operator.

legend: labels of the points. It must match the specified subpopulations.

preHook: A function that, if given, will be called before the figure is draw. The `r` object from the `plotter` module will be passed to this function.

postHook: A function that, if given, will be called after the figure is drawn. The `r` object from the `plotter` module will be passed to this function.

kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) `plot_`, `points_`, `par_`, `legend_` and `dev_print_`, and suffixes (list parameters) `_sp`. Arguments without prefixes are sent to functions `plot` and `points`. String values with a leading `!` will be replaced by its evaluated result against the current population.

3.3.4 Class `infoPlotter`

This operator uses a R function such as `hist` and `qqplot` to plot properties of one or more information fields of individuals in one or more (virtual) subpopulations. Separate subplots are used for different information fields and subpopulations.

This operator essentially gets values of information fields and sends them to a R function such as `hist`. The resulting figures could be customized by additional keyword parameters and various hook functions. For example, a `qqline` function could be called in a `plotHook` function to add a QQ line to a `qqnorm` plot. The `plotHook` can be used to draw the whole (sub)plot if no R function is specified for parameter `func`.

Besides regular keyword parameters, keyword parameters ending in `_sp`, `_fld` or `_spfld` are expected to have multiple values which will be used for different subpopulations, information fields, and their combinations. You can also specify which function the keyword should be sent by prefixing a function name to the parameter name. For example, `pch_fld=[1, 2]` will use different symbols for different information fields, and `par_mar=[1]*4` will send parameter `mar=[1]*4` to function `par`. In addition, if the value of a parameter is a string starting with `!`, the evaluated result of the remaining string will be used as parameter value.

This operator calls R functions `par`, `dev.print`, and a user-specified function. Additional keyword arguments without function prefix will be sent to this function.

```
class infoPlotter (func=None, infoFields=[], saveAs="", leaveOpen=False, preHook=None, postHook=None,  

plotHook=None, stage=4, begin=0, end=-1, step=1, at=[], reps=True, sub-  

Pops=<simuPOP.simuPOP.subPopList>, **kwargs)
```

func: Name of the R function that will be called to draw figures from values of given information fields. No R function will be called if it is not specified. In this case, a `plotHook` can be used to plot passed values.

infoFields: Information fields whose values will be sent to the specified plotting function.

subPops: A list of subpopulations and virtual subpopulations. Each subpopulation will be plotted in a separate subplot.

saveAs: Save figures in files `saveAs_gen_rep.ext` (e.g. `figure_10_0.eps` if `saveAs='figure.eps'`). If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used. Currently supported formats include `.pdf`, `.png`, `.bmp`, `.jpg`, and `.tif`. The default filename could be overridden by derived argument `dev_print_file`.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to `False` functions. If this option is set to `True`, you will have to close the graphic device explicitly using function `r.dev_off()`. Note that leaving the device open allows further manipulation of the figures outside of this operator.

preHook: A function that, if given, will be called before the figure is draw. The `r` object from the `plotter` module will be passed to this function.

postHook: A function that, if given, will be called after the figure is drawn. The `r` object from the `plotter` module will be passed to this function.

plotHook: A function that, if given, will be called after each specified plot function. The `r` object from the `plotter` module, data being plotted, name of the information field and index of subpopulation (in parameter `subPops`, if applicable) will be passed with keywords `r`, `data`, `field` and `subPop` (optional) respectively.

kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) `par_`, `dev_print_` and the function you specify (parameter `func`), and suffixes (list parameters) `_sp`, `_fld`, and `_spfld`. Arguments without prefixes are sent to the user specified function. String values with a leading `!` will be replaced by its evaluated result against the current population.

histPlotter (**args, **kwargs*)

A `infoPlotter` that uses R function `hist` to draw histogram of individual information fields of specified (virtual) subpopulations. Please see `infoPlotter` for details.

qqPlotter (**args, **kwargs*)

A `infoPlotter` that uses R function `qqnorm` to draw qq plot of individual information fields of specified (virtual) subpopulations. Please see `infoPlotter` for details.

3.3.5 Class `boxPlotter`

This operator draws boxplots of one or more information fields of individuals in one or more (virtual) subpopulations of a population. Although a `infoPlotter` with `func=boxplot` could be used to plot boxplots for each information field and/or subpopulation, this class allows multiple whiskers to share one plot. How the whiskers are organized is controlled by parameters `byField` and `bySubPop`.

This operator essentially gets values of information fields and sends them to boxplots. Individual ownerships (subpopulation or field) are also passed so that multiple whiskers could be drawn in the same plot. The resulting figures could be customized by additional keyword parameters and various hook functions.

Besides regular keyword parameters, keyword parameters ending in `_sp`, `_fld` or `_spfld` are expected to have multiple values which will be used for different subpopulations, information fields, and their combinations. You can

also specify which function the keyword should be sent by prefixing a function name to the parameter name. For example, `pch_fld=[1, 2]` will use different symbols for different information fields, and `par_mar=[1]*4` will send parameter `mar=[1]*4` to function `par`. In addition, if the value of a parameter is a string starting with `!`, the evaluated result of the remaining string will be used as parameter value.

This operator calls R functions `par`, `boxplot` and `dev.print`. Keyword parameters without function prefix will be passed to `boxplot`.

```
class boxPlotter (infoFields=[], byField=False, bySubPop=False, saveAs="", leaveOpen=False, preHook=None,
                  postHook=None, plotHook=None, stage=4, begin=0, end=-1, step=1, at=[], reps=True, sub-
                  Pops=<simuPOP.simuPOP.subPopList>, **kwargs)
```

infoFields: Information fields whose values will be sent to R function `boxplot`.

subPops: A list of subpopulations and virtual subpopulations. Separate whiskers will be drawn for individuals in these subpopulations.

byField: If multiple information fields are specified, separate the whiskers different subplots if this parameter is `True`.

bySubPop: If multiple (virtual) subpopulations are specified, separate the whiskers to different subplots if this parameter is `True`.

saveAs: Save figures in files `saveAs_gen_rep.ext` (e.g. `figure_10_0.eps` if `saveAs='figure.eps'`). If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used. Currently supported formats include `.pdf`, `.png`, `.bmp`, `.jpg`, and `.tif`. The default filename could be overridden by derived argument `dev_print_file`.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to `False` functions. If this option is set to `True`, you will have to close the graphic device explicitly using function `r.dev_off()`. Note that leaving the device open allows further manipulation of the figures outside of this operator.

preHook: A function that, if given, will be called before the figure is draw. The `r` object from the `plotter` module will be passed to this function.

postHook: A function that, if given, will be called after the figure is drawn. The `r` object from the `plotter` module will be passed to this function.

plotHook: A function that, if given, will be called after each specified plot function. The `r` object from the `plotter` module, current field and subpopulation will be passed with keywords `r`, `field` and `subPop` if applicable.

kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) `plot_`, `boxplot_`, `par_`, and `dev_print_`, and suffixes (list parameters) `_sp`, `_fld` and `_spfld`. Arguments without prefixes are sent to function `boxplot`. String values with a leading `!` will be replaced by its evaluated result against the current population.

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