# simuPOP Reference Manual

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#### Abstract

simuPOP is a general-purpose individual-based 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. In contrast to competing applications that use command-line options or configuration files to direct the execution of a limited number of predefined evolutionary scenarios, users of simuPOP's scripting interface could make use of many of its unique features, such as customized chromosome types, arbitrary nonrandom mating schemes, virtual subpopulations, information fields and Python operators, to construct and study almost arbitrarily complex evolutionary scenarios.

simuPOP is provided as a number of Python modules, which consist of a large number of Python objects and functions, including population, mating schemes, operators (objects that manipulate populations) and simulators to coordinate the evolutionary processes. It is the users' responsibility to write a Python script to glue these pieces together and form a simulation. At a more user-friendly level, an increasing number of functions and scripts contributed by simuPOP users is available in the online simuPOP cookbook. They provide useful functions for different applications (e.g. load and manipulate HapMap samples, import and export files from another application) and allow users who are unfamiliar with simuPOP to perform a large number of simulations ranging from basic population genetics models to generating datasets under complex evolutionary scenarios.

This document provides complete references to all classes and functions of simuPOP and its utility modules. 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. All resources, including a pdf version of this guide and a mailing list can be found at the simuPOP homepage http://simupop.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, pedigree 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 both Individual and Population 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, which can either be shared by all loci or be specified for each locus.
- Names of loci and chromosomes.
- Names of information fields attached to each individual.

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

### class GenoStruTrait()

A GenoStruTrait object is created with the construction of a Population object and cannot be initialized directly.

# absLocusIndex(chrom, locus)

Return the absolute index of locus locus on chromosome chrom. c.f. chromLocusPair.

# alleleName(allele, locus=0)

Return the name of allele *allele* at *lcous* 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 value ('0', '1', '2', etc) is returned.

### 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).

### 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.

### chromLocusPair(locus)

Return the chromosome and relative index of a locus using its absolute index locus. c.f. absLocusIndex.

#### chromName(chrom)

Return the name of a chromosome chrom.

### chromNames()

Return a list of the names of all chromosomes.

### chromType(chrom)

Return the type of a chromosome *chrom* (CUSTOMIZED, AUTOSOME, CHROMOSOME\_X, CHROMOSOME\_Y or MITOCHONDRIAL.

### chromTypes()

Return the type of all chromosomes (CUSTOMIZED, AUTOSOME, CHROMOSOME\_X, CHROMOSOME\_Y, or MITOCHONDRIAL).

# $indexesOfLoci(loci=ALL\_AVAIL)$

Return the indexes of loci with positions *positions* (list of (chr, pos) pairs). Raise a ValueError if any of the loci cannot be found.

### 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.

### 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* prameter 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.

### numChrom()

Return the number of chromosomes.

### numLoci(chrom)

Return the number of loci on chromosome *chrom*.

#### numLoci()

Return a list of the number of loci on all chromosomes.

#### 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 #-ploid where # is the ploidy number.

#### totNumLoci()

Return the total number of loci on all chromosomes.

### 1.1.2 Class Individual

A Population consists of individuals with the same genotypic structure. An Individual object cannot be created independently, but referces to inidividuals 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 chromsome, 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, is 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).

### affected()

Return True if this individual is affected.

# 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 is 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).

# alleleChar(idx, ploidy=-1, chrom=-1)

Return the name of allele(idx, ploidy, chrom). If idx is invalid (e.g. second homologus copy of chromosome Y), ' is returned.

### alleleLineage(idx, ploidy=-1, chrom=-1)

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

This function returns 0 for modules without lineage information.

# $\__{cmp}$ $\_(rhs)$

A python function used to compare the individual objects

# genotype(ploidy=ALL\_AVAIL, chroms=ALL\_AVAIL)

Return an editable array (a carray object) that represents all alleles of an individual. If *ploidy* or *chroms* is given, only alleles on the specified chromosomes and homologous copy of chromosomes will be returned.

If multiple chromosomes are specified, there should not be gaps between chromosomes. This function ignores type of chromosomes so it will return unused alleles for sex and mitochondrial chromosomes.

### info(field)

Return the value of an information field *filed* (by index or name). ind.info(name) is equivalent to ind.name although the function form allows the use of indexes of information fieldes.

### lineage(ploidy=ALL\_AVAIL, chroms=ALL\_AVAIL)

Return an editable array (a carray\_lineage object) that represents the lineages of all alleles of an individual. If *ploidy* or *chroms* is given, only lineages on the specified chromosomes and homologous copy of chromosomes will be returned. If multiple chromosomes are specified, there should not be gaps between chromosomes. This function ignores type of chromosomes so it will return lineage of unused alleles for sex and mitochondrial chromosomes. A None object will be returned for modules without lineage information.

# mutants(ploidy=ALL\_AVAIL, chroms=ALL\_AVAIL)

Return an itertor that iterate through all mutants (non-zero alleles) of an individual. Each mutant is presented as a tuple of (index, value) where index is the index of mutant ranging from zero to totNumLoci() \* ploidy() - 1, so you will have to adjust indexes to check multiple alleles at a locus. If *ploidy* or *chroms* is given, only alleles on the specified chromosomes and homologous copy of chromosomes will be iterated. If multiple chromosomes are specified, there should not be gaps between chromosomes. This function ignores type of chromosomes so it will return unused alleles for sex and mitochondrial chromosomes.

### setAffected(affected)

Set affection status to affected (True or False).

### 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).

# setAlleleLineage(lineage, idx, ploidy=-1, chrom=-1)

Set lineage *lineage* to an allele, 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). This function does nothing for modules without lineage information.

# setGenotype(geno, ploidy=ALL\_AVAIL, chroms=ALL\_AVAIL)

Fill the genotype of an individual using a list of alleles *geno*. If parameters *ploidy* and/or *chroms* are specified, alleles will be copied to only all or specified chromosomes on selected homologous copies of chromosomes. geno will be reused if its length is less than number of alleles to be filled. This function ignores type of chromosomes so it will set genotype for unused alleles for sex and mitochondrial chromosomes.

### setInfo(value, field)

Set the value of an information field *field* (by index or name) to *value*. ind.setInfo(value, field) is equivalent to ind.field = value although the function form allows the use of indexes of information fieldes.

### setLineage(lineage, ploidy=ALL\_AVAIL, chroms=ALL\_AVAIL)

Fill the lineage of an individual using a list of IDs *lineage*. If parameters *ploidy* and/or *chroms* are specified, lineages will be copied to only all or specified chromosomes on selected homologous copies of chromosomes. Lineage will be reused if its length is less than number of allelic lineage to be filled. This function ignores type of chromosomes so it will set lineage to unused alleles for sex and mitochondrial chromosomes. It does nothing for modules without lineage information.

### setSex(sex)

Set individual sex to MALE or FEMALE.

# sex()

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

# 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 arragement 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.

- *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. If there is only one chromosome, numLoci instead of [numLoci] can be used.
- chromTypes: A list that specifies the type of each chromosome, which can be AUTOSOME, CHROMOSOME\_X, CHROMOSOME\_Y, 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.

# 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. The newly added alleles will have zero lineage in modules with lineage information.

### 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. Chromosomes of *pop*, if named, should not conflict with names of existing chromosome. 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.

# addInfoFields(fields, init=0)

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

# 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. Newly inserted alleles will have zero lineage in modules with lineage information.

### addLociFrom(pop, byName=False)

Add loci from population *pop*. By default, chromosomes are merged by index and names of merged chromosomes of population *pop* will be ignored (merge of two chromosomes with different names will yield a warning). If *byName* is set to True, chromosomes in *pop* will be merged to chromosomes with identical names. 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. Allele lineages are also copied from *pop* in modules with lineage information.

# 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. Note that a float *idx* is acceptable as long as it rounds closely to an integer.

### ancestralGens()

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

#### clone()

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

### $\__{cmp}_{(rhs)}$

A python function used to compare the population objects

# dvars(subPop=[])

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

# extractIndividuals(indexes=[], IDs=[], idField="ind\_id", filter=None)

Extract individuals with given absolute indexes (parameter *indexes*), IDs (parameter *IDs*, stored in information field *idField*, default to ind\_id), or a filter function (parameter *filter*). If a list of absolute indexes are specified, the present generation will be extracted and form a one-generational population. If a list of IDs are specified, this function will look through all ancestral generations and extract individuals with given ID. Individuals with shared IDs are allowed. In the last case, a user-defined Python function should be provided. This function should accept parameter "ind" or one or more of the information fields. All individuals, including ancestors if there are multiple ancestral generations, will be passed to this function. Individuals that returns True will be extracted. Extracted individuals will be in their original ancestral generations and subpopulations, even if some subpopulations or generations are empty. An IndexError will be raised if an index is out of bound but no error will be given if an invalid ID is encountered.

# $extractSubPops (subPops = ALL\_AVAIL, rearrange = False)$

Extract a list of (virtual) subpopulations from a population and create a new population. If *rearrange* is False (default), structure and names of extracted subpopulations are kept although extracted subpopulations can have fewer individuals if they are created from extracted virtual subpopulations. (e.g. it is possible to extract all male individuals from a subpopulation using a SexSplitter()). If *rearrange* is True, each (virtual) subpopulation in *subPops* becomes a new subpopulation in the extracted population in the order at which they are specified. Because each virtual subpopulation becomes a subpopulation, this function could be used, for example, to separate male and female individuals to two subpopulations ( subPops=[(0,0), (0,1)]). If overlapping (virtual) subpopulations are specified, individuals will be copied multiple times. This function only extract individuals from the present generation.

# 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.

# indByID(id, ancGens=ALL\_AVAIL, 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=ALL\_AVAIL), but you can limit the search in specific generations if you know which generations to search (ancGens=[0,1] for present and parental generations) or UNSPECIFIED to search only the current generation. If no individual with *id* is found, an IndexError will be raised. A float *id* is acceptable as long as it rounds closely to an integer. Note that this function uses a dynamic searching algorithm which tends to be slow. If you need to look for multiple individuals from a static population, you might want to convert a population object to a pedigree object and use function Pedigree.indByID.

### 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)).

### 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. Note that a float idx is acceptable as long as it rounds closely to an integer.

# 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)). If you would like to iterate through multiple subpopulations in multiple ancestral generations, please use function Population.allIndividuals().

### lineage(subPop=[])

Return an editable array of the lineage of alleles for all individuals in a population (if subPop=[], default), or individuals in a subpopulation *subPop*. Virtual subpopulation is unsupported. **This function returns** None **for modules without lineage information.** 

# $mergeSubPops(subPops=ALL\_AVAIL, name="")$

Merge subpopulations *subPops*. If *subPops* is ALL\_AVAIL (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.

### mutants(subPop=[])

Return an iterator that iterate through mutants of all individuals in a population (if subPop=[], default), or individuals in a subpopulation *subPop*. Virtual subpopulation is unsupported. Each mutant is presented as a tuple of (index, value) where index is the index of mutant (from 0 to totNumLoci()\*ploidy()) so you will have to adjust its value to check multiple alleles at a locus. This function ignores type of chromosomes so non-zero alleles in unused alleles of sex and mitochondrial chromosomes are also iterated.

# numSubPop()

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

### numVirtualSubPop()

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

# popSize(ancGen=-1)

Return the total number of individuals in all subpopulations of the current generation (default) or the an ancestral generation *ancGen*.

# 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. Otherise, the current population will become the parental generation of *pop*. If *ancGen* of a population is positive and there are already *ancGen* ancestral generations (c.f. 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.

# recodeAlleles(alleles, loci=ALL\_AVAIL, alleleNames=[])

Recode alleles at *loci* (can be a list of loci indexes or names, or all loci in a population (ALL\_AVAIL)) 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], x outside of the range of *newAlleles* will not be recoded, although a warning will be given if DBG\_WARNING is defined) or a Python function, which should accept one or both parameters allele (existing allele) and locus (index of locus). The return value will become the new allele. This function is intended to recode some alleles without listing all alleles in a list. It will be called once for each existing allele so it is not possible to recode an allele to different alleles. 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(indexes=[], IDs=[], idField="ind\_id", filter=None)

Remove individual(s) by absolute indexes (parameter *index*) or their IDs (parameter *IDs*), or using a filter function (parameter *filter*). If indexes are used, only individuals at the current generation will be removed. If IDs are used, all individuals with one of the IDs at information field *idField* (default to "ind\_id") will be removed. Although "ind\_id" usually stores unique IDs of individuals, this function is frequently used to remove groups of individuals with the same value at an information field. An IndexError will be raised if an index is out of bound, but no error will be given if an invalid ID is specified. In the last case, a user-defined function should be provided. This function should accept parameter "ind" or one or more of the information fields. All individuals, including ancestors if there are multiple ancestral generations, will be passed to this function. Individuals that returns True will be removed. This function does not affect subpopulation structure in the sense that a subpopulation will be kept even if all individuals from it are removed.

### removeInfoFields(fields)

Remove information fields *fields* from a population.

# $\verb"removeLoci" (loci=UNSPECIFIED") keep=UNSPECIFIED")$

Remove *loci* (absolute indexes or names) 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 (virtual) subpopulation(s) *subPops* and all their individuals. This function can be used to remove complete subpopulations (with shifted subpopulation indexes) or individuals belonging to virtual subpopulations of a subpopulation. In the latter case, the subpopulations are kept even if all individuals have been removed. This function only handles the present generation.

# 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.

# save(filename)

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

### setAncestralDepth(depth)

Set the intended ancestral depth of a population to *depth*, which can be  $\theta$  (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.

# 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().

# 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.

# setLineage(geno, subPop=[])

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

subPopSize(subPop)\*totNumLoci()\*ploidy(). This function returns directly for modules without lineage information.

### setSubPopByIndInfo(field)

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

# setSubPopName(name, subPop)

Assign a name name to subpopulation subPop. Note that subpopulation names do not have to be unique.

### 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.

# sortIndividuals(infoFields)

Sort individuals according to values at specified information fields (*infoFields*). Individuals will be sorted at an increasing order.

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

Split subpopulation *subPop* into subpopulations of given *sizes*, which should add up to the size of subpopulation *subPop* or 1, in which case *sizes* are treated as proportions. 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.

### subPopBegin(subPop)

Return the index of the first individual in subpopulation subPop.

#### 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.

### 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.

### 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.

# subPopSizes(ancGen=-1)

Return the sizes of all subpopulations at the current generation (default) or specified ancestral generation *ancGen*. Virtual subpopulations are not considered.

# swap(rhs)

Swap the content of two population objects, which can be handy in some particular circumstances. For example, you could swap out a population in a simulator.

# ${\tt updateInfoFieldsFrom} (fields, pop, from Fields = [], anc Gens = ALL\_AVAIL)$

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 *ancGens* is not ALL\_AVAIL, only the specified ancestral generations are updated.

### 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.

### 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"].

#### virtualSplitter()

Return the virtual splitter associated with the population, None will be returned if there is no splitter.

# ${\tt asPedigree} (idField = 'ind\_id', fatherField = 'father\_id', motherField = 'mother\_id')$

Convert the existing population object to a pedigree. After this function pedigree function should magically be usable for this function.

### subPopSize(subPop=[], ancGen=-1)

Return the size of a subpopulation (subPopSize(sp)) or a virtual subpopulation (subPopSize([sp, vsp])) in the current generation (default) or a specified ancestral generation *ancGen*. If no *subpop* is given, it is the same as popSize(ancGen). Population and virtual subpopulation names can be used. <group>2-subpopsize</grouplociList()>

# $allIndividuals(subPops=ALL\_AVAIL, ancGens=True)$

Return an iterator that iterat through all (virtual) subpopulations in all ancestral generations. A list of (virtual) subpopulations (\*subPops\*) and a list of ancestral generations (\*ancGens\*, can be a single number) could be specified to iterate through only selected subpopulation and generations. Value "ALL\_AVAIL" is acceptable in the specification of "sp" and/or "vsp" in specifying a virtual subpopulation "(sp, vsp)" for the iteration through all or specific virtual subpopulation in all or specific subpopulations.

evolve (initOps=[], preOps=[], matingScheme=MatingScheme(), postOps=[], finalOps=[], gen=-1, dryrun=False)
Evolve the current population \*gen\* generations using mating scheme \*matingScheme\* and operators
\*initOps\* (applied before evolution), \*preOps\* (applied to the parental population at the beginning of each
life cycle), \*postOps\* (applied to the offspring population at the end of each life cycle) and \*finalOps\*
(applied at the end of evolution). More specifically, this function creates a \*Simulator\* using the current
population, call its \*evolve\* function using passed parameters and then replace the current population with
the evolved population. Please refer to function "Simulator.evolve" for more details about each parameter.

# 1.1.4 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. An unique ID for all individuals is needed to create a pedigree object from a population object. Compared to the Population class, a Pedigree object is optimized for access individuals by their IDs, regardless of population structure and ancestral generations. Note that the implementation of some algorithms rely on the fact that parental IDs are smaller than their offspring because individual IDs are assigned sequentially during evolution. Pedigrees with manually assigned IDs should try to obey such a rule.

class Pedigree(pop, loci=[], infoFields=[], ancGens=ALL\_AVAIL, idField="ind\_id", fatherField="father\_id", motherField="mother id", stealPop=False)

Create a pedigree object from a population, using a subset of loci (parameter *loci*, can be a list of loci indexes, names, or ALL\_AVAIL, default to no locus), information fields (parameter *infoFields*, default to no information field besides *idField*, *fatherField* and *motherField*), and ancestral generations (parameter *ancGens*, default to all ancestral generations). By default, information field father\_id (parameter *fatherField*) and mother\_id (parameter *motherField*) are used to locate parents identified by ind\_id (parameter *idField*), which should store an unique

ID for all individuals. Multiple individuls with the same ID are allowed and will be considered as the same individual, but a warning will be given if they actually differ in genotype or information fields. Operators IdTagger and PedigreeTagger are usually used to assign such IDs, although function sampling.indexToID could be used to assign unique IDs and construct parental IDs from index based relationship recorded by operator ParentsTagger. A pedigree object could be constructed with one or no parent but certain functions such as relative tracking will not be available for such pedigrees. In case that your are no longer using your population object, you could steal the content from the population by setting *stealPop* to True.

#### clone()

Create a cloned copy of a Pedigree.

# $identifyAncestors(IDs=ALL\_AVAIL, subPops=ALL\_AVAIL, ancGens=ALL\_AVAIL)$

If a list of individuals (*IDs*) is given, this function traces backward in time and find all ancestors of these individuals. If *IDs* is ALL\_AVAIL, ancestors of all individuals in the present generation will be located. If a list of (virtual) subpopulations (*subPops*) or ancestral geneartions (*ancGens*) is given, the search will be limited to individuals in these subpopulations and generations. This could be used to, for example, find all fathers of *IDs*. This function returns a list of IDs, which includes valid specified IDs. Invalid IDs will be silently ignored. Note that parameters *subPops* and *ancGens* will limit starting IDs if IDs is set to ALL\_AVAIL, but specified IDs will not be trimmed according to these parameters.

# ${\tt identifyFamilies}(pedField="", subPops=ALL\_AVAIL, ancGens=ALL\_AVAIL)$

This function goes through all individuals in a pedigree and group related individuals into families. If an information field *pedField* is given, indexes of families will be assigned to this field of each family member. The return value is a list of family sizes corresponding to families 0, 1, 2, ... etc. If a list of (virtual) subpopulations (parameter *subPops*) or ancestral generations are specified (parameter *ancGens*), the search will be limited to individuals in these subpopulations and generations.

### identifyOffspring(IDs=[], subPops=ALL\_AVAIL, ancGens=ALL\_AVAIL)

This function traces forward in time and find all offspring of individuals specified in parameter *IDs*. If a list of (virtual) subpopulations (*subPops*) or ancestral geneartions (*ancGens*) is given, the search will be limited to individuals in these subpopulations and generations. This could be used to, for example, find all male offspring of *IDs*. This function returns a list of *IDs*, which includes valid starting *IDs*. Invalid *IDs* are silently ignored. Note that parameters *subPops* and *ancGens* will limit search result but will not be used to trim specified *IDs*.

# indByID(id)

Return a reference to individual with *id*. An IndexError will be raised if no individual with *id* is found. An float *id* is acceptable as long as it rounds closely to an integer.

individualsWithRelatives (infoFields, sex=[], affectionStatus=[], subPops=ALL\_AVAIL, ancGens=ALL\_AVAIL)

Return a list of IDs of individuals who have non-negative values at information fields infoFields. Additional requirements could be specified by parameters sex and affectionStatus. sex can be ANY\_SEX (default), MALE\_ONLY, FEMALE\_ONLY, SAME\_SEX or OPPOSITE\_SEX, and affectionStatus can be AFFECTED, UNAFFECTED or ANY\_AFFECTION\_STATUS (default). This function by default check all individuals in all ancestral generations, but you could limit the search using parameter subPops (a list of (virtual) subpopulations) and ancestral generations ancGens. Relatives fall out of specified subpopulations and ancestral generations will be considered invalid.

 $\label{locateRelatives} \begin{tabular}{ll} locateRelatives (relType, resultFields=[], sex=ANY\_SEX, affectionStatus=ANY\_AFFECTION\_STATUS, anc-Gens=ALL\ AVAIL) \end{tabular}$ 

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

Parameter relType specifies what type of relative to locate, which can be

- •SPOUSE locate spouses with whom an individual has at least one common offspring.
- •OUTBRED\_SPOUSE locate non-slibling spouses, namely spouses with no shared parent.
- •OFFSPRING all offspring of each individual.
- •COMMON\_OFFSPRING common offspring between each individual and its spouse (located by SPOUSE or OUTBRED\_SPOUSE). *relFields* should consist of an information field for spouse and m-1 fields for offspring where m is the number of fields.

- •FULLSIBLING siblings with common father and mother,
- •SIBLING siblings with at least one common parent.

Optionally, you can specify the sex and affection status of relatives you would like to locate, using parameters *sex* and *affectionStatus*. *sex* can be ANY\_SEX (default), MALE\_ONLY, FEMALE\_ONLY, SAME\_SEX or OPPOSITE\_SEX, and *affectionStatus* can be AFFECTED, UNAFFECTED or ANY\_AFFECTION\_STATUS (default). Only relatives with specified properties will be located.

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

# save(filename, infoFields=[], loci=[])

Save a pedigree to file *filename*. This function goes through all individuals of a pedigree and outputs in each line the ID of individual, IDs of his or her parents, sex ('M' or 'F'), affection status ('A' or 'U'), values of specified information fields *infoFields* and genotypes at specified loci (parameter loci, which can be a list of loci indexes, names, or ALL\_AVAIL). Allele numbers, instead of their names are outputed. Two columns are used for each locus if the population is diploid. This file can be loaded using function loadPedigree although additional information such as names of information fields need to be specified. This format differs from a .ped file used in some genetic analysis software in that there is no family ID and IDs of all individuals have to be unique. Note that parental IDs will be set to zero if the parent is not in the pedigree object. Therefore, the parents of individuals in the top-most ancestral generation will always be zero.

# traceRelatives(fieldPath, sex=[], affectionStatus=[], resultFields=[], ancGens=ALL\_AVAIL)

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* consits of a *fieldPath* that specifies which information fields to look for at each step, a *sex* specifies sex choices at each generation, and a *affectionStatus* that specifies affection status at each generation. *fieldPath* should be a list of information fields, *sex* and *affectionStatus* are optional. If specified, they should be a list of ANY\_SEX, MALE\_ONLY, FEMALE\_ONLY, SAME\_SEX and OppsiteSex for parameter *sex*, and a list of UNAFFECTED, AFFECTED and ANY\_AFFECTION\_STATUS for parameter *affectionStatus*.

For example, if fieldPath = [['father\_id', 'mother\_id'], ['sib1', 'sib2'], ['off1', 'off2']], and sex = [ANY\_SEX, MALE\_ONLY, FEMALE\_ONLY], this function will locate father\_id and mother\_id for each individual, find all individuals referred by father\_id and mother\_id, 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. The results are father or mother's brother's daughters. Their indexes will be saved in each individuals information fields resultFields. If a list of ancestral generations is given in parameter ancGens is given, only individuals in these ancestral generations will be processed.

### asPopulation()

Convert the existing pedigree object to a population. This function will behave like a regular population after this function call.

### 1.1.5 Class Simulator

A simuPOP simulator is responsible for evolving one or more populations forward in time, subject to various *operators*. Populations in a simulator are created from one or more replicates of specified populations. A number of functions are provided to access and manipulate populations, and most importantly, to evolve them.

### class Simulator(pops, rep=1, stealPops=True)

Create a simulator with *rep* (default to 1) replicates of populations *pops*, which is a list of populations although a single population object is also acceptable. Contents of passed populations are by default moved to the simulator to avoid duplication of potentially large population objects, leaving empty populations behind. This behavior can be changed by setting *stealPops* to False, in which case populations are copied to the simulator.

### add(pop, stealPop=True)

Add a population *pop* to the end of an existing simulator. This function by default moves *pop* to the simulator, leaving an empty population for passed population object. If *steal* is set to False, the population will be copied to the simulator, and thus unchanged.

### clone()

Clone a simulator, along with all its populations. Note that Python assign statement simu1 = simu only creates a symbolic link to an existing simulator.

### $\__{cmp}_{(rhs)}$

A Pyton function used to compare the simulator objects Note that mating schemes are not tested.

# dvars(rep, subPop=[])

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

evolve(initOps=[], preOps=[], matingScheme=MatingScheme, postOps=[], finalOps=[], gen=-1, dryrun=False) Evolve all populations gen generations, subject to several lists of operators which are applied at different stages of an evolutionary process. Operators initOps are applied to all populations (subject to applicability restrictions of the operators, imposed by the rep parameter of these operators) before evolution. They are used to initialize populations before evolution. Operators finalOps are applied to all populations after the evolution.

Operators *preOps*, and *postOps* are applied during the life cycle of each generation. These operators can be applied at all or some of the generations, to all or some of the evolving populations, depending the *begin*, *end*, *step*, *at* and *reps* parameters of these operators. These operators are applied in the order at which they are specified. populations in a simulator are evolved one by one. At each generation, operators *preOps* are applied to the parental generations. 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. After an offspring generation is successfully generated and becomes the current generation, operators *postOps* are applied to the offspring generation. If any of the *preOps* and *postOps* fails (return False), the evolution of a population will be stopped. The generation number of a population, which is the variable "gen" in each populations local namespace, is increased by one if an offspring generation has been successfully populated even if a post-mating operator fails. Another variable "rep" will also be set to indicate the index of each population in the simulator. Note that populations in a simulator does not have to have the same generation number. You could reset a population's generation number by changing this variable.

Parameter *gen* can be set to a non-negative number, which is the number of generations to evolve. If a simulator starts at the beginning of a generation g (for example 0), a simulator will stop at the beginning (instead of the end) of generation g + gen (for example gen). If *gen* is negative (default), the evolution will continue indefinitely, until all replicates are stopped by operators that return False at some point (these operators are called *terminators*). At the end of the evolution, the generations that each replicates have evolved are returned. Note that *finalOps* are applied to all applicable population, including those that have stopped before others.

If parameter *dryrun* is set to True, this function will print a description of the evolutionary process generated by function describeEvolProcess() and exits.

# $\mathtt{extract}(\mathit{rep})$

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). If an independent copy of the population is needed, you can use population.clone() to create a cloned copy or simulator.extract() to remove the population from the simulator.

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

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

# 1.2 Virtual splitters

# 1.2.1 Class BaseVspSplitter

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.

Each VSP has a name. A default name is determined by each splitter but you can also assign a name to each VSP. The name of a VSP can be retrieved by function BaseVspSplitter.name() or Population.subPopName().

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 can be used.

```
class BaseVspSplitter(names=[])
```

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.

### vspByName(name)

Return the index of a virtual subpopulation from its name. If multiple virtual subpopulations share the same name, the first vsp is returned.

# 1.2.2 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(names=[])
```

Create a sex splitter that defines male and female VSPs. These VSPs are named Male and Female unless a new set of names are specified by parameter *names*.

```
name(vsp)
```

Return "Male" if vsp=0 and "Female" otherwise, unless a new set of names are specified.

# numVirtualSubPop()

Return 2.

# 1.2.3 Class AffectionSplitter

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

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### class AffectionSplitter(names=[])

Create a splitter that defined two VSPs by affection status. These VSPs are named Unaffected and Affected unless a new set of names are specified by parameter *names*.

#### name(vsp)

Return "Unaffected" if vsp=0 and "Affected" if vsp=1, unless a new set of names are specified.

### numVirtualSubPop()

Return 2.

# 1.2.4 Class InfoSplitter

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

```
class InfoSplitter(field, values=[], cutoff=[], ranges=[], names=[])
```

Create an infomration 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 <= v < 2 and v >= 2 where v is the value of an individual at information field *field*. If parameter ranges is specified, each range defines a VSP. For example, ranges=[[1, 3], [2, 5]] defines two VSPs with 1 <= v < 3 and 2 <= 3 < 5. Of course, only one of the parameters *values*, *cutoff* and *ranges* should be defined, and values in *cutoff* should be distinct, and in an increasing order. A default set of names are given to each VSP unless a new set of names is given by parameter *names*.

#### 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. A user-specified name, if specified, will be returned instead.

### 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.

# 1.2.5 Class ProportionSplitter

This splitter divides subpopulations into several VSPs by proportion.

```
class ProportionSplitter(proportions=[], names=[])
```

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. A default set of names are given to each VSP unless a new set of names is given by parameter *names*.

### name(vsp)

Return the name of VSP *vsp*, which is "Prop p" where p=propotions[vsp]. A user specified name will be returned if specified.

### numVirtualSubPop()

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

# 1.2.6 Class RangeSplitter

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

```
class RangeSplitter(ranges, names=[])
```

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. A default set of names are given to each VSP unless a new set of names is given by parameter *names*.

name(*vsp*)

Return the name of VSP vsp, which is "Range [a, b)" where [a, b) is range ranges[vsp]. A user specified name will be returned if specified.

numVirtualSubPop()

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

# 1.2.7 Class GenotypeSplitter

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

class GenotypeSplitter(loci, alleles, phase=False, names=[])

Create a splitter that defines VSPs by individual genotype at *loci* (can be indexes or names of one or more loci). 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 if 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 has 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.

A default set of names are given to each VSP unless a new set of names is given by parameter names.

name(vsp)

Return name of VSP *vsp*, which is "Genotype loc1, loc2: genotype" as defined by parameters *loci* and *alleles*. A user provided name will be returned if specified.

numVirtualSubPop()

Number of virtual subpops of subpopulation sp

# 1.2.8 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. In addition, a new set of VSPs could be defined as the union of one or more of the original VSPs. This splitter is usually used to define different types of VSPs to a population.

```
class CombinedSplitter(splitters=[], vspMap=[], names=[])
```

Create a combined splitter using a list of *splitters*. For example, CombinedSplitter([SexSplitter(), AffectionSplitter()]) defines a combined splitter with four VSPs, defined by male (vsp 0), female (vsp 1), unaffected (vsp 2) and affected individuals (vsp 3). Optionally, a new set of VSPs could be defined by parameter *vspMap*. Each item in this parameter is a list of VSPs that will be combined to a single VSP. For example, vspMap=[(0, 2), (1, 3)] in the previous example will define two VSPs defined by male or unaffected, and female or affected individuals. VSP names are usually determined by splitters, but can also be specified using parameter *names*.

name(vsp)

Return the name of a VSP *vsp*, which is the name a VSP defined by one of the combined splitters unless a new set of names is specified. If a *vspMap* was used, names from different VSPs will be joined by "or".

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#### numVirtualSubPop()

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

# 1.2.9 Class ProductSplitter

This splitter takes several splitters and take their intersections as new VSPs. For example, if the first splitter defines 3 VSPs and the second splitter defines 2, 6 VSPs will be defined by splitting 3 VSPs defined by the first splitter each to two VSPs. This splitter is usually used to define finer VSPs from existing VSPs.

### class ProductSplitter(splitters=[], names=[])

Create a product splitter using a list of *splitters*. For example, ProductSplitter([SexSplitter(), AffectionSplitter()]) defines four VSPs by male unaffected, male affected, female unaffected, and female affected individuals. VSP names are usually determined by splitters, but can also be specified using parameter *names*.

### name(vsp)

Return the name of a VSP *vsp*, which is the names of indivdual VSPs separated by a comma, unless a new set of names is specified for each VSP.

### numVirtualSubPop()

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

# 1.3 Mating Schemes

# 1.3.1 Class MatingScheme

This mating scheme is the base class of all mating schemes. It evolves a population generation by generation but does not actually transmit genotype.

### class MatingScheme(subPopSize=[])

Create a base mating scheme that evolves a population without transmitting genotypes. At each generation, this mating scheme creates an offspring generation according to parameter *subPopSize*, which can be a list of subpopulation sizes (or a number if there is only one subpopulation) or a Python function which will be called at each generation, just before mating, to determine the subpopulation sizes of the offspring generation. The function should be defined with one or both parameters of gen and pop where gen is the current generation number and pop is the parental population just before mating. The return value of this function should be a list of subpopulation sizes for the offspring generation. A single number can be returned if there is only one subpopulation. The passed parental population is usually used to determine offspring population size from parental population size but you can also modify this population to prepare for mating. A common practice is to split and merge parental populations in this function so that you demographic related information and actions could be implemented in the same function.

# 1.3.2 Class HomoMating

A homogeneous mating scheme that uses a parent chooser to choose parents from a prental 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=[], subPops=ALL\_AVAIL, 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 which will be called at each generation to determine the subpopulation sizes of the offspring generation. Please refer to class MatingScheme for details about this parameter.

If this mating shome is used within a heterogeneous mating scheme. Parameters *subPops* and *weight* are used to determine which (virtual) subpopulations 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.

# 1.3.3 Class HeteroMating

A heterogeneous mating scheme that applies a list of homogeneous mating schemes to different (virtual) subpopula-

 ${\bf class} \ {\bf HeteroMating} (matingSchemes, \ subPopSize=[], \ shuffleOffspring=True)$ 

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 class MatingScheme for a detailed explanation of this parameter.

Each mating scheme defined in *matingSchemes* can be applied to one or more (virtual) subpopulation. If parameter *subPops* is not specified, a mating scheme will be applied to all subpopulations. If a list of (virtual) subpopulation is specified, the mating scheme will be applied to specific (virtual) 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 *shuffleOff-spring* to False.

# 1.3.4 Class Conditional Mating

A conditional mating scheme that applies different mating schemes according to a condition (similar to operator IfElse). The condition can be a fixed condition, an expression or a user-defined function, to determine which mating scheme to be used.

class ConditionalMating(cond, ifMatingScheme, elseMatingScheme)

Create a conditional mating scheme that applies mating scheme *ifMatingScheme* if the condition *cond* is True, or *elseMatingScheme* if *cond* is False. If a Python expression (a string) is given to parameter *cond*, the expression will be evalulated in parental population's local namespace. When a Python function is specified, it accepts parameter pop for the parental population. The return value of this function should be True or False. Otherwise, parameter *cond* will be treated as a fixed condition (converted to True or False) upon which *ifMatingScheme* or *elseMatingScheme* will alway be applied.

# 1.3.5 Class PedigreeMating

This mating scheme evolves a population following an existing pedigree structure. If the Pedigree object has N ancestral generations and a present generation, it can be used to evolve a population for N generations, starting from the topmost ancestral generation. At the k-th generation, this mating scheme produces an offspring generation according to subpopulation structure of the N-k-1 ancestral generation in the pedigree object (e.g. producing the offspring population of generation 0 according to the N-1 ancestral generation of the pedigree object). For each offspring, this

mating scheme copies individual ID and sex from the corresponing individual in the pedigree object. It then locates the parents of each offspring using their IDs in the pedigree object. A list of during mating operators are then used to transmit parental genotype to the offspring. The population being evolved must have an information field 'ind\_id'.

# class PedigreeMating(ped, ops, idField="ind id")

Creates a pedigree mating scheme that evolves a population according to Pedigree object *ped*. The evolved population should contain individuals with ID (at information field *idField*, default to 'ind\_id') that match those individual in the topmost ancestral generation who have offspring. After parents of each individuals are determined from their IDs, a list of during-mating operators *ops* are applied to transmit genotypes. The return value of these operators are not checked.

parallelizable()

FIXME: No document

# 1.3.6 Class SequentialParentChooser

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

# class SequentialParentChooser(sexChoice=ANY\_SEX)

Create a parent chooser that chooses a parent from a parental (virtual) subpopulation sequentially. Parameter *choice* can be ANY\_SEX (default), MALE\_ONLY and FEMALE\_ONLY. In the latter two cases, only male or female individuals are selected. A RuntimeError will be raised if there is no male or female individual from the population.

#### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

### initialize(pop, subPop)

Initialize a parent chooser for subpopulation subPop of population pop.

# 1.3.7 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.

# 1.3.8 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 individual fitness values are assigned to individuals ( stored in an information field *selectionField* (default to "fitness"), individuals will be chosen at a probability proportional to his or her fitness value. If parents are chosen without replacement, a parent can be chosen only once. An RuntimeError will be raised if all parents are exhausted. Natural selection is disabled in the without-replacement case.

# ${\bf class} \ {\bf RandomParentChooser} (replacement = True, \ selectionField = "fitness", \ sexChoice = ANY\_SEX)$

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*. This parent chooser by default chooses parent from all individuals (ANY\_SEX), but it can be made to select only male (MALE\_ONLY) or female (FEMALE\_ONLY) individuals by setting parameter *sexChoice*.

#### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

# initialize(pop, subPop)

Initialize a parent chooser for subpopulation *subPop* of *population* pop.

### 1.3.9 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 individual fitness values are assigned (stored in information field selectionField, default to "fitness", the probability that an individual is chosen is proportional to his/her fitness value among all individuals with the same sex. 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. Natural selection is disabled in the without-replacement case.

# ${\bf class} \ {\bf RandomParentsChooser} (replacement = True, \ selectionField = "fitness")$

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*.

#### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

### initialize(pop, subPop)

Initialize a parent chooser for subpopulation *subPop* of *population* pop.

# 1.3.10 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.

```
{\bf 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 FE-MALE) has *polyNum* spouses. The parents are chosen with replacement. If individual fitness values are assigned (stored to information field selectionField, default to "fitness"), the probability that an individual is chosen is proportional to his/her fitness value among all individuals with the same sex.

### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

### initialize(pop, subPop)

Initialize a parent chooser for subpopulation *subPop* of *population* pop.

# 1.3.11 Class CombinedParentsChooser

This parent chooser accepts two parent choosers. It takes one parent from each parent chooser and return them as father and mother. Because two parent choosers do not have to choose parents from the same virtual subpopulation, this parent chooser allows you to choose parents from different subpopulations.

# ${\bf class} \ {\bf CombinedParentsChooser} (fatherChooser, \ motherChooser)$

Create a Python parent chooser using two parent choosers *fatherChooser* and *motherChooser*. It takes one parent from each parent chooser and return them as father and mother. If two valid parents are returned, the first valid parent (father) will be used for *fatherChooser*, the second valid parent (mother) will be used for *motherChooser*. Although these two parent choosers are supposed to return a father and a mother respectively, the sex of returned parents are not checked so it is possible to return parents with the same sex using this parents chooser.

#### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

### initialize(pop, subPop)

Initialize a parent chooser for subpopulation *subPop* of *population* pop.

# 1.3.12 Class PyParentsChooser

This parent chooser accepts 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. 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(generator)

Create a Python parent chooser using a Python generator function *parentsGenerator*. This function should accept one or both of parameters *pop* (the parental population) and *subPop* (index of subpopulation) 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.

### chooseParents()

Return chosen parents from a population if the parent chooser object is created with a population.

### initialize(pop, subPop)

Initialize a parent chooser for subpopulation *subPop* of *population* pop.

# 1.3.13 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=RANDOM_SEX)
```

Create a basic offspring generator. This offspring generator uses *ops* genotype transmitters to transmit genotypes from parents to offspring.

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. 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. Note that applicability parameters begin, step, end, at and reps could be used in these operators but negative population and generation indexes are unsupported.

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 Python function or generator, 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. When a generator function is specified, it will be called for each subpopulation to provide number of offspring for all mating events during the populating of this subpopulation. Current generation number will be passed to this function or generator function if parameter "gen" is used in this function. In the last case, a tuple (or a list) in one of the following forms can be given:

- ●(GEOMETRIC\_DISTRIBUTION, p)
- (POISSON\_DISTRIBUTION, p), p > 0
- (BINOMIAL\_DISTRIBUTION, p, N), 0 , <math>N > 0

• (UNIFORM\_DISTRIBUTION, a, b),  $0 \le a \le b$ .

In this case, the number of offspring will be determined randomly following the specified statistical distributions. Because families with zero offspring are silently ignored, the distribution of the observed number of offspring per mating event (excluding zero) follows zero-truncated versions of these distributions.

Parameter *numOffspring* specifies the number of offspring per mating event but the actual surviving offspring can be less than specified. More spefically, if any during-mating operator returns False, an offspring will be discarded so the actually number of offspring of a mating event will be reduced. This is essentially how during-mating selector works.

Parameter *sexMode* is used to control the sex of each offspring. Its default value is usually *RANDOM\_SEX* which assign MALE or FEMALE to each individual randomly, with equal probabilities. If NO\_SEX is given, offspring sex will not be changed. *sexMode* can also be one of

- (PROB\_OF\_MALES, p) where p is the probability of male for each offspring,
- (NUM\_OF\_MALES, n) where n is the number of males in a mating event. If n is greater than or equal to the number of offspring in this family, all offspring in this family will be MALE.
- (NUM\_OF\_FEMALES, n) where n is the number of females in a mating event,
- •(SEQUENCE\_OF\_SEX, s1, s2 ...) where s1, s2 etc are MALE or FEMALE. The sequence will be used for each mating event. It will be reused if the number of offspring in a mating event is greater than the length of sequence.
- •(GLOBAL\_SEQUENCE\_OF\_SEX, s1, s2, ...) where s1, s2 etc are MALE or FEMALE. The sequence will be used across mating events. It will be reused if the number of offspring in a subpopulation is greater than the length of sequence.

Finally, parameter *sexMode* accepts a function or a generator function. A function will be called whenever an offspring is produced. A generator will be created at each subpopulation and will be used to produce sex for all offspring in this subpopulation. No parameter is accepted.

# 1.3.14 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) PLoS Genetics".

class ControlledOffspringGenerator(loci, alleles, freqFunc, ops=[], numOffspring=1,  $sexMode=RANDOM\_SEX$ )

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*. Parameter *loci* can be a list of loci indexes, names, or ALL\_AVAIL. 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 frequecies 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*.

# 1.4 Pre-defined mating schemes

# 1.4.1 Class CloneMating

A homogeneous mating scheme that uses a sequential parent chooser and a clone offspring generator.

 $\textbf{class CloneMating} (numOffspring=1, sexMode=None, ops=CloneGenoTransmitter(), subPopSize=[], sub-Pops=ALL\_AVAIL, weight=0, selectionField=None)$ 

Create a clonal mating scheme that clones parents to offspring using a CloneGenoTransmitter. Please refer to class OffspringGenerator for parameters *ops* and *numOffspring*, and to class HomoMating for parameters *subPop-Size*, *subPops* and *weight*. Parameters *sexMode* and *selectionField* are ignored because this mating scheme does not support natural selection, and CloneGenoTransmitter copies sex from parents to offspring. Note that CloneGenoTransmitter by default also copies all parental information fields to offspring.

### 1.4.2 Class RandomSelection

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.

class RandomSelection (numOffspring=1, sexMode=None, ops=CloneGenoTransmitter(), subPopSize=[], sub-Pops=ALL AVAIL, weight=0, selectionField='fitness')

Create a mating scheme that select a parent randomly and copy him or her to the offspring population. Please refer to class RandomParentChooser for parameter *selectionField*, to class OffspringGenerator for parameters *ops* and *numOffspring*, and to class HomoMating for parameters *subPopSize*, *subPops* and *weight*. Parameter *sexMode* is ignored because cloneOffspringGenerator copies sex from parents to offspring.

# 1.4.3 Class RandomMating

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.

 $\textbf{class RandomMating} (numOffspring=1, sexMode=RANDOM\_SEX, ops=MendelianGenoTransmitter(), subPopSize=[], subPops=ALL AVAIL, weight=0, selectionField='fitness')$ 

Creates a random mating ssheme that selects two parents randomly and transmit genotypes according to Mendelian laws. Please refer to class RandomParentsChooser for parameter selectionField, to class OffspringGenerator for parameters ops, sexMode and numOffspring, and to class HomoMating for parameters sub-PopSize, subPops and weight.

### 1.4.4 Class Monogamous Mating

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.

 $\textbf{class MonogamousMating} (numOffspring=1, sexMode=RANDOM\_SEX, ops=MendelianGenoTransmitter(), subPop-Size=[], subPops=ALL\_AVAIL, weight=0, selectionField=None)$ 

Creates a monogamous mating scheme that selects each parent only once. Please refer to class OffspringGenerator for parameters *ops*, *sexMode* and *numOffspring*, and to class HomoMating for parameters *sub-PopSize*, *subPops* and *weight*. Parameter *selectionField* is ignored because this mating scheme does not support natural selection.

# 1.4.5 Class Polygamous Mating

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.

 $\begin{array}{ll} \textbf{class PolygamousMating}(polySex=MALE, & polyNum=1, & numOffspring=1, & sexMode=RANDOM\_SEX, \\ ops=MendelianGenoTransmitter(), & subPopSize=[], & subPops=ALL\_AVAIL, & weight=0, & selectionField='fitness') \end{array}$ 

Creates a polygamous mating scheme that each parent mates with multiple 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*, *subPops* and *weight*.

# 1.4.6 Class HaplodiploidMating

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.

 $\textbf{class HaplodiploidMating} (numOffspring=1.0, sexMode=RANDOM\_SEX, ops=HaplodiploidGenoTransmitter(), sub-PopSize=[], subPops=ALL\_AVAIL, weight=0, selectionField='fitness')$ 

Creates a mating scheme in haplodiploid populations. Please refer to class RandomParentsChooser for parameter selectionField, to class OffspringGenerator for parameters ops, sexMode and numOffspring, and to class HomoMating for parameters subPopSize, subPops and weight.

# 1.4.7 Class SelfMating

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.

 $\textbf{class SelfMating} (replacement = True, numOffspring = 1, sexMode = RANDOM\_SEX, ops = SelfingGenoTransmitter(), subPopSize = [], subPops = ALL\_AVAIL, weight = 0, selectionField = 'fitness')$ 

Creates a selfing mating scheme where two homologous copies of parental chromosomes are transmitted to offspring according to Mendelian laws. 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*, *subPops* and *weight*.

# 1.4.8 Class ControlledRandomMating

A homogeneous mating scheme that uses a random sexual parents chooser with replacement and a controlled offspring generator using Mendelian genotype transmitter. It falls back to a regular random mating scheme if there is no locus to control or no trajectory is defined.

 $\textbf{class ControlledRandomMating}(loci=[], \ alleles=[], \ freqFunc=None, \ numOffspring=1, \ sexMode=RANDOM\_SEX, \\ ops=MendelianGenoTransmitter(), \ subPopSize=[], \ subPops=ALL\_AVAIL, \ weight=0, \\ selectionField='fitness')$ 

Creates a random mating scheme that controls allele frequency at loci *loci*. At each generation, function *freqFunc* will be called to 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. If *loci* is empty or *freqFunc* is None, this mating scheme works identically to a RandomMating scheme. 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*, *subPops* and *weight*.

# 1.5 Utility Classes

# 1.5.1 Class WithArgs

This class wraps around a user-provided function and provides an attribute args so that simuPOP knows which parameters to send to the function. This is only needed if the function can not be defined with allowed parameters.

# class WithArgs(func, args)

Return a callable object that wraps around function func. Parameter args should be a list of parameter names.

# 1.5.2 Class WithMode

This class wraps around a user-provided output string, function or file handle (acceptable by parameter output of operators) so that simuPOP knows which mode the output should be written to. For example, if the output of the operator is a binary compressed stream, WithMode(output, 'b') could be used to tell the operators to output bytes instead of string. This is most needed for Python 3 because files in Python 2 accepts string even if they are opened in binary mode.

### class WithMode(output, mode=")

Return an object that wraps around output and tells simuPOP to output string in mode. This class currently only support mode='' for text mode and mode='b' for binary output.

# 1.5.3 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, generator mt19937 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. Names of supported random number generators are available from moduleInfo()['availableRNGs'].

### 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.

### randChisq(nu)

Generate a random number following a Chi-squared distribution with *nu* degrees of freedom.

### randExponential(mu)

Generate a random number following a exponential distribution with parameter mu.

### randGamma(a, b)

Generate a random number following a gamma distribution with a shape parameters *a* and scale parameter *b*.

### randGeometric(p)

Generate a random number following a geometric distribution with parameter p.

### randInt(n)

Return a random number in the range of [0, 1, 2, ... n-1]

#### randMultinomial(N, p)

Generate a random number following a multinomial distribution with parameters N and p (a list of probabilities).

#### randNormal(mu, sigma)

Generate a random number following a normal distribution with mean mu and standard deviation sigma.

#### randPoisson(*mu*)

Generate a random number following a Poisson distribution with parameter mu.

#### randTruncatedBinomial(n, p)

Generate a positive random number following a zero-truncated binomial distribution with parameters n and p.

#### randTruncatedPoisson(mu)

Generate a positive random number following a zero-truncated Poisson distribution with parameter mu.

#### randUniform()

Generate a random number following a rng uniform [0, 1) distribution.

#### seed()

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

```
set(name=None, seed=0)
```

Replace the existing random number generator using RNG*name* with seed *seed*. If *seed* is 0, a random seed will be used. If *name* is empty, use the existing RNG but reset the seed.

# 1.5.4 Class WeightedSampler

A random number generator that returns 0, 1, ..., k-1 with probabilites that are proportional to their weights. For example, a weighted sampler with weights 4, 3, 2 and 1 will return numbers 0, 1, 2 and 3 with probabilities 0.4, 0.3, 0.2 and 0.1, respectively. If an additional parameter N is specified, the weighted sampler will return exact proportions of numbers if N numbers are returned. The version without additional parameter is similar to the sample(prob, replace=FALSE) function of the R statistical package.

#### **class** WeightedSampler(weights=[], N=0)

Creates a weighted sampler that returns 0, 1, ... k-1 when a list of k weights are specified (weights). weights do not have to add up to 1. If a non-zero N is specified, exact proportions of numbers will be returned in N returned numbers.

#### draw()

Returns a random number between 0 and k-1 with probabilities that are proportional to specified weights.

#### drawSamples(n=1)

Returns a list of *n* random numbers

# 1.6 Global functions

#### 1.6.1 Function closeOutput

# 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.

1.6. Global functions

#### 1.6.2 Function describeEvolProcess

 $\label{lem:describeEvolProcess} \begin{subarray}{l} describeEvolProcess (initOps=[], preOps=[], matingScheme=MatingScheme, postOps=[], finalOps=[], gen=-1, num-Rep=1) \end{subarray}$ 

This function takes the same parameters as Simulator.evolve and output a description of how an evolutionary process will be executed. It is recommended that you call this function if you have any doubt how your simulation will proceed.

# 1.6.3 Function loadPopulation

loadPopulation(file)

Load a population from a file saved by Population::save().

### 1.6.4 Function loadPedigree

loadPedigree(file, idField="ind\_id", fatherField="father\_id", motherField="mother\_id", ploidy=2, loci=[], chrom-Types=[], lociPos=[], chromNames=[], alleleNames=[], lociNames=[], subPopNames=[], infoFields=[])

Load a pedigree from a file saved by operator PedigreeTagger or function Pedigree.save. This file contains the ID of each offspring and their parent(s) and optionally sex ('M' or 'F'), affection status ('A' or 'U'), values of information fields and genotype at some loci. IDs of each individual and their parents are loaded to information fields *idField*, *fatherField* and *motherField*. Only numeric IDs are allowed, and individual IDs must be unique across all generations.

Because this file does not contain generation information, generations to which offspring belong are determined by the parent-offspring relationships. Individuals without parents are assumed to be in the top-most ancestral generation. This is the case for individuals in the top-most ancestral generation if the file is saved by function "Pedigree.save()", and for individuals who only appear as another individual's parent, if the file is saved by operator "PedigreeTagger". The order at which offspring is specified is not important because this function essentially creates a top-most ancestral generation using IDs without parents, and creates the next generation using offspring of these parents, and so on until all generations are recreated. That is to say, if you have a mixture of pedigrees with different generations, they will be lined up from the top most ancestral generation.

If individual sex is not specified, sex of of parents are determined by their parental roles (father or mother) but the sex of individuals in the last generation can not be determined so they will all be males. If additional information fields are given, their names have to be specified using parameter *infoFields*. The rest of the columns are assued to be alleles, arranged *ploidy* consecutive columns for each locus. If paraemter *loci* is not specified, the number of loci is calculated by number of columns divided by *ploidy* (default to 2). All loci are assumed to be on one chromosome unless parameter *loci* is used to specified number of loci on each chromosome. Additional parameters such as *ploidy*, *chromTypes*, *lociPos*, *chromNames*, *alleleNames*, *lociNames* could be used to specified the genotype structured of the loaded pedigree. Please refer to class Population for details about these parameters.

# 1.6.5 Function moduleInfo

#### 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.
- •wordsize: size of word, can be either 32 or 64.
- •alleleBits: the number of bits used to store an allele
- •maxNumSubPop: maximum number of subpopulations.
- •maxIndex: maximum index size (limits population size \* total number of marker).
- debug: A dictionary with debugging codes as keys and the status of each debugging code (True or False)
  as their values.

# 1.6.6 Function getRNG

#### getRNG()

Return the currently used random number generator

#### 1.6.7 Function setRNG

```
setRNG(name=", seed=0)
```

Set random number generator. This function is obsolete but is provided for compatibility purposes. Please use setOptions instead

# 1.6.8 Function setOptions

```
setOptions(numThreads=-1, name=None, seed=0)
```

First argument is to set number of thread in openMP. The number of threads can be be positive, integer (number of threads) or 0, which implies all available cores, or a number set by environmental variable OMP\_NUM\_THREADS. Second and third argument is to set the type or seed of existing random number generator using RNG*name* with *seed*. If using openMP, it sets the type or seed of random number generator of each thread.

# 1.6.9 Function turnOnDebug

```
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 moduleInfo()['debug'].keys().

# 1.6.10 Function turnOffDebug

```
{\tt turn0ffDebug}(code {\tt = "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.

1.6. Global functions

# Chapter 2

# **Operator References**

# 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 begging 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 a 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. Lastly, if the output stream only accept a binary output (e.g. a gzip stream), withMode(output, 'b') should be used to let simuPOP convert string to bytes before writing to the output.

class BaseOperator(output, begin, end, step, at, reps, 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 an Python expression prefixed by an exclamation mark

('!expr'). If a file object, or any Python object with a write function is provided, the output will be write to this file. Alternatively, a Python function or a file object (any Python object with a write function) can be given which will be called with a string of output content. A global function WithMode can be used to let simuPOP output bytes instead of string.

*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 ALL\_AVAIL 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 simplied as subPops=sp1. Negative indexes are not supported. A common default value (ALL\_AVAIL) of this parameter reprents all subpopulations of the population being aplied. Suport 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

This operator initializes sex of individuals, either randomly or use a list of sexes.

class InitSex(maleFreq=0.5, maleProp=-1, sex=[], begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Create an operator that initializes individual sex to MALE or FEMALE. By default, it assigns sex to individuals randomly, with equal probability of having a male or a female. This probabability can be adjusted through parameter maleFreq or be made to exact proportions by specifying parameter maleProp. 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 or maleProp are 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 (virtual) subpopulation boundaries so that you can assign sex to all individuals in a population.

### 2.2.2 Class InitInfo

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

**class InitInfo**(*values*, *begin=0*, *end=-1*, *step=1*, *at=[]*, *reps=ALL\_AVAIL*, *subPops=ALL\_AVAIL*, *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.

# 2.2.3 Class InitGenotype

This operator assigns alleles at all or part of loci with given allele frequencies, proportions or values. This operator initializes all chromosomes, including unused genotype locations and customized chromosomes.

 $\textbf{class InitGenotype}(freq=[], \ genotype=[], \ prop=[], \ haplotypes=[], \ loci=ALL\_AVAIL, \ ploidy=ALL\_AVAIL, \ begin=0, \\ end=1, \ step=1, \ at=[], \ reps=ALL\_AVAIL, \ subPops=ALL\_AVAIL, \ infoFields=[])$ 

This function creates an initializer that initializes individual genotypes with random alleles or haplotypes with specified frequencies (parameter *freq*) or proportions (parameter *prop*). If parameter *haplotypes* is not specified, *freq* specifies the allele frequencies of alleles 0, 1, ... respectively. Alternatively, you can use parameter *prop* to specified the exact proportions of alleles 0, 1, ..., although alleles with small proportions might not be assigned at all. Values of parameter *prob* or *prop* should add up to 1. If parameter *haplotypes* is specified, it should contain a list of haplotypes and parameter *prob* or *prop* specifies frequencies or proportions of each haplotype. If *loci*, *ploidy* and/or *subPop* are specified, only specified loci, ploidy, and individuals in these (virtual) subpopulations will be initialized. Parameter *loci* can be a list of loci indexes, names or ALL\_AVAIL. If the length of a haplotype is not enough to fill all loci, the haplotype will be reused. If a list (or a single) haplotypes are specified without *freq* or *prop*, they are used with equal probability.

In the last case, if a sequence of genotype is specified, it will be used repeatedly to initialize all alleles sequentially. This works similar to function Population.setGenotype() except that you can limit the initialization to certain *loci* and *ploidy*.

# 2.2.4 Class InitLineage

This operator assigns lineages at all or part of loci with given values. This operator initializes all chromosomes, including unused lineage locations and customized chromosomes.

 $\textbf{class InitLineage} (lineage=[], mode=PER\_ALLELE, loci=ALL\_AVAIL, ploidy=ALL\_AVAIL, begin=0, end=1, step=1, \\ at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields="ind_id")$ 

This function creates an initializer that initializes lineages with either a specified set of values or from the field *infoFields* (default to ind\_id), whose value will be saved as the lineage of modified alleles. If a list of values is specified in parameter *lineage*, each value in this list is applied to one or more alleles so that each allele (PER\_ALLELE, default mode), alleles on each chromosome (PER\_CHROMOSOME), on chromosomes of each ploidy (PER\_PLOIDY), or for each individual (PER\_INDIVIDUAL) have the same lineage. A single value is allowed and values in *lineage* will be re-used if not enough values are provided. If an empty list is provided, values 1, 2, 3, ... will be used to provide an unique identify for each allele, genotype, chromosome, etc. If a valid field is specified (default to ind\_id), the value of this field will be used for all alleles of each individual if *mode* is set to FROM\_INFO, or be adjusted to produce positive values for alleles on the frist ploidy, and negative values for the second ploidy (and so on) if *mode* equals to FROM\_INFO\_SIGNED. If *loci*, *ploidy* and/or *subPops* are specified, only specified loci, ploidy, and individuals in these (virtual) subpopulations will be initialized.

# 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=">", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, 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*.

# 2.3.2 Class 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=">", begin=0, end=-1, step=1, at=[], reps=ALL_AVAIL, sub-Pops=Py_False, infoFields=[])
```

Create a PyEval operator that evaluates a Python expression *expr* in a population's local namespaces when it is applied to this population. This namespace can either be the population's local namespace (pop.vars()), or namespaces subPop[sp] for (virtual) subpop (pop.vars(subpop)) in specified *subPops*. If Python statements *stmts* is given (a single or multi-line string), the statement will be executed before *expr*. If *exposePop* is set to an 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.

# 2.3.3 Class 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=">", begin=0, end=-1, step=1, at=[], reps=ALL_AVAIL, sub-Pops=Py_False, infoFields=[])
```

Create a PyExec operator that executes statements *stmts* in a population's local namespace when it is applied to this population. This namespace can either be the population's local namespace (pop.vars()), or namespaces subPop[sp] for each (virtual) subpop (pop.vars(subpop)) in specified *subPops*. 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 once. Note that exposed population variables will be removed after the statements are executed.

#### 2.3.4 Class InfoEval

Unlike operator PyEval and PyExac 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 the local namespace of the population. A Python expression is then evaluated for each individual. The result is written to an output.

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

Create an operator that evaluate a Python expression *expr* using individual information fields and population variables as variables. If *exposeInd* is not empty, the individual itself will be exposed in the population's local namespace as a variable with name specified by *exposeInd*.

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. The evaluation of this statement may change the value of information fields.

Parameter usePopVars is obsolete because population variables are always usable in such expressions.

#### 2.3.5 Class InfoExec

Operator InfoExec is similar to InfoEval in that it works at the individual level, using individual information fields as variables. This is usually used to change the value of information fields. For example, "b=a\*2" will set the value of information field b to a\*a for all individuals.

class InfoExec(stmts="", usePopVars=False, exposeInd="", output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])

Create an operator that executes Python statements *stmts* using individual information fields and population variables as variables. If *exposeInd* is not empty, the individual itself will be exposed in the population's local namespace as a variable with name specified by *exposeInd*.

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 a or a population variable a if a is not an information field but a population variable, and a=ind.sex() will set information field a of all individuals to its sex (needs exposeInd='ind'.

Parameter usePopVars is obsolete because population variables will always be usable.

# 2.4 Demographic models

# 2.4.1 Class Migrator

This operator migrates individuals from (virtual) subpopulations to other subpopulations, according to either prespecified 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 intepreted as probabilities to migrate to each destination subpopulation. Each individual's defination 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 indidividuals are chosen to migrate.

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

This operator goes through all source (virtual) subpopulations and assign detination subpopulation of each individual to an information field. Unexpected results may happen if individuals migrate from overlapping virtual subpopulations.

class Migrator(rate=[], mode=BY\_PROBABILITY, toSubPops=ALL\_AVAIL, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, 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* = BY\_PROBABILITY), proportions of individuals in the source (virtual) subpopulations to the destination subpopulations (*mode* = BY\_PROPORTION), numbers of migrants in the source (virtual) subpopulations (*mode* = BY\_COUNTS), or ignored completely (*mode* = BY\_IND\_INFO). 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.

# 2.4.2 Class 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 ( $subPops=ALL\_AVAIL$ , sizes=[], proportions=[], names=[], randomize=True, begin=0, end=-1, step=1, at=[],  $reps=ALL\_AVAIL$ , 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.

# 2.4.3 Class 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 ( $subPops=ALL\_AVAIL$ ,  $name="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, infoFields=[])$ 

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.

### 2.4.4 Class ResizeSubPops

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

 $\textbf{class ResizeSubPops}(subPops=ALL\_AVAIL, \ sizes=[], \ proportions=[], \ propagate=True, \ begin=0, \ end=-1, \ step=1, \\ at=[], \ reps=ALL\_AVAIL, \ infoFields=[])$ 

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.

# 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.

 $\textbf{class GenoTransmitter}(output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])$ 

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), except that it also clears allele lineage if it is executed in a module with lineage allele type.

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), polidy, chrom), except that it also copies allelic lineage when it is executed in a module with lineage allele type.

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), except that it also copies allelic lineage when it is executed in a module with lineage allele type.

# 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. In addition to genotypes on all non-customized or specified chromosomes, sex and information fields are by default also coped copied from parent to offspring.

 $\textbf{class CloneGenoTransmitter}(output="", chroms=ALL\_AVAIL, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=ALL\_AVAIL) \\$ 

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. After genotype transmission, offspring sex and affection status is copied from the parent even if sex has been determined by an offspring generator. All or specified information fields (parameter *infoFields*, default to ALL\_AVAIL) will also be copied from parent to offspring. Parameters *subPops* is ignored. This operator by default copies genotypes on all autosome and sex chromosomes (excluding customized chromosomes), unless a parameter *chroms* is used to specify which chromosomes to copy. This operator also copies allelic lineage when it is executed in a module with lineage allele type.

# 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=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, 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. This operator also copies allelic lineage when it is executed in a module with lineage allele type.

```
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=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])
```

Create a self-fertilization genotype transmitter that transmits genotypes of a parent to an offspring through self-fertilization. Cutsomized chromosomes are not handled. Parameters *subPops* and *infoFields* are ignored. This operator also copies allelic lineage when it is executed in a module with lineage allele type.

#### 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=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, 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. This operator also copies allelic lineage when it is executed in a module with lineage allele type.

#### 2.5.6 Class MitochondrialGenoTransmitter

This geno transmitter transmits the first homologous copy of a Mitochondrial chromosome. If no mitochondrial chromosome is present, it assumes that the first homologous copy of several (or all) Customized chromosomes are copies of mitochondrial chromosomes. This operator transmits the mitochondrial chromosome from the female parent to offspring for sexsual reproduction, and any parent to offspring for asexual reproduction. If there are multiple chromosomes, the organelles are selected randomly. 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( $output="", chroms=ALL\_AVAIL, begin=0, end=-1, step=1, at=[]$  $reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[]$ 

Createa a mitochondrial genotype transmitter that treats the Mitochondiral chromosome, or Customized chromosomes if no Mitochondrial chromosome is specified, 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. It also copies allelic lineage when it is executed in a module with lineage allele type.

#### 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 uses 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 differntly (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.

 $\textbf{class Recombinator}(rates=[], intensity=-1, loci=ALL\_AVAIL, convMode=NO\_CONVERSION, output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])$ 

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*, which can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. Each locus in this list specifies a recombination point between the locus and the locus immediately **after** it. Loci that are the last locus on each chromosome are ignored.

If a single recombination rate (parameter *rates*) is specified, it will 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*, different recombination rates could be applied after a list of specified loci (between loci and their immediate neighbor to the right). The loci should be specified by parameter *loci* as a list with the same length as *rates*, or *ALL\_AVAIL* (default) in which case the length of *rates* should equal to the total number of loci. Note that recombination rates specified for the last locus on each chromosome are ignored because simuPOP assumes free recombination between chromosomes.

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 assume for loci position and recombination intensity.

Gene conversion is controlled using parameter convMode, which can be

- •NoConversion: no gene conversion (default).
- •(NUM\_MARKERS, prob, n): With probability prob, convert a fixed number (n) of markers if a recombination event happens.
- •(GEOMETRIC\_DISTRIBUTION, prob, p): With probability *prob*, convert a random number of markers if a recombination event happens. The number of markes converted follows a geometric distribution with probability *p*.
- (TRACT\_LENGTH, 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.
- (EXPONENTIAL\_DISTRIBUTION, prob, p): With probability *prob*, convert a region of random tract length if a recombination event happens. The distribution of tract length follows a 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 if the Holliday junction is resolved/repaired successfully, or a conversion event if the junction is not resolved/repaired. 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 translate to 0.1/0.90.1 to 15/160.94 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 an 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 happens. 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 an 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.

In addition to genotypes, this operator also copies alleleic lineage if it is executed in a module with lineage allele type.

**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 pesudoautosomal regions on these chromosomes. If such a feature is required, you will have to simulate the pesudoautosomal regions as separate chromosomes.

#### 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 BaseMutator

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 BaseMutator(rates=[], loci=ALL\_AVAIL, mapIn=[], mapOut=[], context=0, output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields="ind\_id", lineage-Mode=FROM\_INFO)

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*). Parameter *loci* can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. Please refer to class BaseOperator for a detailed explanation of these parameters.

Parameter *rate* or its equivalence specifies the probability that a 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.

If a valid information field is specified for parameter *infoFields* (default to ind\_id) for modules with lineage allele type, the lineage of the mutated alleles will be the ID (stored in the first field of *infoFields*) of individuals that harbor the mutated alleles if *lineageMode* is set to FROM\_INFO (default). If *lineageMode* is set to FROM\_INFO\_SIGNED, the IDs will be assigned a sign depending on the ploidy the mutation happens (1 for ploidy 0, -1 for ploidy 1, etc). The lineage information will be transmitted along with the alleles so this feature allows you to track the source of mutants during evolution.A

A mutator by default does not produce any output. However, if an non-empty output is specified, the operator will output generation number, locus, ploidy, original allele, mutant, and values of all information field specified by parameter infoFields (e.g. individual ID if ind\_id is specified).

Some mutation models are context dependent. Namely, how an allele mutates will depend on its adjecent 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.

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# 2.6.2 Class MatrixMutator

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. #

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*. Diagnal 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*. If alleles other than 0, 1, ..., n-1 exist in the population, they will not be mutated although a warning message will be given if debugging code DBG\_WARNING is turned on. Please refer to classes mutator and BaseOperator for detailed explanation of other parameters.

# 2.6.3 Class KAlleleMutator

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

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*. If the mutated allele is larger than or equal to k, it will not be mutated. A warning message will be displayed if debugging code DBG\_WARNING is turned on. Please refer to classes mutator and BaseOperator for descriptions of other parameters.

# 2.6.4 Class StepwiseMutator

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 of 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).

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.
- (GEOMETRIC\_DISTRIBUTION, p): The number of steps follows a 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.

# 2.6.5 Class PyMutator

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

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 as parameter allele, locus index locus, and optional array of alleles as parameter context, which are *context* alleles the left and right of the mutated allele. Invalid context alleles (e.g. left allele to the first locus of a chromosome) will be marked by -1. The return value of this function will be used to mutate the passed allele. The passed, returned and context alleles might be altered if parameter *mapIn* and *mapOut* are used. 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.

#### 2.6.6 Class MixedMutator

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

Create a mutator that randomly chooses one of the specified *mutators* to mutate an allele when a mutation event happens. The mutators are choosen 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.

#### 2.6.7 Class ContextMutator

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.

Create a mutator that choose one of the specified *mutators* to mutate an allele when a mutation event happens. The mutators are choosen 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

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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.

#### 2.6.8 Class PointMutator

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="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=0, infoFields="ind\_id", lineageMode=FROM\_INFO)

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.

# 2.6.9 Class SNPMutator

A mutator model that assumes two alleles 0 and 1 and accepts mutation rate from 0 to 1, and from 1 to 0 alleles.

**class** SNPMutator(*u*=0, *v*=0, loci=True, mapIn=[], mapOut=[], output=", begin=0, end=-1, step=1, at=[], reps=True, subPops=ALL\_AVAIL, infoFields=['ind\_id'], lineageMode=115)

Return a MatrixMutator with proper mutate matrix for a two-allele mutation model using mutation rate from allele 0 to 1 (parameter u) and from 1 to 0 (parameter v)

# 2.6.10 Class AcgtMutator

This mutation 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.

class AcgtMutator(rate=[], model='general', loci=True, mapIn=[], mapOut=[], output=", begin=0, end=-1, step=1, at=[], reps=True, subPops=ALL\_AVAIL, infoFields=['ind\_id'], lineageMode=115)

Create a mutation model that mutates between nucleotides A, C, G, and T (alleles are coded in that order as 0, 1, 2 and 3). Currently supported models are Jukes and Cantor 1969 model (JC69), Kimura's 2-parameter model (K80), Felsenstein 1981 model (F81), Hasgawa, 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.

#### 2.6.11 Class RevertFixedSites

This operator checks all or specified loci of a population and revert all mutants at loci to wildtype alleles if they are fixed in the population. If a list of (virtual) subpopulations are specified, alleles are reverted if they are fixed in each subpopulation, regardless if the alleles are fixed in other subpopulations.

 $\textbf{class RevertFixedSites} (loci=ALL\_AVAIL, \ output="", \ begin=0, \ end=-1, \ step=1, \ at=[], \ reps=ALL\_AVAIL, \ sub-Pops=ALL\_AVAIL, \ infoFields="ind_id")$ 

Create an operator to set all alleles to zero at specified (parameter *loci*) or all loci if they are fixed (having one non-zero allele) at these loci. If parameter *subPops* are specified, only individuals in these subpopulations are considered.

# 2.7 Penetrance

#### 2.7.1 Class BasePenetrance

A penetrance model models the probability that an individual has a certain disease provided that he or she has certain genetic (genotype) and environmental (information field) riske factors. A penetrance operator calculates this probability according to provided information and set his or her affection status randomly. For example, an individual will have probability 0.8 to be affected if the penetrance is 0.8. This class is the base class to all penetrance operators and defines a common interface for all penetrance operators.

A penetrance operator can be applied at any stage of an evolutionary cycle. If it is applied before or after mating, it will set affection status of all parents and offspring, respectively. If it is applied during mating, it will set the affection status of each offspring. You can also apply a penetrance operator to an individual using its applyToIndividual member function.

By default, a penetrance operator assigns affection status of individuals but does not save the actual penetrance value. However, if an information field is specified, penetrance values will be saved to this field for future analysis.

When a penetrance operator is applied to a population, it is only applied to the current generation. You can, however, use parameter *ancGens* to set affection status for all ancestral generations (ALL\_AVAIL), or individuals in specified generations if a list of ancestral generations is specified. Note that this parameter is ignored if the operator is applied during mating.

 $\textbf{class BasePenetrance} (anc Gens = UNSPECIFIED, begin = 0, end = -1, step = 1, at = [], reps = ALL\_AVAIL, sub-Pops = ALL\_AVAIL, infoFields = [])$ 

Create a base penetrance operator. This operator assign individual affection status in the present generation (default). If ALL\_AVAIL or a list of ancestral generations are specified in parameter *ancGens*, individuals in specified ancestral generations will be processed. A penetrance operator can be applied to specified (virtual) subpopulations (parameter *subPops*) and replicates (parameter *reps*). If an information field is given, penetrance value will be stored in this information field of each individual.

apply(pop)

Set penetrance to all individuals and record penetrance if requested

applyToIndividual(ind, pop=None)

Apply the penetrance operator to a single individual *ind* and set his or her affection status. A population reference can be passed if the penetrance model depends on population properties such as generation number. This function returns the affection status.

### 2.7.2 Class MapPenetrance

This penetrance operator assigns individual affection status using a user-specified penetrance dictionary.

 $\textbf{class MapPenetrance}, \ anc Gens = UNSPECIFIED, \ begin = 0, \ end = -1, \ step = 1, \ at = [], \ reps = ALL\_AVAIL, \ subPops = ALL\_AVAIL, \ infoFields = [])$ 

Create a penetrance operator that get penetrance value from a dictionary *penetrance* with genotype at *loci* as keys, and *penetrance* as values. For each individual, genotypes at *loci* are collected one by one (e.g. p0\_loc0, p1\_loc0, p0\_loc1, p1\_loc1... for a diploid individual) and are looked up in the dictionary. Parameter *loci* can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. If a genotype cannot be found, it will be looked up again without phase information (e.g. (1,0) will match key (0,1)). If the genotype still can not be found, a ValueError will be raised. This operator supports sex chromosomes and haplodiploid populations. In these cases, only valid genotypes should be used to generator the dictionary keys.

#### 2.7.3 Class MaPenetrance

This operator is called a 'multi-allele' penetrance operator because it groups multiple alleles into two groups: wildtype

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and non-wildtype alleles. Alleles in each allele group are assumed to have the same effect on individual penetrance. If we denote all wildtype alleles as A, and all non-wildtype alleles a, this operator assign Individual penetrance according to genotype AA, Aa, aa in the diploid case, and A and a in the haploid case.

class MaPenetrance (loci, penetrance, wildtype=0, ancGens=UNSPECIFIED, begin=0, end=-1, step=1, at=[],  $reps=ALL\_AVAIL$ ,  $subPops=ALL\_AVAIL$ , infoFields=[])

Creates a multi-allele penetrance operator that groups multiple alleles into a wildtype group (with alleles *wildtype*, default to [0]), and a non-wildtype group. A list of penetrance values is specified through parameter *penetrance*, for genotypes at one or more *loci*. Parameter *loci* can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. If we denote wildtype alleles using capital letters A, B ... and non-wildtype alleles using small letters a, b ..., the penetrance values should be for

- •genotypes A and a for the haploid single-locus case,
- •genotypes AB, Ab, aB and bb for haploid two=locus cases,
- •genotypes AA, Aa and aa for diploid single-locus cases,
- •genotypes AABB, AABb, AABb, AaBB, AaBb, aaBb, aaBb, and aabb for diploid two-locus cases,
- •and in general 2\*\*n for diploid and 3\*\*n for haploid cases if there are n loci.

This operator does not support haplodiploid populations and sex chromosomes.

#### 2.7.4 Class MlPenetrance

This penetrance operator is created by a list of penetrance operators. When it is applied to an individual, it applies these penetrance operators to the individual, obtain a list of penetrance values, and compute a combined penetrance value from them and assign affection status accordingly. ADDITIVE, multiplicative, and a heterogeneour multi-locus model are supported. Please refer to Neil Rish (1989) "Linkage Strategies for Genetically Complex Traits" for some analysis of these models.

Create a multiple-locus penetrance operator from a list penetrance operator *ops*. When this operator is applied to an individual (parents when used before mating and offspring when used during mating), it applies these operators to the individual and obtain a list of (usually single-locus) penetrance values. These penetrance values are combined to a single penetrance value using

- $Prod(f \ i)$ , namely the product of individual penetrance if mode = MULTIPLICATIVE,
- • $sum(f_i)$  if mode = ADDITIVE, and
- •1- $Prod(1 f_i)$  if mode = HETEROGENEITY

0 or 1 will be returned if the combined penetrance value is less than zero or greater than 1.

Applicability parameters (begin, end, step, at, reps, subPops) could be used in both MlSelector and selectors in parameter *ops*, but parameters in MlSelector will be interpreted first.

# 2.7.5 Class PyPenetrance

This penetrance operator assigns penetrance values by calling a user provided function. It accepts a list of loci (parameter loci), and a Python function func which should be defined with one or more of parameters geno, mut, gen, ind, pop, or names of information fields. When this operator is applied to a population, it passes genotypes or mutants (non-zero alleles) at specified loci at specified loci, generation number, a reference to an individual, a reference to the current population (usually used to retrieve population variables) and values at specified information fields to respective parameters of this function. Genotypes of each individual are passed as a tuple of alleles arranged locus by locus (in the order of A1,A2,B1,B2 for loci A and B). Mutants are passed as a default dictionary of loci index (with respect to all

genotype of individuals, not just the first ploidy) and alleles. The returned penetrance values will be used to determine the affection status of each individual.

class PyPenetrance(func, loci=[], ancGens=UNSPECIFIED, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Create a Python hybrid penetrance operator that passes genotype at specified *loci*, values at specified information fields (if requested), and a generation number to a user-defined function *func*. Parameter *loci* can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. The return value will be treated as Individual penetrance.

# 2.7.6 Class PyMlPenetrance

This penetrance operator is a multi-locus Python penetrance operator that assigns penetrance values by combining locus and genotype specific penetrance values. It differs from a PyPenetrance in that the python function is responsible for penetrance values values for each gentoype type at each locus, which can potentially be random, and locus or gentoype-specific.

class PyMlPenetrance(func, mode=MULTIPLICATIVE, loci=ALL\_AVAIL, ancGens=UNSPECIFIED, output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])

Create a penetrance operator that assigns individual affection status according to penetrance values combined from locus-specific penetrance values that are determined by a Python call-back function. The callback function accepts parameter *loc*, *alleles* (both optional) and returns location- or genotype-specific penetrance values that can be constant or random. The penetrance values for each genotype will be cached so the same penetrance values will be assigned to genotypes with previously assigned values. Note that a function that does not examine the genotype naturally assumes a dominant model where genotypes with one or two mutants have the same penetrance value. Because genotypes at a locus are passed separately and in no particular order, this function is also responsible for assigning consistent fitness values for genotypes at the same locus (a class is usually used). This operator currently ignores chromosome types so unused alleles will be passed for loci on sex or mitochondrial chromosomes. This operator also ignores the phase of genotype so genotypes (a,b) and (b,a) are assumed to have the same fitness effect.

Individual penetrance will be combined in ADDITIVE, MULTIPLICATIVE, or HETEROGENEITY mode from penetrance values of loci with at least one non-zero allele (See MlPenetrance for details).

# 2.8 Quantitative Trait

# 2.8.1 Class BaseQuanTrait

A quantitative trait in simuPOP is simply an information field. A quantitative trait model simply assigns values to one or more information fields (called trait fields) of each individual according to its genetic (genotype) and environmental (information field) factors. It can be applied at any stage of an evolutionary cycle. If a quantitative trait operator is applied before or after mating, it will set the trait fields of all parents and offspring. If it is applied during mating, it will set the trait fields of each offspring.

When a quantitative trait operator is applied to a population, it is only applied to the current generation. You can, however, use parameter ancGen=-1 to set the trait field of all ancestral generations, or a generation index to apply to only ancestral generation younger than ancGen. Note that this parameter is ignored if the operator is applied during mating.

class BaseQuanTrait(ancGens=UNSPECIFIED, begin=0, end=-1, step=1, at=[],  $reps=ALL\_AVAIL$ ,  $sub-Pops=ALL\_AVAIL$ , infoFields=[])

Create a base quantitative trait operator. This operator assigns one or more quantitative traits to trait fields in the present generation (default). If ALL\_AVAIL or a list of ancestral generations are specified, this operator will be applied to individuals in these generations as well. A quantitative trait operator can be applied to specified

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```
(virtual) subpopulations (parameter subPops) and replicates (parameter reps).
apply(pop)
    Set qtrait to all individual
```

### 2.8.2 Class PyQuanTrait

This quantitative trait operator assigns a trait field by calling a user provided function. It accepts a list of loci (parameter *loci*), and a Python function func which should be defined with one or more of parameters geno, mut, gen, ind, or names of information fields. When this operator is applied to a population, it passes genotypes or mutants (non-zero alleles) of each individual at specified loci, generation number, a reference to an individual, and values at specified information fields to respective parameters of this function. Genotypes of each individual are passed as a tuple of alleles arranged locus by locus (in the order of A1,A2,B1,B2 for loci A and B). Mutants are passed as a default dictionary of loci index (with respect to all genotype of individuals, not just the first ploidy) and alleles. The return values will be assigned to specified trait fields.

class PyQuanTrait(func, loci=[], ancGens=UNSPECIFIED, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Create a Python hybrid quantitative trait operator that passes genotype at specified *loci*, optional values at specified information fields (if requested), and an optional generation number to a user-defined function *func*. Parameter *loci* can be a list of loci indexes, names, or ALL\_AVAIL. The return value will be assigned to specified trait fields (*infoField*). If only one trait field is specified, a number or a sequence of one element is acceptable. Otherwise, a sequence of values will be accepted and be assigned to each trait field.

# 2.9 Natural selection

# 2.9.1 Class BaseSelector

This class is the base class to all selectors, namely operators that perform natural selection. It defines a common interface for all selectors.

A selector can be applied before mating or during mating. If a selector is applied to one or more (virtual) subpopulations of a parental population before mating, it sets individual fitness values to all involved parents to an information field (default to *fitness*). When a mating scheme that supports natural selection is applied to the parental population, it will select parents with probabilities that are proportional to individual fitness stored in an information field (default to *fitness*). Individual fitness is considered **relative** fitness and can be any non-negative number. This simple process has some implications that can lead to advanced usages of natural selection in simuPOP:

- It is up to the mating scheme how to handle individual fitness. Some mating schemes do not support natural selection at all.
- A mating scheme performs natural selection according to fitness values stored in an information field. It does
  not care how these values are set. For example, fitness values can be inherited from a parent using a tagging
  operator, or set directly using a Python operator.
- A mating scheme can treat any information field as fitness field. If an specified information field does not exist, or if all individuals have the same fitness values (e.g. 0), the mating scheme selects parents randomly.
- Multiple selectors can be applied to the same parental generation. individual fitness is determined by the last fitness value it is assigned.
- A selection operator can be applied to virtual subpopulations and set fitness values only to part of the individuals.
- individuals with zero fitness in a subpopulation with anyone having a positive fitness value will not be selected to produce offspring. This can sometimes lead to unexpected behaviors. For example, if you only assign fitness

value to part of the individuals in a subpopulation, the rest of them will be effectively discarded. If you migrate individuals with valid fitness values to a subpopulation with all individuals having zero fitness, the migrants will be the only mating parents.

- It is possible to assign multiple fitness values to different information fields so that different homogeneous mating schemes can react to different fitness schemes when they are used in a heterogeneous mating scheme.
- You can apply a selector to the offspring generation using the *postOps* parameter of Simulator.evolve, these fitness values will be used when the offspring generation becomes parental generation in the next generation.

Alternatively, a selector can be used as a during mating operator. In this case, it caculates fitness value for each offspring which will be treated as **absolute** fitness, namely the probability for each offspring to survive. This process uses the fact that an individual will be discarded when any of the during mating operators returns *False*. It is important to remember that:

- individual fitness needs to be between 0 and 1 in this case.
- Fitness values are not stored so the population does not need an information field *fitness*.
- This method applies natural selection to offspring instead of parents. These two implementation can be identical or different depending on the mating scheme used.
- Seleting offspring is less efficient than the selecting parents, especially when fitness values are low.
- Parameter *subPops* are applied to the offspring population and is used to judge if an operator should be applied. It thus does not make sense to apply a selector to a virtual subpopulation with affected individuals.

class BaseSelector(output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=ALL\_AVAIL)
Create a base selector object. This operator should not be created directly.

# 2.9.2 Class MapSelector

This selector assigns individual fitness values using a user-specified dictionary. This operator can be applied to populations with arbitrary number of homologous chromosomes.

class MapSelector(loci, fitness, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, in-foFields=ALL\_AVAIL)

Create a selector that assigns individual fitness values using a dictionary *fitness* with genotype at *loci* as keys, and fitness as values. Parameter *loci* can be a list of indexes, loci names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. For each individual (parents if this operator is applied before mating, and offspring if this operator is applied during mating), genotypes at *loci* are collected one by one (e.g. p0\_loc0, p1\_loc0, p0\_loc1, p1\_loc1... for a diploid individual, with number of alleles varying for sex and mitochondrial DNAs) and are looked up in the dictionary. If a genotype cannot be found, it will be looked up again without phase information (e.g. (1,0) will match key (0,1)). If the genotype still can not be found, a ValueError will be raised. This operator supports sex chromosomes and haplodiploid populations. In these cases, only valid genotypes should be used to generator the dictionary keys.

#### 2.9.3 Class MaSelector

This operator is called a 'multi-allele' selector because it groups multiple alleles into two groups: wildtype and non-wildtype alleles. Alleles in each allele group are assumed to have the same effect on individual fitness. If we denote all wildtype alleles as A, and all non-wildtype alleles a, this operator assign individual fitness according to genotype AA, Aa, aa in the diploid case, and A and a in the haploid case.

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Creates a multi-allele selector that groups multiple alleles into a wildtype group (with alleles *wildtype*, default to [0]), and a non-wildtype group. A list of fitness values is specified through parameter *fitness*, for genotypes at one or more *loci*. Parameter *loci* can be a list of indexes, loci names , list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. If we denote wildtype alleles using capital letters A, B ... and non-wildtype alleles using small letters a, b ...., the fitness values should be for

- •genotypes A and a for the haploid single-locus case,
- •genotypes AB, Ab, aB and bb for haploid two=locus cases,
- •genotypes AA, Aa and aa for diploid single-locus cases,
- •genotypes AABB, AABb, AAbb, AaBB, AaBb, Aabb, aaBB, aaBb, and aabb for diploid two-locus cases,
- •and in general 2\*\*n for diploid and 3\*\*n for haploid cases if there are n loci.

This operator does not support haplodiploid populations, sex and mitochondrial chromosomes.

# 2.9.4 Class MlSelector

This selector is created by a list of selectors. When it is applied to an individual, it applies these selectors to the individual, obtain a list of fitness values, and compute a combined fitness value from them. ADDITIVE, multiplicative, and a heterogeneour multi-locus model are supported.

class MISelector(ops, mode=MULTIPLICATIVE, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=ALL\_AVAIL)

Create a multiple-locus selector from a list selection operator *selectors*. When this operator is applied to an individual (parents when used before mating and offspring when used during mating), it applies these operators to the individual and obtain a list of (usually single-locus) fitness values. These fitness values are combined to a single fitness value using

- $Prod(f_i)$ , namely the product of individual fitness if mode = MULTIPLICATIVE,
- •1- $sum(1 f_i)$  if mode = ADDITIVE,
- •1- $Prod(1 f_i)$  if mode = HETEROGENEITY, and
- exp(-sum(1 f i)) if mode = EXPONENTIAL,

zero will be returned if the combined fitness value is less than zero.

Applicability parameters (begin, end, step, at, reps, subPops) could be used in both MlSelector and selectors in parameter *ops*, but parameters in MlSelector will be interpreted first.

# 2.9.5 Class PySelector

This selector assigns fitness values by calling a user provided function. It accepts a list of loci (parameter *loci*) and a Python function func which should be defined with one or more of parameters geno, mut, gen, ind, pop or names of information fields. Parameter *loci* can be a list of loci indexes, names, list of chromosome position pairs, ALL\_AVAIL, or a function with optional parameter pop that will be called at each ganeeration to determine indexes of loci. When this operator is applied to a population, it passes genotypes or mutants at specified loci, generation number, a reference to an individual, a reference to the current population (usually used to retrieve population variable), and values at specified information fields to respective parameters of this function. Genotypes are passed as a tuple of alleles arranged locus by locus (in the order of A1,A2,B1,B2 for loci A and B). Mutants are passed as a default dictionary of loci index (with respect to all genotype of individuals, not just the first ploidy) and alleles. The returned value will be used to determine the fitness of each individual.

 $\textbf{class PySelector}(func,\ loci=[],\ begin=0,\ end=-1,\ step=1,\ at=[],\ reps=ALL\_AVAIL,\ subPops=ALL\_AVAIL,\ infoFields=ALL\_AVAIL)$ 

Create a Python hybrid selector that passes genotype at specified *loci*, values at specified information fields (if requested) and a generation number to a user-defined function *func*. The return value will be treated as individual fitness.

# 2.9.6 Class PyMlSelector

This selector is a multi-locus Python selector that assigns fitness to individuals by combining locus and genotype specific fitness values. It differs from a PySelector in that the python function is responsible for assigning fitness values for each gentoype type at each locus, which can potentially be random, and locus or gentoype-specific.

class PyMlSelector(func, mode=EXPONENTIAL, loci=ALL\_AVAIL, output="", begin=0, end=-1, step=1, at=[], reps=ALL AVAIL, subPops=ALL AVAIL, infoFields=ALL AVAIL)

Create a selector that assigns individual fitness values by combining locus-specific fitness values that are determined by a Python call-back function. The callback function accepts parameter *loc*, *alleles* (both optional) and returns location- or genotype-specific fitness values that can be constant or random. The fitness values for each genotype will be cached so the same fitness values will be assigned to genotypes with previously assigned values. Note that a function that does not examine the genotype naturally assumes a dominant model where genotypes with one or two mutants have the same fitness effect. Because genotypes at a locus are passed separately and in no particular order, this function is also responsible for assigning consistent fitness values for genotypes at the same locus (a class is usually used). This operator currently ignores chromosome types so unused alleles will be passed for loci on sex or mitochondrial chromosomes. It also ignores phase of genotype so it will use the same fitness value for genotype (a,b) and (b,a).

Individual fitness will be combined in ADDITIVE, MULTIPLICATIVE, HETEROGENEITY, or EXPONENTIAL mode from fitness values of loci with at least one non-zero allele (See MlSelector for details). If an output is given, location, genotype, fitness and generation at which the new genotype is assgined the value will be written to the output, in the format of 'loc a1 a2 fitness gen' for loci on autosomes of diploid populations.

# **2.10** Tagging operators

# 2.10.1 Class IdTagger

An IdTagger gives a unique ID for each individual it is applies 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 1. Value 1 instead of 0 is used because most software applications use 0 as missing values for parentship. 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 pre0ps parameter of function Simulator.evolve to assign initial ID to a population.

 $\textbf{class IdTagger}(begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, output="", infoFields="ind_id")$ 

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.

reset(startID=1)

Reset the global individual ID number so that IdTaggers will start from id (default to 1) again.

# 2.10.2 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.

 $\textbf{class InheritTagger}(mode=PATERNAL,\ begin=0,\ end=-1,\ step=1,\ at=[],\ reps=ALL\_AVAIL,\ subPops=ALL\_AVAIL,\ output="",\ infoFields=[])$ 

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=MINIMUM 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.

# 2.10.3 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.

 $\textbf{class SummaryTagger}(mode=MEAN,\ begin=0,\ end=-1,\ step=1,\ at=[],\ reps=ALL\_AVAIL,\ subPops=ALL\_AVAIL,\ out-put="",\ infoFields=[])$ 

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.

# 2.10.4 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 asexsual 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.

 $\textbf{class ParentsTagger}(begin=0, \ end=-1, \ step=1, \ at=[], \ reps=ALL\_AVAIL, \ subPops=ALL\_AVAIL, \ output="", \ infoFields=["father\_idx", "mother\_idx"])$ 

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 *output* and *subPops*.

# 2.10.5 Class OffspringTagger

This tagging operator records the indexes of offspring within a family (sharing the same parent or parents) in specified information field (default to offspring\_idx). This tagger can be used to control the number of offspring during mating.

 $\textbf{class 0ffspringTagger}(begin=0,\ end=-1,\ step=1,\ at=[],\ reps=ALL\_AVAIL,\ subPops=ALL\_AVAIL,\ output="",\ infoFields=ALL\_AVAIL)$ 

Create an offspring tagger that records the indexes of offspring within a family. The index is determined by successful production of offspring during a mating events so the it does not increase the index if a previous offspring is discarded, and it resets index even if adjacent families share the same parents. This operator ignores parameters *stage*, *output*, and *subPops*.

# 2.10.6 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 asexsual 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.

 $\textbf{class PedigreeTagger}(idField="ind\_id", output="", outputFields=[], outputLoci=[], begin=0, end=-1, step=1, at=[], \\ reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=["father\_id", "mother\_id"])$ 

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. If a valid output stream is given (should be in the form of '>>filename' so that output will be concatenated), this operator will output the ID of offspring, IDs of his or her parent(s), sex and affection status of offspring, and values at specified information fields (*outputFields*) and loci (*outputLoci*) in the format of off\_id father\_id mother\_id M/F A/U fields genotype. father\_id or mother\_id will be ignored if only one parent is involved. This file format can be loaded using function loadPedigree.

Because only offspring will be outputed, individuals in the top-most ancestral generation will not be outputed. This is usually not a problem because individuals who have offspring in the next generation will be constructed by function loadPedigree, although their information fields and genotype will be missing. If you would like to create a file with complete pedigree information, you can apply this operator before evolution in the *initOps* parameter of functions Population.evolve or Simulator.evolve. This will output all individuals in the initial population (the top-most ancestral population after evolution) in the same format. Note that sex, affection status and genotype can be changed by other operators so this operator should usually be applied after all other operators are applied.

# 2.10.7 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, begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, output="", infoFields=[])

Create a hybrid tagger that provides an user provided function func with values of specified information fields

(determined by parameter names of this function) of parents and assign corresponding information fields of offspring with its return value. If more than one parent are available, maternal values are passed after paternal values. For example, if a function func(A, B) is passed, this operator will send two tuples with parental values of information fields 'A' and 'B' to this function and assign its return values to fields 'A' and 'B' of each offspring. 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*.

# 2.11 Statistics Calculation

#### **2.11.1** Class 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 evalulate expressions in this local namespace after Stat is applied.

class Stat(popSize=False, numOfMales=False, numOfAffected=False, numOfSegSites=[], numOfMutants=[], alleleFreq=[], heteroFreq=[], homoFreq=[], genoFreq=[], haploFreq=[], haploHeteroFreq=[], haplo-HomoFreq=[], sumOfInfo=[], meanOfInfo=[], varOfInfo=[], maxOfInfo=[], minOfInfo=[], LD=[], association=[], neutrality=[], structure=[], HWE=[], inbreeding=[], effectiveSize=[], vars=ALL\_AVAIL, suffix="", output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])

Create a Stat operator that calculates specified statistics of a population when it is applied to this population. This operator 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 evalulate 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.

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

- •num0fMales (default): Total number of male individuals in all or specified (virtual) subpopulations.
- •num0fFemales (default): Total number of female individuals in all or specified (virtual) subpopulations.
- •prop0fMales: Proportion of male individuals.
- •prop0fFemales: Proportion of female individuals.
- •numOfMales\_sp: Number of male individuals in each (virtual) subpopulation.
- •numOfFemales\_sp: Number of female individuals in each (virtual) subpopulation.
- •prop0fMales\_sp: Proportion of male individuals in each (virtual) subpopulation.
- •prop0fFemales\_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:

- •num0fAffected (default): Total number of affected individuals in all or specified (virtual) subpopulations.
- •num0fUnaffected (default): Total number of unaffected individuals in all or specified (virtual) subpopulations
- •prop0fAffected: Proportion of affected individuals.
- •prop0fUnaffected: Proportion of unaffected individuals.
- •num0fAffected\_sp: Number of affected individuals in each (virtual) subpopulation.
- •num0fUnaffected\_sp: Number of unaffected individuals in each (virtual) subpopulation.
- prop0fAffected\_sp: Proportion of affected individuals in each (virtual) subpopulation.
- $\bullet \texttt{prop0fUnaffected\_sp:} \ Proportion \ of \ unaffected \ individuals \ in \ each \ (virtual) \ subpopulation.$

**numOfSegSites**: Parameter *numOfSegSites* accepts a list of loci (loci indexes, names, or ALL\_AVAIL) and count the number of loci with at least two different alleles (segregating sites) or loci with only one non-zero allele (no zero allele, not segragating) for individuals in all or specified (virtual) subpopulations. This parameter sets variables

- •num0fSegSites (default): Number of segregating sites in all or specified (virtual) subpopulations.
- •numOfSegSites\_sp: Number of segregating sites in each (virtual) subpopulation.
- •num0fFixedSites: Number of sites with one non-zero allele in all or specified (virtual) subpopulations.
- •num0fFixedSites\_sp: Number of sites with one non-zero allele in in each (virtual) subpopulations.
- •seqSites: A list of segregating sites in all or specified (virtual) subpopulations.
- •segSites\_sp: A list of segregating sites in each (virtual) subpopulation.
- •fixedSites: A list of sites with one non-zero allele in all or specified (virtual) subpopulations.
- •fixedSites\_sp: A list of sites with one non-zero allele in in each (virtual) subpopulations.

**numOfMutants**: Parameter *numOfMutants* accepts a list of loci (loci indexes, names, or ALL\_AVAIL) and count the number of mutants (non-zero alleles) for individuals in all or specified (virtual) subpopulations. It sets variables

•num0fMutants (default): Number of mutants in all or specified (virtual) subpopulations.

•num0fMutants\_sp: Number of mutants in each (virtual) subpopulations.

alleleFreq: This parameter accepts a list of loci (loci indexes, names, or ALL\_AVAIL), 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 or names), 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.
- $\bullet \texttt{heteroFreq\_sp:} \ A \ dictionary \ of \ proportion \ of \ heterozygotes \ in \ each \ (virtual) \ subpopulation.$
- $\bullet {\tt homoFreq\_sp:}\ A\ dictionary\ of\ proportion\ of\ homozygotes\ in\ each\ (virtual)\ subpopulation.$
- •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 indexes or names) at which number and frequency of all genotypes are outputed 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: Halptype frequencies in each (virtual) subpopulation.
- •haploNum\_sp: Halptype count in each (virtual) subpopulation.

**haploHeteroFreq** and **haploHomoFreq**: These parameters accept a list of haplotypes (list of loci), at which the number and frequency of haplotype homozygotes and/or heterozygotes will be calculated. Note that these statistics are **observed** count of haplotype heterozygote. The following variables will be outputted:

- •haploHeteroFreq (default for parameter *haploHeteroFreq*): A dictionary of proportion of haplotype heterozygotes in all or specified (virtual) subpopulations, with haplotype indexes as dictionary keys.
- •haploHomoFreq (default for parameter *haploHomoFreq*): A dictionary of proportion of homozygotes in all or specified (virtual) subpopulations.
- •haploHeteroNum: A dictionary of number of heterozygotes in all or specified (virtual) subpopulations.
- •haploHomoNum: A dictionary of number of homozygotes in all or specified (virtual) subpopulations.
- •haploHeteroFreq\_sp: A dictionary of proportion of heterozygotes in each (virtual) subpopulation.
- •haploHomoFreq\_sp: A dictionary of proportion of homozygotes in each (virtual) subpopulation.
- •haploHeteroNum\_sp: A dictionary of number of heterozygotes in each (virtual) subpopulation.
- •haploHomoNum\_sp: A dictionary of number of homozygotes in each (virtual) subpopulation.

**sumOfinfo**, **warOfInfo**, **warOfInfo** 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 iddividuals in all or specified (virtual) subpopulations will be calculated. The results will be put into the following population variables:

- •sum0fInfo (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.
- •sum0fInfo\_sp: A dictionary of the sum of information fields of individuals in each subpopulation.
- •mean0fInfo\_sp: A dictionary of the mean of information fields of individuals in each subpopulation.
- •var0fInfo\_sp: A dictionary of the sample variance of information fields of individuals in each subpopulation.
- •max0fInfo\_sp: A dictionary of the maximum value of information fields of individuals in each subpopulation.
- •min0fInfo\_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 contigency 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 contigency 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 R2 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, which can be a list of indexes, names, or ALL\_AVAIL. 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, which can be a list of loci indexes, names or ALL\_AVAIL. 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 paiewise 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. *structure* accepts a list of loci indexes, names or ALL\_AVAIL. 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. Nei's Gst uses only allele frequency information so it is available for all population type (haploid, diploid etc). Weir and Cockerham's Fst uses heterozygosity frequency so it is best for autosome of diploid populations. For non-diploid population, sex, and mitochondrial DNAs, simuPOP uses expected heterozygosity (1 sum p\_i2) when heterozygosity is needed. These statistics output the following variables:
- •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. *HWE* can be a list of loci indexes, names or ALL\_AVAIL. This statistic 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.

**inbreeding**: Inbreeding measured by Identitcal by Decent (and by State). This statistics go through all loci of individuals in a diploid population and calculate the number and proportions of alleles that are identitcal by decent and by state. Because ancestral information is only available in lineage module, variables IBD\_freq are always set to zero in other modules. Loci on sex and mitochondrial chromosomes, and non-diploid populations are currently not supported. This statistic outputs the following variables:

- •IBD\_freq (default) The frequency of IBD pairs among all allele pairs. To use this statistic, the population must be initialized by operator InitLineage() to assign each ancestral allele an unique identify.
- •IBS\_freq (default) The proportion of IBS pairs among all allele pairs.
- •IBD\_freq\_sp frequency of IBD in each (virtual) subpopulations.
- •IBS\_freq\_sp frequency of IBS in each (virtual) subpopulations.

**effectiveSize**: Parameter effectiveSize accepts a list of loci at which the effective population size for the whole or specified (virtual) subpopulations is calculated. *effectiveSize* can be a list of loci indexes, names or ALL\_AVAIL. Parameter *subPops* is usually used to define samples from which effective sizes are estimated. This statistic allows the calculation of true effective size based on number of gametes each parents transmit to the offspring population (per-locus before and after mating), and estimated effective size based on sample genotypes. Due to the temporal natural of some methods, more than one Stat operators might be needed to calculate effective size. The *vars* parameter specified which method to use and which variable to set. Acceptable values include:

- •Ne\_demo\_base When this variable is set before mating, it stores IDs of breeding parents and, more importantly, assign an unique lineage value to alleles at specified loci of each individual. This feature is only available for lineage modules and will change lineage values at specified loci of all individuals.
- •Ne\_demo\_base\_sp Pre-mating information for each (virtual) subpopulation, used by variable Ne\_demo\_sp.
- •Ne\_demo A dictionary of locus-specific demographic effective population size, calculated using number of gemetes each parent transmits to the offspring population. The method is vased on Crow & Denniston 1988 (Ne = KN-1/k-1+Vk/k) and need variable Ne\_demo\_base set before mating. Effective size estimated from this formula is model dependent and might not be applicable to your mating schemes.
- •Ne\_demo\_sp Calculate subpopulation-specific effective size.
- •Ne\_temporal\_base When this variable is set in parameter *vars*, the Stat operator saves baseline allele frequencies and other information in this variable, which are used by temporary methods to estimate effective population size according to changes in allele frequency between the baseline and present generations. This variable could be set repeatedly to change baselines.
- •Ne\_temporal\_base\_sp Set baseline information for each (virtual) subpopulation specified.
- •Ne\_tempoFS\_P1 Effective population size, 2.5% and 97.5% confidence interval for sampling plan 1 as a list of size 3, estimated using a temporal method as described in Jorde & Ryman (2007), and as implemented by software tempoFS (http://www.zoologi.su.se/ryman/). This variable is set to census population size if no baseline has been set, and to the temporal effective size between the present and the baseline generation otherwise. This method uses population size or sum of subpopulation sizes of specified (virtual) subpopulations as census population size for the calculation based on plan 1.
- •Ne\_tempoFS\_P2 Effective population size, 2.5% and 97.5% confidence interval for sampling plan 2 as a list of size 6, estimated using a temporal method as described in Jorde & Ryman (2007). This variable is set to census population size no baseline has been set, and to the temporal effective size between the present and the baseline generation otherwise. This method assumes that the sample is drawn from an infinitely-sized population.
- •Ne\_tempoFS deprecated, use Ne\_tempoFS\_P2 instead.
- •Ne\_tempoFS\_P1\_sp Estimate effective size of each (virtual) subpopulation using method Jorde & Ryman 2007, assuming sampling plan 1. The census population sizes for sampling plan 1 are the sizes for each subpopulation that contain the specified (virtual) subpopulations.
- •Ne\_tempoFS\_P2\_sp Estimate effective size of each (virtual) subpopulation using method Jorde & Ryman 2007, assuming sampling plan 2.
- •Ne\_tempoFS\_sp deprecated, use Ne\_tempoFS\_P2\_sp instead.
- •Ne\_waples89\_P1 Effective population size, 2.5% and 97.5% confidence interval for sampling plan 1 as a list of size 6, estimated using a temporal method as described in Waples 1989, Genetics. Because this is a temporal method, Ne\_waples89 estimates effective size between the present and the baseline generation set by variable Ne\_temporal\_base. Census population size will be resutned if no baseline has been set. This method uses population size or sum of subpopulation sizes of specified (virtual) subpopulations as census population size for the calculation based on plan 1.
- •Ne\_waples89\_P2 Effective population size, 2.5% and 97.5% confidence interval for sampling plan 2 as a list of size 6, estimated using a temporal method as described in Waples 1989, Genetics. Because this is a temporal method, Ne\_waples89 estimates effective size between the present and the baseline generation set by variable Ne\_temporal\_base. Census population size will be returned if no baseline has been set.

- •Ne\_waples89\_P1\_sp Estimate effective size for each (virtual) subpopulation using method Waples 89, assuming sampling plan 1. The census population sizes are the sizes for each subpopulation that contain the specified (virtual) subpopulation.
- •Ne\_waples89\_P2\_sp Estimate effective size for each (virtual) subpopulation using method Waples 89, assuming sampling plan 2.
- •Ne\_waples89\_sp deprecated, use Ne\_waples89\_P2\_sp instead.
- •Ne\_LD Lists of length three for effective population size, 2.5% and 97.% confidence interval for cutoff allele frequency 0., 0.01, 0.02 and 0.05 (as dictionary keys), using a parametric method, estimated from linkage disequilibrim information of one sample, using LD method developed by Waples & Do 2006 (LDNe). This method assumes unlinked loci and uses LD measured from genotypes at loci. Because this is a sample based method, it should better be applied to a random sample of the population. 95% CI is calculated using a Jackknife estimated effective number of independent alleles. Please refer to relevant papers and the LDNe user's guide for details.
- •Ne\_LD\_sp Estimate LD-based effective population size for each specified (virtual) subpopulation.
- •Ne\_LD\_mono A version of Ne\_LD that assumes monogamy (see Waples 2006 for details.
- •Ne\_LD\_mono\_sp Ne\_LD\_mono calculated for each (virtual) subpopulation.

# 2.12 Conditional operators

#### 2.12.1 Class IfElse

This operator uses a condition, which can be a fixed condition, an expression or a user-defined function, to determine which operators to be applied when this operator is applied. A list of if-operators will be applied when the condition is True. Otherwise a list of else-operators will be applied.

class IfElse(cond, ifOps=[], elseOps=[], output=">", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Create a conditional operator that will apply operators *ifOps* if condition *cond* is met and *elseOps* otherwise. If a Python expression (a string) is given to parameter *cond*, the expression will be evalulated in each population's local namespace when this operator is applied. When a Python function is specified, it accepts parameter pop when it is applied to a population, and one or more parameters pop, off, dad or mom when it is applied during mating. The return value of this function should be True or False. Otherwise, parameter *cond* will be treated as a fixed condition (converted to True or False) upon which one set of operators is always applied. The applicability of *ifOps* and *elseOps* are controlled by parameters *begin*, *end*, *step*, *at* and *rep* of both the IfElse operator and individual operators but *ifOps* and *elseOps* opeartors does not support negative indexes for replicate and generation numbers.

# 2.12.2 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="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[])

Create a terminator with an expression *condition*, which will be evalulated 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*.

# 2.12.3 Class RevertIf

This operator replaces the current evolving population by a population loaded from a specified filename if certain condition is met. It is mostly used to return to a previously saved state if the simulation process fails to met a condition (e.g. a disease allele is lost).

class RevertIf(cond, fromPop="", ops=[], output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Replaces the current evolving population by a population loaded from *fromPop*, which should be a file saved by function Population.save() or operator SavePopulation. If a Python expression (a string) is given to parameter *cond*, the expression will be evalulated in each population's local namespace when this operator is applied. When a Python function with optional parameter pop is specified, it should accept the current population (to parameter pop) and converts and return True or False. Otherwise, parameter *cond* will be treated as a fixed condition (converted to True or False) upon which the population is reverted. After the population is reverted, an optional list of operators *ops* could be applied to the population.

#### 2.12.4 Class DiscardIf

This operator discards individuals according to either an expression that evaluates according to individual information field, or a Python function that accepts individual and its information fields.

**class DiscardIf**(cond, exposeInd="", output="", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, sub-Pops=ALL\_AVAIL, infoFields=[])

Create an operator that discard individuals according to an expression or the return value of a Python function (parameter *cond*). This operator can be applied to a population before or after mating, or to offspring during mating. If an expression is passed to *cond*, it will be evaluated with each individual's information fields (see operator InfoEval for details). If *exposeInd* is non-empty, individuals will be available for evaluation in the expression as an variable with name spacied by *exposeInd*. If the expression is evaluated to be True, individuals (if applied before or after mating) or offspring (if applied during mating) will be removed or discard. If a function is passed to *cond*, it should accept parameters *ind* and *pop* or names of information fields when it is applied to a population (pre or post mating), or parameters *off*, *dad*, *mom*, *pop* (parental population), or names of information fields if the operator is applied during mating. Individuals will be discarded if this function returns True. A constant expression (e.g. True) is also acceptable). Because this operator supports parameter *subPops*, only individuals belonging to specified (virtual) subpopulations will be screened.

# 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 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.

 $\textbf{class PyOperator}(func, \ param=None, \ begin=0, \ end=-1, \ step=1, \ at=[], \ reps=ALL\_AVAIL, \ subPops=ALL\_AVAIL, \ infoFields=[])$ 

Create a pure-Python operator that calls a user-defined function when it is applied. If this operator is applied before or after mating, your function should have form func(pop) or func(pop, param) where pop is the population to which the operator is applied, param is the value specified in parameter *param*. param will be ignored if your function only accepts one parameter. Althernatively, the function should have form func(ind) with optional parameters pop and param. In this case, the function will be called for all individuals, or individuals in subpopulations *subPops*. Individuals for which the function returns False will be removed from the population. This operator can therefore perform similar functions as operator DiscardIf.

If this operator is applied during mating, your function should accept parameters pop, off (or ind), dad, mom and

param where pop is the parental population, and off or ind, dad, and mom are offspring and their parents for each mating event, and param is an optional parameter. If *subPops* are provided, only offspring in specified (virtual) subpopulations are acceptable.

This operator does not support parameters *output*, 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.

# 2.14 Miscellaneous operators

## 2.14.1 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.

 $\textbf{class NoneOp}(output=">", begin=0, end=0, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, infoFields=[]) \\ Create a NoneOp.$ 

## 2.14.2 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, ancGens=UNSPECIFIED, width=1, max=100, loci=[], output=">", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL\_AVAIL, 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 *ancGens*). All loci will be outputed 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*.

# 2.14.3 Class SavePopulation

An operator that save populations to specified files.

class SavePopulation(output=""", begin=0, end=-1, step=1, at=[],  $reps=ALL\_AVAIL$ ,  $subPops=ALL\_AVAIL$ , infoFields=[])

Create an operator that saves a population to *output* when it is applied to the population. This operator supports 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*.

## 2.14.4 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=">", begin=0, end=-1, step=1, at=[], reps=ALL\_AVAIL, subPops=ALL AVAIL, infoFields=[])

Create an operator that pause the evolution of a population when it is applied to this population. If *stopOn-KeyStroke* 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.

# 2.14.5 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. As an advanced feature that mainly used for performance testing, this operator accepts a parameter *stopAfter* (seconds), and will stop the evolution of a population if the overall time exceeds *stopAfter*. Note that elapsed time is only checked when this operator is applied to a population so it might not be able to stop the evolution process right after *stopAfter* seconds. This operator can also be applied during mating. Note that to avoid excessive time checking, this operator does not always check system time accurately.

Create a TicToc operator that outputs the elapsed since the last time it was applied, and the overall time since the first time this operator is applied.

# 2.15 Function form of operators

# 2.15.1 Function acgtMutate

acgtMutate(pop, \*args, \*\*kwargs)
Function form of operator AcgtMutator

## 2.15.2 Function contextMutate

contextMutate(pop, \*args, \*\*kwargs)
Function form of operator ContextMutator

# 2.15.3 Function discardIf

discardIf(pop, \*args, \*\*kwargs)

Apply operator DiscardIf to population *pop* to remove individuals according to an expression or a Python function.

#### 2.15.4 Function dump

dump(pop, \*args, \*\*kwargs)
Apply operator Dumper to population pop.

# 2.15.5 Function infoEval

infoEval(pop, \*args, \*\*kwargs)

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

#### 2.15.6 Function infoExec

infoExec(pop, \*args, \*\*kwargs)

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

# 2.15.7 Function initGenotype

initGenotype(pop, \*args, \*\*kwargs)

Apply operator InitGenotype to population pop.

# 2.15.8 Function initInfo

initInfo(pop, \*args, \*\*kwargs)

Apply operator InitInfo to population pop.

# 2.15.9 Function initSex

initSex(pop, \*args, \*\*kwargs)

Apply operator InitSex to population pop.

#### 2.15.10 Function kAlleleMutate

kAlleleMutate(pop, \*args, \*\*kwargs)

Function form of operator KAlleleMutator

#### 2.15.11 Function maPenetrance

maPenetrance(pop, loci, penetrance, wildtype=0, ancGens=True, \*args, \*\*kwargs)

Apply opertor MaPenetrance to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

# 2.15.12 Function mapPenetrance

mapPenetrance(pop, loci, penetrance, ancGens=True, \*args, \*\*kwargs)

Apply opertor MapPenetrance to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

#### 2.15.13 Function matrixMutate

matrixMutate(pop, \*args, \*\*kwargs)

Function form of operator MatrixMutator

# 2.15.14 Function mergeSubPops

mergeSubPops(pop, \*args, \*\*kwargs)

Merge subpopulations *subPops* of population *pop* into a single subpopulation. Please refer to the operator form of this funciton (MergeSubPops) for details

# 2.15.15 Function migrate

migrate(pop, \*args, \*\*kwargs)

Function form of operator Migrator.

#### 2.15.16 Function mixedMutate

mixedMutate(pop, \*args, \*\*kwargs)

Function form of operator MixedMutator

#### 2.15.17 Function mlPenetrance

mlPenetrance(pop, ops, mode, ancGens=True, \*args, \*\*kwargs)

Apply opertor MapPenetrance to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

# 2.15.18 Function pointMutate

pointMutate(pop, \*args, \*\*kwargs)

Function form of operator PointMutator

# 2.15.19 Function pyEval

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

# 2.15.20 Function pyExec

pyExec(pop, \*args, \*\*kwargs)

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

# 2.15.21 Function pyMutate

pyMutate(pop, \*args, \*\*kwargs)

Function form of operator PyMutator

## 2.15.22 Function pyPenetrance

pyPenetrance(pop, func, loci=[], ancGens=True, \*args, \*\*kwargs)

Apply opertor PyPenetrance to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

# 2.15.23 Function pyMlPenetrance

pyMlPenetrance(pop, func, mode, loci=[], ancGens=True, \*args, \*\*kwargs)

Apply opertor PyMlPenetrance to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

# 2.15.24 Function pyQuanTrait

pyQuanTrait(pop, func, loci=[], ancGens=True, \*args, \*\*kwargs)

Apply opertor PyQuanTrait to population *pop*. Unlike the operator form of this operator that only handles the current generation, this function by default assign affection status to all generations.

## 2.15.25 Function resizeSubPops

resizeSubPops(pop, \*args, \*\*kwargs)

Resize subpopulations *subPops* of population *pop* into new sizes *size*. Individuals will be added or removed accordingly. Please refer to the operator form of this function (ResizeSubPops) for details

# 2.15.26 Function snpMutate

snpMutate(pop, \*args, \*\*kwargs)

Function form of operator SNPMutator

#### 2.15.27 Function splitSubPops

splitSubPops(pop, \*args, \*\*kwargs)

Split subpopulations (*subPops*) of population *pop* according to either *sizes* or *proportions* of the resulting subpopulations, or an information field. Please refer to the operator form of this function (splitSubPop) for details.

# 2.15.28 Function stat

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()

#### 2.15.29 Function stepwiseMutate

stepwiseMutate(pop, \*args, \*\*kwargs)

Function form of operator StepwiseMutator

# 2.15.30 Function tagID

tagID(pop, reset=False, \*args, \*\*kwargs)

Apply operator IdTagger to population *pop* to assign a unique ID to all individuals in the population. Individuals ID will starts from a system wide index. You can reset this start ID using parameter reset which can be True (reset to 1) or a non-negative number (start from this number).

# **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.Params that helps users manage simulation parameters.

When simuPOP is loaded, it checkes 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 version of simuPOP for your script. simuPOP recognize the following commandline arguments

- --optimized: Load the optimized version of a simuPOP module.
- --gui=None|batch|interactive|True|wxPython|Tkinter: Whether or not use a graphical toolkit and which one to use.
  --gui=batch is usually used to run a script in batch mode (do not start a parameter input dialog and use all default values unless a parameter is specified from command line or a configuration file. If --gui=interactive, an interactive shell will be used to solicit input from users. Otherwise, simuPOP will try to use a graphical parameter input dialog, and falls to an interactive mode when no graphical Toolkit is available. Please refer to parameter gui for simuOpt.setOptions for details.

class params. Params provides a powerful way to handle commandline arguments. Briefly speaking, a Params 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 Params.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, version=None, revision=None, numThreads=None, plotter=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,long or mutant allele version of the simuPOP module if alleleType is set to 'short', 'binary', 'long', 'mutant', or 'lineage' 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, which graphical toolkit to use and how to process parameters in non-GUI mode. If this parameter is None (default), this function will check environmental variable SIMUGUI or commandline option --gui for a value, and assume True if such an option is unavailable. If gui=True, simuPOP will use wxPython-based dialogs if wxPython is available, and use Tkinter-based dialogs if Tkinter is available and use an interactive shell if no graphical toolkit is available. gui='Tkinter' or 'wxPython' can be used to specify the graphical toolkit to use. If gui='interactive', a simuPOP script prompt users to input values of parameters. If gui='batch', default values of unspecified parameters will be used. In any case, commandline arguments and a configuration file specified by parameter --config will be processed. This option is usually left to None so that the same script can be run in both GUI and batch mode using commandline option --gui.

*plotter:* The plotting library used to draw figures. simuPOP will by default use rpy (NOT rpy2), and matplotlib if rpy is not available. You can set this parameter to one of them to force the use a particular library.

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.

*version:* A version string (e.g. 1.0.0) indicating the required version number for the simuPOP module to be loaded. simuPOP will fail to load if the installed version is older than the required version.

revision: Obsolete with the introduction of parameter version.

numThreads: Number of Threads that will be used to execute a simuPOP script. The values can be a positive number (number of threads) or 0 (all available cores of the computer, or whatever number set by environmental variable OMP\_NUM\_THREADS). If this parameter is not set, the number of threads will be set to 1, or a value set by environmental variable OMP\_NUM\_THREADS.

#### 3.1.2 Class Params

class Params 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 interative input. This class provides parameter validation, conversion and and some utility functions to print, save and restore parameters.

A Params 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:

name: Long command line option name. For example 'version' checks the presence of argument --version. 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 identified as a single BooleanType in allowedTypes or a default value False when no allowedTypes is defined. Such a value should have default value False and the presence of this argument in the command line (e.g. --verbose) change it to True.

*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.

- 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 outputed as is without the leading 'l' symbol.
- allowedTypes: A list of acceptable types of this option. class Params will try to convert user input to these types. For example, if allowedTypes is list or tuple 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. If only one type is acceptable, a single value can be used as input (ignore []).
- validator: An expression or a function to validate the parameter. If an expression (a string) is used, it will be evaluated using current values of parameters as inputs. If a function is specified, it will be called with the value of the parameter. The option will not be accepted if the expression is evaluated as "False" or if the function returns False. This module defines a large number of such validation functions but user defined functions are also acceptable.
- type: Type of the input parameter. Which can be a datatype (e.g. bool), a list of acceptable types (e.g. (int, long)), or one of 'chooseOneOf', values, 'chooseFrom', values, 'filename' (a valid filename), 'dirname' (a valid directory name), 'integer' (int or long), 'integers' (list of integers), 'number' (int, long or float), 'numbers' (list of numbers), 'string' (the same as str), 'strings' (list of strings). These types will advise class simuOpt.Params how to accept parameters, and how to convert user input to appropriate types. For example, a file browser will be used to browse for a valid filename in a parameter input dialog (if --gui=True) for a parameter of type 'filename', and input '52' will be automatically converted to (52,) for a parameter of type 'integers'.

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

arg, longarg, useDefault, chooseFrom, chooseOneOf, allowedTypes: These parameters are deprecated because of the introduction of the 'name', 'gui\_type' keys and the 'batch' mode.

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

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

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

Create a Params oject 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 Params 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(name=", default=None, **kwargs)
```

Append an entry to the parameter specification list. Dictionary entries should be specified as keyword arguments such as name='option'. More specifically, you can specify parameters name (required), label, default (required), description, validator, type, and separator. This option will have a name specified by name and an initial default value specified by default.

```
asDict()
```

Return parameters as a dictionary.

asList()

Return parameters as a list.

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

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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 chekArgs 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 optimaly 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.

If Params.valueValidFile or Params.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 (deprecated)
- 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]).

#### 3.1.3 Function param

```
param(name=", default=None, **kwargs)
```

A simple wrapper that allows the specification of a parameter using a function instead of a dictionary. Please refer to class simuOpt.Params for allowed keyword arguments and their meanings.

# 3.1.4 Function valueNot

valueNot(t)

Return a function that returns true if passed option does not equal t, or does not passes validator t

#### 3.1.5 Function valueOr

valueOr(t1, t2)

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

# 3.1.6 Function valueAnd

valueAnd(t1, t2)

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

# 3.1.7 Function valueOneOf

valueOneOf(\*args)

Return a function that returns true if passed option is one of the parameters, or one of the values in the only parameter

# 3.1.8 Function valueTrueFalse

valueTrueFalse()

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

# 3.1.9 Function valueBetween

valueBetween(a, b)

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

#### 3.1.10 Function valueGT

valueGT(a)

Return a function that returns true if passed option is greater than a

# 3.1.11 Function valueGE

 $\mathbf{valueGE}(a)$ 

Return a function that returns true if passed option is greater than or equal to a

# 3.1.12 Function valueLT

 ${\tt valueLT}(a)$ 

Return a function that returns true if passed option is less than a

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# 3.1.13 Function valueLE

#### valueLE(a)

Return a function that returns true if passed option is less than or equal to a

## 3.1.14 Function valueEqual

#### valueEqual(a)

Return a function that returns true if passed option equals a

# 3.1.15 Function valueNotEqual

#### valueNotEqual(a)

Return a function that returns true if passed option does not equal a

# 3.1.16 Function valueIsNum

#### valueIsNum()

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

## 3.1.17 Function valueIsInteger

#### valueIsInteger()

Return a function that returns true if passed option is an integer (int, long)

# 3.1.18 Function valueIsList

#### valueIsList(size=None)

Return a function that returns true if passed option is a sequence. If a size is given, the sequence must have the specified size (e.g. size=3), or within the range of sizes (e.g. size=[1, 5]). A None can be used as unspecified lower or upper bound.

#### 3.1.19 Function valueListOf

#### valueListOf(t, size=None)

Return a function that returns true if passed option val is a list of type t if t is a type, if v is one of t if t is a list, or if v passes test t if t is a validator (a function). If a size is given, the sequence must have the specified size (e.g. size=3), or within the range of sizes (e.g. size=[1, 5]). A None can be used as unspecified lower or upper bound.

#### 3.1.20 Function valueSumTo

#### valueSumTo(a, eps=1e-07)

Return a function that returns true if passed option sum up to a. An eps value can be specified to allowed for numerical error.

#### 3.1.21 Function valueValidDir

#### valueValidDir()

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

#### 3.1.22 Function valueValidFile

#### 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 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 simulateForwardTrajectory and simulateBackwardTrajectory.

The Trajectory object provides several member functions to facilitate the use of Trajectory-simulation techiniques. 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).

#### mutants()

Return a list of mutants in the form of (loc, gen, subPop)

# 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 preOps 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 keyward parameters.

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

Plot simulated Trajectory using R through a Python module rpy, or matplotlib if rpy is not available. The function will return silently if module rpy and matplotlib 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 or functions of matplotlib.

This function makes use of the derived keyword parameter feature of module plotter. The rpy version allows prefixes par, plot, lines and dev\_print, and suffixes loc and sp. For example, you could use parameter plot\_ylim to reset the default value of ylim in R function plot. The matplotlib version allows prefix figure, plot, set\_title, set\_ylim, set\_xlabel, and set\_ylabel, and suffixes loc and sp.

# 3.2.2 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 attemps.

#### 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 frequecies are considered as frequencies at the beginning of this generation.

endGen: Ending generation. The ending frequencies are considerd 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.

# 3.2.3 Function simulateForwardTrajectory

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. If a logger object is given, it will send detailed debug information at DEBUG level and ending allele frequencies at the INFO level. The latter can be used to adjust your fitness model and/or ending allele frequency if a trajectory is difficult to obtain because of parameter mismatch.

## 3.2.4 Function simulateBackwardTrajectory

 $\label{eq:simulateBackwardTrajectory} simulateBackwardTrajectory (N, endGen, endFreq, nLoci=1, fitness=None, minMutAge=None, maxMutAge=None, maxMutAge=None, maxMutAge=None)$ 

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. If a logger object is given, it will send detailed debug information at

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DEBUG level and ending generation and frequency at the INFO level. The latter can be used to adjust your fitness model and/or ending allele frequency if a trajectory is difficult to obtain because of parameter mismatch.

## 3.2.5 Class ProgressBar

The ProgressBar 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 simu0pt.set0ptions).

This class is usually used as follows:

```
progress = ProgressBar("Start simulation", 500)
for i in range(500):
    # i+1 can be ignored if the progress bar is updated by 1 step
    progress.update(i+1)
# if you would like to make sure the done message is displayed.
progress.done()
```

class ProgressBar(message, totalCount, progressChar='.', block=2, done=' Done.

n', gui=None)

Create a progress bar with message, which will be the title of a progress dialog or a message for textbased progress bar. Parameter totalCount specifies total expected steps. If a text-based progress bar is used, you could specified progress character and intervals at which progresses will be displayed using parameters progressChar and block. A ending message will also be displayed in text mode.

done()

Finish progressbar, print 'done' message if in text-mode.

```
update(count=None)
```

Update the progreebar with count steps done. The dialog or textbar may not be updated if it is updated by full percent(s). If count is None, the progressbar increases by one step (not percent).

#### 3.2.6 Function viewVars

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).

# 3.2.7 Function saveCSV

saveCSV(pop, filename=", infoFields=[], loci=True, header=True, subPops=ALL\_AVAIL, genoFormatter=None, infoFormatter=None, sexFormatter={1: 'M', 2: 'F'}, affectionFormatter={False: 'U', True: 'A'}, sep=', ', \*\*kwargs)

This function is deprecated. Please use export(format='csv') instead. Save a simuPOP population pop in csv format. Columns of this file is arranged in the order of information fields (infoFields), sex (if sexFormatter is not None), affection status (if affectionFormatter is not None), and genotype (if genoFormatter is not None). This function only output individuals in the present generation of population pop. This function accepts the following parameters:

- pop: A simuPOP population object.
- *filename:* Output filename. Leading '>' characters are ignored. However, if the first character of this filename is '!', the rest of the name will be evaluated in the population's local namespace. If filename is empty, the content will be written to the standard output.
- infoFileds: Information fields to be outputted. Default to none.
- *loci:* If a list of loci is given, only genotype at these loci will be written. Default to ALL\_AVAIL, meaning all available loci. You can set this parameter to [] if you do not want to output any genotype.
- header: Whether or not a header should be written. These headers will include information fields, sex (if sexFormatter is not None), affection status (if affectionFormatter is not None) and loci names. If genotype at a locus needs more than one column, \_1, \_2 etc will be appended to loci names. Alternatively, a complete header (a string) or a list of column names could be specified directly.
- subPops: A list of (virtual) subpopulations. If specified, only individuals from these subpopulations will be outputed.
- *infoFormatter:* A format string that is used to format all information fields. If unspecified, str(value) will be used for each information field.
- genoFormatter: How to output genotype at specified loci. Acceptable values include None (output allele names), a dictionary with genotype as keys, (e.g. genoFormatter={(0,0):1, (0,1):2, (1,0):2, (1,1):3}, or a function with genotype (as a tuple of integers) as inputs. The dictionary value or the return value of this function can be a single or a list of number or strings.
- *sexFormatter:* How to output individual sex. Acceptable values include None (no output) or a dictionary with keys MALE and FEMALE.
- affectionFormatter: How to output individual affection status. Acceptable values include None (no output) or a dictionary with keys True and False.

Parameters genoCode, sexCode, and affectionCode from version 1.0.0 have been renamed to genoFormatter, sexFormatter and affectionFormatter but can still be used.

# 3.2.8 Class Exporter

An operator to export the current population in specified format. Currently supported file formats include:

STRUCTURE (http://pritch.bsd.uchicago.edu/structure.html). This format accepts the following parameters:

markerNames: If set to True (default), output names of loci that are specified by parameter *lociNames* of the Population class. No names will be outputted if loci are anonymous. A list of loci names are acceptable which will be outputted directly.

recessiveAlleles: If specified, value of this parameter will be outputted after the marker names line.

*interMarkerDistances:* If set to True (default), output distances between markers. The first marker of each chromosome has distance -1, as required by this format.

*phaseInformation:* If specified, output the value (0 or 1) of this parameter after the inter marker distances line. Note that simuPOP populations always have phase information.

label: Output 1-based indexes of individuals if this parameter is true (default)

popData: Output 1-based index of subpopulation if this parameter is set to true (default).

popFlag: Output value of this parameter (0 or 1) after popData if this parameter specified.

locData: Name of an information field with location information of each individual. Default to None (no location data)

*phenotype:* Name of an information field with phenotype information of each individual. Default to None (no phenotype)

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Genotype information are always outputted. Alleles are coded the same way (0, 1, 2, etc) as they are stored in simuPOP.

GENEPOP (http://genepop.curtin.edu.au/). The genepop format accepts the following parameters:

title: The tile line. If unspecified, a line similar to 'produced by simuPOP on XXX' will be outputted.

adjust: Adjust values of alleles by specified value (1 as default). This adjustment is necessary in many cases because GENEPOP treats allele 0 as missing values, and simuPOP treats allele 0 as a valid allele. Exporting alleles 0 and 1 as 1 and 2 will allow GENEPOP to analyze simuPOP-exported files correctly.

Because 0 is reserved as missing data in this format, allele A is outputted as A+adjust. simuPOP will use subpopulation names (if available) and 1-based individual index to output individual label (e.g. SubPop2-3). If parameter subPops is used to output selected individuals, each subpop will be outputted as a separate subpopulation even if there are multiple virtual subpopulations from the same subpopulation. simuPOP currently only export diploid populations to this format.

FSTAT (http://www2.unil.ch/popgen/softwares/fstat.htm). The fstat format accepts the following parameters:

*lociNames*: Names of loci that will be outputted. If unspecified, simuPOP will try to use names of loci that are specified by parameter *lociNames* of the Population class, or names in the form of chrX-Y.

*adjust:* Adjust values of alleles by specified value (1 as default). This adjustment is necessary in many cases because FSTAT treats allele 0 as missing values, and simuPOP treats allele 0 as a valid allele. Exporting alleles 0 and 1 as 1 and 2 will allow FSTAT to analyze simuPOP-exported files correctly.

MAP (marker information format) output information about each loci. Each line of the map file describes a single marker and contains chromosome name, locus name, and position. Chromosome and loci names will be the names specified by parameters chromNames and lociNames of the Population object, and will be chromosome index + 1, and '.' if these parameters are not specified. This format output loci position to the third column. If the unit assumed in your population does not match the intended unit in the MAP file, (e.g. you would like to output position in basepair while the population uses Mbp), you can use parameter posMultiplier to adjust it. This format accepts the following parameters:

*posMultiplier:* A number that will be multiplied to loci positions (default to 1). The result will be outputted in the third column of the output.

PED (Linkage Pedigree pre MAKEPED format), with columns of family, individual, father mother, gender, affection status and genotypes. The output should be acceptable by HaploView or plink, which provides more details of this format in their documentation. If a population does not have ind\_id, father\_id or mother\_id, this format will output individuals in specified (virtual) subpopulations in the current generation (parental generations are ignored) as unrelated individuals with 0, 0 as parent IDs. An incremental family ID will be assigned for each individual. If a population have ind\_id, father\_id and mother\_id, parents will be recursively traced to separate all individuals in a (multigenerational) population into families of related individuals. father and mother id will be set to zero if one of them does not exist. This format uses 1 for MALE, 2 for FEMALE. If phenoField is None, individual affection status will be outputted with 1 for Unaffected and 2 for affected. Otherwise, values of an information field will be outputted as phenotype. Because 0 value indicates missing value, values of alleles will be adjusted by 1 by default, which should be avoided if you are using non-zero alleles to model ACTG alleles in simuPOP. This format will ignore subpopulation structure because parents might belong to different subpopulations. This format accepts the following parameters:

idField: A field for individual id, default to ind\_id. Value at this field will be individual ID inside a pedigree.

fatherField: A field for father id, default to father\_id. Value at this field will be used to output father of an individual, if an individual with this ID exists in the population.

*motherField:* A field for mother id, default to mother\_id. Value at this field will be used to output mother of an individual, if an individual with this ID exists in the population.

phenoField: A field for individual phenotype that will be outputted as the sixth column of the PED file. If None is specified (default), individual affection status will be outputted (1 for unaffected and 2 for affected).

adjust: Adjust values of alleles by specified value (1 as default). This adjustment is necessary in many cases because LINKAGE/PED format treats allele 0 as missing values, and simuPOP treats allele 0 as a valid allele. You should

set this paremter to zero if you have already used alleles 1, 2, 3, 4 to model A, C, T, and G alleles.

Phylip (Joseph Felsenstein's Phylip format). Phylip is generally used for nuclotide sequences and protein sequences. This makes this format suitable for simulations of haploid populations (ploidy=1) with nucleotide or protein sequences (number of alleles = 4 or 24 with alleleNames as nucleotide or amino acid names). If your population does satisfy these conditions, you can still export it, with homologous chromosomes in a diploid population as two sequences, and with specified allele names for allele 0, 1, 2, .... This function outputs sequence name as SXXX where XXX is the 1-based index of individual and SXXX\_Y (Y=1 or 2) for diploid individuals, unless names of sequences are provided by parameter seqNames. This format supports the following parameters:

- alleleNames: Names of alleles 0, 1, 2, ... as a single string (e.g. 'ACTG') or a list of single-character strings (e.g. ['A', 'C', 'T', 'G']). If this parameter is unspecified (default), this program will try to use names of alleles specified in alleleNames parameter of a Population, and raise an error if no name could be found.
- *seqNames:* Names of each sequence outputted, for each individual, or for each sequences for non-haploid population. If unspecified, default names such as SXXX or SXXX\_Y will be used.
- *style:* Output style, can be 'sequential' (default) or 'interleaved'. For sequential output, each sequence consists of for the first line a name and 90 symbols starting from column 11, and subsequent lines of 100 symbols. The interleaved style have subsequent lines as separate blocks.

MS (output from Richard R. Hudson's MS or msHOT program). This format records genotypes of SNP markers at segregating site so all non-zero genotypes are recorded as 1. simuPOP by default outputs a single block of genotypes at all loci on the first chromosome, and for all individuals, unless parameter splitBy is specified to separate genotypes by chromosome or subpopulations.

splitBy:: simuPOP by default output segregating sites at all loci on the first chromosome for all individuals. If splitBy is set to 'subPop', genotypes for individuals in all or specified (parameter subPops) subpopulations are outputted in separate blocks. The subpopulations should have the same number of individuals to produce blocks of the same number of sequences. Alternatively, splitBy can be set to chrom, for which genotypes on different chromosomes will be outputted separately.

CSV (comma separated values). This is a general format that output genotypes in comma (or tab etc) separated formats. The function form of this operator <code>export(format='csv')</code> is similar to the now-deprecated <code>saveCSV</code> function, but its interface has been adjusted to match other formats supported by this operator. This format outputs a header (optiona), and one line for each individual with values of specified information fields, sex, affection status, and genotypes. All fields except for genotypes are optional. The output format is controlled by the following parameters:

infoFileds: Information fields to be outputted. Default to none.

- header: Whether or not a header should be written. These headers will include information fields, sex (if sexFormatter is not None), affection status (if affectionFormatter is not None) and loci names. If genotype at a locus needs more than one column, \_1, \_2 etc will be appended to loci names. Alternatively, a complete header (a string) or a list of column names could be specified directly.
- *infoFormatter:* A format string that is used to format all information fields. If unspecified, str(value) will be used for each information field.
- genoFormatter: How to output genotype at specified loci. Acceptable values include None (output allele values), a dictionary with genotype as keys, (e.g. genoFormatter={(0,0):1, (0,1):2, (1,0):2, (1,1):3}, or a function with genotype (as a tuple of integers) as inputs. The dictionary value or the return value of this function can be a single or a list of number or strings.
- sexFormatter: How to output individual sex. Acceptable values include None (no output) or a dictionary with keys MALE and FEMALE.
- affectionFormatter: How to output individual affection status. Acceptable values include None (no output) or a dictionary with keys True and False.

delimiter: Delimiter used to separate values, default to ','.

This operator supports the usual applicability parameters such as begin, end, step, at, reps, and subPops. If subPops

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are specified, only individuals from specified (virtual) subPops are exported. Similar to other operators, parameter output can be an output specification string (filename, >>filename, !expr), filehandle (or any Python object with a write function), any python function. Unless explicitly stated for a particular format, this operator exports individuals from the current generation if there are multiple ancestral generations in the population.

The Exporter class will make use of a progress bar to show the progress. The interface of the progress bar is by default determined by the global GUI status but you can also set it to, for example, gui=False to forcefully use a text-based progress bar.

## 3.2.9 Function importPopulation

importPopulation(format, filename, \*args, \*\*kwargs)

This function import and return a population from a file *filename* in specified *format*. Format-specific parameters can be used to define how the input should be interpreted and imported. This function supports the following file format.

GENEPOP (http://genepop.curtin.edu.au/). For input file of this format, this function ignores the first title line, load the second line as loci names, and import genotypes of different POP sections as different subpopulations. This format accepts the following parameters:

adjust: Adjust alleles by specified value (default to 0 for no adjustment). This parameter is mostly used to convert alleles 1 and 2 in a GenePop file to alleles 0 and 1 (with adjust=-1) in simuPOP.

FSTAT (http://www2.unil.ch/popgen/softwares/fstat.htm). This format accepts the following parameters:

adjust: Adjust alleles by specified value (default to 0 for no adjustment). This parameter is mostly used to convert alleles 1 and 2 in a GenePop file to alleles 0 and 1 (with adjust=-1) in simuPOP.

Phylip (Joseph Felsenstein's Phylip format). This function ignores sequence names and import sequences in a haploid (default) or diploid population (if there are even number of sequences). An list of allele names are required to translate symbols to allele names. This format accepts the following parameters:

alleleNames: Names of alleles 0, 1, 2, ... as a single string (e.g. 'ACTG') or a list of single-character strings (e.g. ['A', 'C', 'T', 'G']). This will be used to translate symbols into numeric alleles in simuPOP. Allele names will continue to be used as allele names of the returned population.

*ploidy:* Ploidy of the returned population, default to 1 (haploid). There should be even number of sequences if ploidy=2 (haploid) is specified.

MS (output from Richard R. Hudson's MS or msHOT program). The ms program generates npop blocks of nseq haploid chromosomes for command starting with ms nsample nrepeat. By default, the result is imported as a haploid population of size nsample. The population will have nrepeat subpopulations each with the same number of loci but different number of segregating sites. This behavior could be changed by the following parameters:

*ploidy:* If ploidy is set to 2, the sequenences will be paired so the population will have nseq/2 individuals. An error will be raised if an odd number of sequences are simulated.

mergeBy: By default, replicate samples will be presented as subpopulations. All individuals have the same number of loci but individuals in different subpopulations have different segregating sites. If mergeBy is set to "chrom", the replicates will be presented as separate chromosomes, each with a different set of loci determined by segregating sites.

# 3.2.10 Function export

export(pop, format, \*args, \*\*kwargs)

Apply operator Exporter to population *pop* in format *format*.

# 3.3 Module simuPOP.demography

This module provides some commonly used demographic models. In addition to several migration rate generation functions, it provides models that encapsulate complete demographic features of one or more populations (population growth, split, bottleneck, admixture, migration). These models provides:

- 1. The model itself can be passed to parameter subPopSize of a mating scheme to determine the size of the next generation. More importantly, it performs necessary actions of population size change when needed.
- 2. The model provides attribute num\_gens, which can be passed to parameter gens of Simulator.evolve or Population.evolve function. A demographic model can also terminate an evolutionary process by returnning an empty list so gens=model.num\_gens is no longer required.

# 3.3.1 Function migrIslandRates

```
migrIslandRates(r, n)
migration rate matrix

x m/(n-1) m/(n-1) ....
m/(n-1) x ......
....
....
m/(n-1) m/(n-1) x
where x = 1-m
```

# 3.3.2 Function migrHierarchicalIslandRates

#### 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.

# 3.3.3 Function migrSteppingStoneRates

```
migrSteppingStoneRates(r, n, circular=False)
```

migration rate matrix for circular stepping stone model (X=1-m)

or non-circular

This function returns [[1]] when there is only one subpopulation.

# 3.3.4 Function migrtwoDSteppingStoneRates

migr2DSteppingStoneRates(r, m, n, diagonal=False, circular=False)

migration rate matrix for 2D stepping stone model, with or without diagonal neighbors (4 or 8 neighbors for central patches). The boundaries are connected if circular is True. Otherwise individuals from corner and bounary patches will migrate to their neighbors with higher probability.

# 3.3.5 Class BaseDemographicModel

This class is the base class for all demographic models and provides common interface and utility functions for derived classes. A demographic model is essentially a callable Python object that encapsulates required functions of a demographic model, to determine initial population size (Population(size=model.init\_size, infoFields=model.info\_fields), to determine size of offspring population during evolution (subPopSize=model of a mating scheme), and number of generations to evolve (gen=model.num\_gens), although the first and last utility could be relaxed to for models that could be applied to populations with different sizes, and models that evolve indefinitely.

```
class BaseDemographicModel(numGens=-1, initSize=[], ops=[], infoFields=[])
```

Set attributes init\_size, info\_fields, and num\_gens to a demographic model. The initial population will be merged or split to match initSize. For example, N0=[A, [B,C]] is a 3-subpop model where the last two subpopulation will be split (and resize if needed) from the second subpopulation of the initial subpopulation (which should have two subpopulations). The population size can be an integer for fixed population size, None for the size of the population or subpopulation when the demographic model is first applied to, or a float number representing the proportion (can be larger than 1) of individuals for the whole or corresponding subpopulation. A None value will be assigned to attribute init\_size in such a case because the initial population size is determined dynamically. In addition, whenever a population size is allowed, a tuple of (size, name) is acceptable, which assigns name to the corresponding subpopulation. numGens can be a non-negative number or -1, which allows the demographic model to be determinated by a terminator. One or more operators (e.g. a migration operator or a terminator) could be passed (parameter ops) and will be applied to the population. The demographic model will return [] (which will effectively terminate the evolutioonary process) if any of the operator returns False. Information fields required by these operators should be passed to infoFields.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

#### 3.3.6 Class InstantChangeModel

A model for instant population change (growth, resize, merge, split).

class InstantChangeModel(T=None, N0=[], G=[], NG=[], ops=[], infoFields=[], removeEmptySubPops=False)

An instant population growth model that evolves a population from size N0 to NT for T generations with population

size changes at generation G to NT. If G is a list, multiple population size changes are allowed. In that case, a list (or a nested list) of population size should be provided to parameter NT. Both NO and NT supports fixed (an integer), dynamic (keep passed poulation size) and proportional (an float number) population size. Optionally, one or more operators (e.g. a migrator) ops can be applied to population. Required information fields by these operators should be passed to parameter infoFields. If removeEmpty option is set to True, empty subpopulation will be removed. This option can be used to remove subpopulations.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

# 3.3.7 Class ExponentialGrowthModel

A model for exponential population growth with carry capacity

```
class ExponentialGrowthModel(T=None, NO=[], NT=None, r=None, ops=[], infoFields=[])
```

An exponential population growth model that evolves a population from size N0 to NT for T generations with r\*N(t) individuals added at each generation. N0, NT and r can be a list of population sizes or growth rates for multiple subpopulations. The initial population will be resized to N0 (split if necessary). Zero or negative growth rates are allowed. The model will automatically determine T, r or NT if one of them is unspecified. If all of them are specified, NT is interpretted as carrying capacity of the model, namely the population will keep contant after it reaches size NT. Optionally, one or more operators (e.g. a migrator) ops can be applied to population.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

# 3.3.8 Class LinearGrowthModel

A model for linear population growth with carry capacity.

```
class LinearGrowthModel(T=None, NO=[], NT=None, r=None, ops=[], infoFields=[])
```

An linear population growth model that evolves a population from size N0 to NT for T generations with r\*N0 individuals added at each generation. N0, NT and r can be a list of population sizes or growth rates for multiple subpopulations. The initial population will be resized to N0 (split if necessary). Zero or negative growth rates are allowed. The model will automatically determine T, r or NT if one of them is unspecified. If all of them are specified, NT is intepretted as carrying capacity of the model, namely the population will keep contant after it reaches size NT. Optionally, one or more operators (e.g. a migrator) ops can be applied to population.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

## 3.3.9 Class MultiStageModel

A multi-stage demographic model that connects a number of demographic models.

```
class MultiStageModel(models, ops=[], infoFields=[])
```

An multi-stage demographic model that connects specified demographic models models. It applies a model to the population until it reaches num\_gens of the model, or if the model returns []. One or more operators could be specified, which will be applied before a demographic model is applied. Note that the last model will be ignored if it lasts 0 generation.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

#### 3.3.10 Class OutOfAfricaModel

A dempgrahic model for the CHB, CEU, and YRI populations, as defined in Gutenkunst 2009, Plos Genetics. The model is depicted in Figure 2, and the default parameters are listed in Table 1 of this paper.

Counting **backward in time**, this model evolves a population for T0 generations (required parameter). The ancient population A started at size N\_A and expanded at T\_AF generations from now, to pop AF with size N\_AF. Pop B split from pop AF at T\_B generations from now, with size N\_B; Pop AF remains as N\_AF individuals. Pop EU and AS split from pop B at T\_EU\_AS generations from now; with size N\_EU0 individuals and N\_ASO individuals, respectively. Pop EU grew exponentially with rate r\_BU; Pop AS grew exponentially with rate r\_AS. The YRI, CEU and CHB samples are drawn from AF, EU and AS populations respectively. Additional operators could be added to ops. Information fields required by these operators should be passed to infoFields. If a scaling factor scale is specified, all population sizes and generation numbers will be divided by a factor of scale.

This model merges all subpopulations if it is applied to a population with multiple subpopulation.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

# 3.3.11 Class SettlementOfNewWorldModel

A dempgrahic model for settlement of the new world of Americans, as defined in Gutenkunst 2009, Plos Genetics. The model is depicted in Figure 3, and the default parameters are listed in Table 2 of this paper.

Counting **backward in time**, this model evolves a population for T0 generations. The ancient population A started at size N\_A and expanded at T\_AF generations from now, to pop AF with size N\_AF. Pop B split from pop AF at T\_B generations from now, with size N\_B; Pop AF remains as N\_AF individuals. Pop EU and AS split from pop B at T\_EU\_AS generations from now; with size N\_EU0 individuals and N\_ASO individuals, respectively. Pop EU grew exponentially with final population size N\_EU; Pop AS grew exponentially with final population size N\_AS. Pop MX split from pop AS at T\_MX generations from now with size N\_MX0, grew exponentially to final size N\_MX. Migrations are allowed between populations with migration rates m\_AF\_B, m\_EU\_AS, m\_AF\_EU, and m\_AF\_AS. At the end of the evolution, the AF and CHB populations are removed, and the EU and MX populations are merged with f\_MX proportion for MX. The Mexican American<F19> sample could be sampled from the last single population. Additional operators could be added to ops. Information fields required by these operators should be passed to infoFields. If a scaling factor scale is specified, all population sizes and generation numbers will be divided by a factor of scale. This demographic model by default only returns the mixed Mexican America model (outputcom='MXL') but you can specify any combination of AF, EU, AS, MX and MXL.

This model merges all subpopulations if it is applied to a population with multiple subpopulation.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic models that works for particular mating schemes (e.g. genotype dependent).

#### 3.3.12 Class CosiModel

A dempgrahic model for Africa, Asia and Europe, as described in Schaffner et al, Genome Research, 2005, and implemented in the coalescent simulator cosi.

```
 \begin{array}{l} \textbf{class CosiModel} (T0, \, N\_A = 12500, \, N\_AF = 24000, \, N\_OoA = 7700, \, N\_AF1 = 100000, \, N\_AS1 = 100000, \, N\_EU1 = 100000, \\ T\_AF = 17000, \, T\_OoA = 3500, \, T\_EU\_AS = 2000, \, T\_AS\_exp = 400, \, T\_EU\_exp = 350, \, T\_AF\_exp = 200, \\ F\_OoA = 0.085, \, F\_AS = 0.067, \, F\_EU = 0.02, \, F\_AF = 0.02, \, m\_AF\_EU = 3.2e - 05, \, m\_AF\_AS = 8e - 06, \\ ops = [], \, infoFields = [], \, scale = 1) \end{array}
```

Counting **backward in time**, this model evolves a population for a total of T0 generations. The ancient population Ancestral started at size N\_Ancestral and expanded at T\_AF generations from now, to pop AF with size N\_AF. The Out of Africa population split from the AF population at T\_00A generations ago. The 00A population split into two subpopulations AS and EU but keep the same size. At the generations of T\_EU\_exp, T\_AS\_exp, and T\_AF\_exp ago, three populations expanded to modern population sizes of N\_AF1, N\_AS1 and N\_EU1 exponentially, respectively. Migrations are allowed between AF and EU populations with rate m\_AF\_EU, and between AF and AS with rate m\_AF\_AS.

Four bottlenecks happens in the AF, 00A, EU and AS populations. They are supposed to happen 200 generations after population split and last for 200 generations. The intensity is parameterized in F, which is number of generations devided by twice the effective size during bottleneck. So the bottleneck size is 100/F.

This model merges all subpopulations if it is applied to a population with multiple subpopulation. Although parameters are configurable, we assume the order of events so dramatically changes of parameters might need to errors. If a scaling factor scale is specified, all population sizes and generation numbers will be divided by, and migration rates will be multiplied by a factor of scale.

```
plot(filename=", title=", initSize=[])
```

Evolve a haploid population using a RandomSelection mating scheme using the demographic model. Print population size changes duringe evolution. An initial population size could be specified using parameter initSize for a demographic model with dynamic initial population size. If a filename is specified and if matplotlib is available, this function draws a figure to depict the demographic model and save it to filename. An optional title could be specified to the figure. Note that this function can not be plot demographic

# 3.4 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) or matplotlib. Note that rpy2, the successor of rpy, is currently not supported. You can specify the plotting library using simuOpt.setOptions(plotter='matplotlib').

Each operator calls a sequence of R or matplotlib 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 if rpy is used. The help message of each class will describe which and in what sequence these R or matplotlib functions are called to help you figure out which parameters are allowed.

#### 3.4.1 Function newDevice

#### newDevice()

Create a new graphics window and return its device number in R. This function essentially calls getOption('device')() in R.

# 3.4.2 Function saveFigure

#### 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.

#### 3.4.3 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 seperated to subplots by replicates (byRep), by each dimention 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).

If the rpy module is used (default if rpy if available), 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 opertor 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.

- - *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 evalulate 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 manipuation 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 for rpy or Axes object for matplotlib will be passed to this function.
- postHook: A function that, if given, will be called after the figure is drawn. The r object for rpy or Axes object for matplotlib will be passed to this function.
- plotHook: A function that, if given, will be called after each plot function. The r object from the rpy module or Figure object from the matplotlib 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 or matplotlib functions. These arguments could have prefixes (destination function names) plot\_, lines\_, par\_, legend\_ and dev\_print\_, and suffixes (list parameters) rep, dim, and repdim for the rpy option. 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.

#### 3.4.4 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 <code>subPops</code>, 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 <code>\_sp</code>. For example, if you have defined two VSPs by sex and set <code>subPops=[(0, 0), (0, 1)], col\_sp=['blue', 'red']</code> 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 opertor 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.

- *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 overriden 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 manipuation 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 or the Figure object from matplotlib 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 or the Figure object from matplotlib 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.

#### 3.4.5 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 differnt 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 opertor 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, begin=0, end=-1, step=1, at=[], reps=True, subPops=[], \*\*kwargs) func: Name of the R or matplotlib 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 overriden 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 manipuation of the figures outside of this operator.
- *preHook:* A function that, if given, will be called before the figure is draw. The r object for rpy will be passed to this function.
- postHook: A function that, if given, will be called after the figure is drawn. The r object for rpy will be passed to this function.
- plotHook: A function that, if given, will be called after each plot function. The r object from the rpy 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.

#### 3.4.6 Class HistPlotter

An InfoPlotter that uses function hist.

class HistPlotter(\*args, \*\*kwargs)

Returns an InfoPlotter that uses R function hist to draw histogram of individual information fields of specified (virtual) subpopulations. Please see InfoPlotter for details.

# 3.4.7 Class QQPlotter

An InfoPlotter that uses function qqnorm.

class QQPlotter(\*args, \*\*kwargs)

Returns an InfoPlotter that uses R function qqnorm to draw qq plot of individual information fields of specified (virtual) subpopulations. Please see InfoPlotter for details.

# 3.4.8 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 oraganized 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, \_ftd or \_spftd are expected to have multiple values which will be used for differnt 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\_ftd=[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 opertor calls R functions par, boxplot and dev.print. Keyword parameters without function prefix will be passed to boxplot.

- - 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 overriden 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 manipuation of the figures outside of this operator.
- *preHook:* A function that, if given, will be called before the figure is draw. The r object for rpy will be passed to this function.
- postHook: A function that, if given, will be called after the figure is drawn. The r object for rpy will be passed to this function.
- plotHook: A function that, if given, will be called after each plot function. The r object from the rpy 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.

# 3.5 Module simuPOP.sampling

This module provides classes and functions that could be used to draw samples from a simuPOP population. These functions accept a list of parameters such as subPops ((virtual) subpopulations from which samples will be drawn) and numOfSamples (number of samples to draw) and return a list of populations. Both independent individuals and dependent individuals (Pedigrees) are supported.

Independent individuals could be drawn from any Population. pedigree information is not necessary and is usually ignored. Unique IDs are not needed either although such IDs could help you identify samples in the parent Population.

Pedigrees could be drawn from multi-generational populations or age-structured populations. All individuals are required to have a unique ID (usually tracked by operator IdTagger and are stored in information field ind\_id). Parents of individuals are usually tracked by operator PedigreeTagger and are stored in information fields father\_id and mother\_id. If parental information is tracked using operator ParentsTagger and information fields father\_idx and mother\_idx, a function sampling.indexToID can be used to convert index based pedigree to ID based Pedigree. Note that ParentsTagger can not be used to track Pedigrees in age-structured populations because they require parents of each individual resides in a parental generation.

All sampling functions support virtual subpopulations through parameter subpops, although sample size specification might vary. This feature allows you to draw samples with specified properties. For example, you could select only female individuals for cases of a female-only disease, or select individuals within certain age-range. If you specify a list of (virtual) subpopulations, you are usually allowed to draw certain number of individuals from each subpopulation.

# 3.5.1 Class BaseSampler

A sampler extracts individuals from a simuPOP population and return them as separate populations. This base class defines the common interface of all sampling classes, including how samples prepared and returned.

```
class BaseSampler(subPops=ALL_AVAIL)
```

Create a sampler with parameter subPops, which will be used to prepare population for sampling. subPops should be a list of (virtual) subpopulations from which samples are drawn. The default value is ALL\_AVAIL, which means all available subpopulations of a Population.

```
drawSample(pop)
```

Draw and return a sample.

```
drawSamples(pop, numOfSamples)
```

Draw multiple samples and return a list of populations.

```
prepareSample(pop, rearrange)
```

Prepare passed population object for sampling according to parameter subPops. If samples are drawn from the whole population, a Population will be trimmed if only selected (virtual) subpopulations are used. If samples are drawn separately from specified subpopulations, Population pop will be rearranged (if rearrange==True) so that each subpoulation corresponds to one element in parameter subPops.

# 3.5.2 Class RandomSampler

A sampler that draws individuals randomly.

```
class RandomSampler(sizes, subPops=ALL_AVAIL)
```

Creates a random sampler with specified number of individuals.

```
drawSample(input_pop)
```

Draw a random sample from passed population.

```
drawSamples(pop, numOfSamples)
```

Draw multiple samples and return a list of populations.

#### prepareSample(pop, rearrange)

Prepare passed population object for sampling according to parameter subPops. If samples are drawn from the whole population, a Population will be trimmed if only selected (virtual) subpopulations are used. If samples are drawn separately from specified subpopulations, Population pop will be rearranged (if rearrange==True) so that each subpoulation corresponds to one element in parameter subPops.

# 3.5.3 Function drawRandomSample

#### drawRandomSample(pop, sizes, subPops=ALL AVAIL)

Draw sizes random individuals from a population. If a single sizes is given, individuals are drawn randomly from the whole population or from specified (virtual) subpopulations (parameter subPops). Otherwise, a list of numbers should be used to specify number of samples from each subpopulation, which can be all subpopulations if subPops=ALL\_AVAIL (default), or from each of the specified (virtual) subpopulations. This function returns a population with all extracted individuals.

# 3.5.4 Function drawRandomSamples

drawRandomSamples(pop, sizes, numOfSamples=1, subPops=ALL\_AVAIL)

Draw numOfSamples random samples from a population and return a list of populations. Please refer to function drawRandomSample for more details about parameters sizes and subPops.

# 3.5.5 Class CaseControlSampler

A sampler that draws affected and unaffected individuals randomly.

 ${\bf class} \ {\bf CaseControlSampler} (cases,\ controls,\ subPops=ALL\_AVAIL)$ 

Ceates a case-control sampler with specified number of cases and controls.

 ${\tt drawSample}(input\_pop)$ 

Draw a case control sample

drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

prepareSample(input\_pop)

Find out indexes all affected and unaffected individuales.

#### 3.5.6 Function drawCaseControlSample

## ${\tt drawCaseControlSample}(pop,\ cases,\ controls,\ subPops = ALL\_AVAIL)$

Draw a case-control samples from a population with cases affected and controls unaffected individuals. If single cases and controls are given, individuals are drawn randomly from the whole Population or from specified (virtual) subpopulations (parameter subPops). Otherwise, a list of numbers should be used to specify number of cases and controls from each subpopulation, which can be all subpopulations if subPops=ALL\_AVAIL (default), or from each of the specified (virtual) subpopulations. This function returns a population with all extracted individuals.

# 3.5.7 Function drawCaseControlSamples

 $\label{lem:caseControlSamples} {\it drawCaseControlSamples} (pop, \ cases, \ controls, \ numOfSamples = 1, \ subPops = ALL\_AVAIL)$ 

Draw num0fSamples case-control samples from a population with cases affected and controls unaffected individ-

uals and return a list of populations. Please refer to function drawCaseControlSample for a detailed descriptions of parameters.

## 3.5.8 Class PedigreeSampler

The base class of all pedigree based sampler.

class PedigreeSampler (families, subPops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', mother-Field='mother id')

Creates a pedigree sampler with parameters

families: number of families. This can be a number or a list of numbers. In the latter case, specified families are drawn from each subpopulation.

*subPops:* A list of (virtual) subpopulations from which samples are drawn. The default value is ALL\_AVAIL, which means all available subpopulations of a population.

drawSample(input\_pop)

Randomly select Pedigrees

drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

family(id)

Get the family of individual with id.

prepareSample(pop, loci=[], infoFields=[], ancGens=True)

Prepare self.pedigree, some pedigree sampler might need additional loci and information fields for this sampler.

#### 3.5.9 Class AffectedSibpairSampler

A sampler that draws a nuclear family with two affected offspring.

class AffectedSibpairSampler(families, subPops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', mother-Field='mother id')

Initialize an affected sibpair sampler.

drawSample(input\_pop)

Randomly select Pedigrees

drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

family(id)

Return id, its spouse and their children

prepareSample(input\_pop)

Find the father or all affected sibpair families

# 3.5.10 Function drawAffectedSibpairSample

drawAffectedSibpairSample(pop, families, subPops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', mother-Field='mother id')

Draw affected sibpair samples from a population. If a single families is given, affected sibpairs and their parents are drawn randomly from the whole population or from specified (virtual) subpopulations (parameter subPops). Otherwise, a list of numbers should be used to specify number of families from each subpopulation, which can

be all subpopulations if subPops=ALL\_AVAIL (default), or from each of the specified (virtual) subpopulations. This function returns a population that contains extracted individuals.

## 3.5.11 Function drawAffectedSibpairSamples

drawAffectedSibpairSamples(pop, families, numOfSamples=1, subPops=ALL\_AVAIL, idField='ind\_id', father-Field='father id', motherField='mother id')

Draw numOfSamples affected sibpair samples afrom population pop and return a list of populations. Please refer to function drawAffectedSibpairSample for a description of other parameters.

# 3.5.12 Class NuclearFamilySampler

A sampler that draws nuclear families with specified number of affected parents and offspring.

**class** NuclearFamilySampler(families, numOffspring, affectedParents=0, affectedOffspring=0, subPops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', motherField='mother\_id')

Creates a nuclear family sampler with parameters

families: number of families. This can be a number or a list of numbers. In the latter case, specified families are drawn from each subpopulation.

numOffspring: number of offspring. This can be a fixed number or a range [min, max].

affectedParents: number of affected parents. This can be a fixed number or a range [min, max].

affectedOffspring: number of affected offspring. This can be a fixed number of a range [min, max].

*subPops:* A list of (virtual) subpopulations from which samples are drawn. The default value is ALL\_AVAIL, which means all available subpopulations of a population.

drawSample(input\_pop)

Randomly select Pedigrees

drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

family(id

Return id, its spouse and their children

#### 3.5.13 Function drawNuclearFamilySample

drawNuclearFamilySample(pop, families, numOffspring, affectedParents=0, affectedOffspring=0, sub-Pops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', motherField='mother\_id')

Draw nuclear families from a population. Number of offspring, number of affected parents and number of affected offspring should be specified using parameters numOffspring, affectedParents and affectedOffspring, which can all be a single number, or a range [a, b] (b is incldued). If a single families is given, Pedigrees are drawn randomly from the whole population or from specified (virtual) subpopulations (parameter subPops). Otherwise, a list of numbers should be used to specify numbers of families from each subpopulation, which can be all subpopulations if subPops=ALL\_AVAIL (default), or from each of the specified (virtual) subpopulations. This function returns a population that contains extracted individuals.

#### 3.5.14 Function drawNuclearFamilySamples

drawNuclearFamilySamples(pop, families, numOffspring, affectedParents=0, affectedOffspring=0, numOfSamples=1, subPops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', mother-Field='mother id')

Draw numOfSamples affected sibpair samplesa from population pop and return a list of populations. Please refer to function drawNuclearFamilySample for a description of other parameters.

# 3.5.15 Class ThreeGenFamilySampler

A sampler that draws three-generation families with specified pedigree size and number of affected individuals.

class ThreeGenFamilySampler(families, numOffspring, pedSize, numOfAffected=0, subPops=ALL\_AVAIL, id-Field='ind id', fatherField='father id', motherField='mother id')

families: number of families. This can be a number or a list of numbers. In the latter case, specified families are drawn from each subpopulation.

numOffspring: number of offspring. This can be a fixed number or a range [min, max].

pedSize: number of individuals in the Pedigree. This can be a fixed number or a range [min, max].

numAfffected: number of affected individuals in the Pedigree. This can be a fixed number or a range [min, max]

*subPops:* A list of (virtual) subpopulations from which samples are drawn. The default value is ALL\_AVAIL, which means all available subpopulations of a population.

drawSample(input\_pop)

Randomly select Pedigrees

drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

family(id)

Return id, its spouse, their children, children's spouse and grandchildren

# 3.5.16 Function drawThreeGenFamilySample

drawThreeGenFamilySample(pop, families, numOffspring, pedSize, numOfAffected=0, subPops=ALL\_AVAIL, id-Field='ind\_id', fatherField='father\_id', motherField='mother\_id')

Draw three-generation families from a population. Such families consist of grant parents, their children, spouse of these children, and grand children. Number of offspring, total number of individuals, and total number of affected individuals in a pedigree should be specified using parameters numOffspring, pedSize and numOfAffected, which can all be a single number, or a range [a, b] (b is incldued). If a single families is given, Pedigrees are drawn randomly from the whole Population or from specified (virtual) subpopulations (parameter subPops). Otherwise, a list of numbers should be used to specify numbers of families from each subpopulation, which can be all subpopulations if subPops=ALL\_AVAIL (default), or from each of the specified (virtual) subpopulations. This function returns a population that contains extracted individuals.

# 3.5.17 Function drawThreeGenFamilySamples

drawThreeGenFamilySamples (pop, families, numOffspring, pedSize, numOfAffected=0, numOfSamples=1, sub-Pops=ALL\_AVAIL, idField='ind\_id', fatherField='father\_id', motherField='mother\_id')

Draw numOfSamples three-generation pedigree samples from population pop and return a list of populations. Please refer to function drawThreeGenFamilySample for a description of other parameters.

# 3.5.18 Class CombinedSampler

A combined sampler accepts a list of sampler objects, draw samples and combine the returned sample into a single population. An id field is required to use this sampler, which will be used to remove extra copies of individuals who have been drawn by different samplers.

```
class CombinedSampler(samplers=[], idField='ind_id')
    samplers: A list of samplers
```

#### drawSamples(pop, numOfSamples)

Draw multiple samples and return a list of populations.

#### prepareSample(pop, rearrange)

Prepare passed population object for sampling according to parameter subPops. If samples are drawn from the whole population, a Population will be trimmed if only selected (virtual) subpopulations are used. If samples are drawn separately from specified subpopulations, Population pop will be rearranged (if rearrange==True) so that each subpoulation corresponds to one element in parameter subPops.

## 3.5.19 Function drawCombinedSample

drawCombinedSample(pop, samplers, idField='ind\_id')

Draw different types of samples using a list of samplers. A Population consists of all individuals from these samples will be returned. An idField that stores an unique ID for all individuals is needed to remove duplicated individuals who are drawn multiple numOfSamples from these samplers.

## 3.5.20 Function drawCombinedSamples

 ${\tt drawCombinedSamples}(pop, samplers, numOfSamples=1, idField='ind\_id')$ 

Draw combined samples numOfSamples and return a list of populations. Please refer to function drawCombinedSample for details about parameters samplers and idField.

# 3.5.21 Function plotPedigree

A wrapper function that calls R to draw pedigree by outputting the pedigree to a format that is recognizable by R's kinship2 library. *ped* can be a population or a pedigree object, as long as there are valid *idField*, *fatherField* and *motherField* fields in the population. Aliased arguments could be used to pass parameters to functions pedigree, plot and par. Please refer to module simuPOP.plotter for details about aliased arguments. This function returns silently if rpy is not properly installed.

# 3.6 Module simuPOP.gsl

This module exposes the following GSL (GUN Scientific Library) functions used by simuPOP to the user interface. Although more functions may be added from time to time, this module is not intended to become a complete wrapper for GSL. Please refer to the GSL reference manual (http://www.gnu.org/software/gsl/manual/html\_node/) for details about these functions. Note that random number generation functions are wrapped into the simuPOP.RNG class.

- gsl\_cdf\_gaussian\_P(x, sigma)
- gsl\_cdf\_gaussian\_Q(x, sigma)
- qsl\_cdf\_qaussian\_Pinv(P, sigma)
- gsl\_cdf\_gaussian\_Qinv(Q, sigma)
- gsl\_cdf\_ugaussian\_P(x)
- gsl\_cdf\_ugaussian\_Q(x)
- qsl\_cdf\_ugaussian\_Pinv(P)

- gsl\_cdf\_ugaussian\_Qinv(Q)
- gsl\_cdf\_exponential\_P(x, mu)
- gsl\_cdf\_exponential\_Q(x, mu)
- gsl\_cdf\_exponential\_Pinv(P, mu)
- gsl\_cdf\_exponential\_Qinv(Q, mu)
- gsl\_cdf\_chisq\_P(x, nu)
- gsl\_cdf\_chisq\_Q(x, nu)
- gsl\_cdf\_chisq\_Pinv(P, nu)
- gsl\_cdf\_chisq\_Qinv(Q, nu)
- gsl\_cdf\_gamma\_P(x, a, b)
- gsl\_cdf\_gamma\_Q(x, a, b)
- gsl\_cdf\_gamma\_Pinv(P, a, b)
- gsl\_cdf\_gamma\_Qinv(Q, a, b)
- gsl\_ran\_gamma\_pdf(x, a, b)
- gsl\_cdf\_beta\_P(x, a, b)
- gsl\_cdf\_beta\_Q(x, a, b)
- gsl\_cdf\_beta\_Pinv(P, a, b)
- gsl\_cdf\_beta\_Qinv(Q, a, b)
- gsl\_ran\_beta\_pdf(x, a, b)
- gsl\_cdf\_binomial\_P(k, p, n)
- gsl\_cdf\_binomial\_Q(k, p, n)
- gsl\_ran\_binomial\_pdf(k, p, n)
- gsl\_cdf\_poisson\_P(k, mu)
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