simuPOP Reference Manual

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Abstract

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

simuPOP is written in C++ and is provided as Python modules. It provides a large number of building blocks (populations, mating schemes, various genetic forces in the form of operators, simulators and gene mapping methods) to construct a simulation. This provides a R/Splus or Matlab-like environment where users can interactively create, manipulate and evolve populations, monitor and visualize population statistics and apply gene mapping methods. Please refer to the *simuPOP user's guide* for a detailed introduction to simuPOP concepts, and a number of examples on how to use simuPOP to perform various simulations.

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

How to cite simuPOP:

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

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

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Chapter 1

simuPOP Components

1.1 Individual, population and simulator

1.1.1 Class GenoStruTrait

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

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

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

class GenoStruTrait()

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

ploidy()

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

ploidyName()

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

chromBegin (chrom)

Return the index of the first locus on chromosome *chrom*.

chromByName (name)

Return the index of a chromosome by its *name*.

chromEnd(chrom)

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

chromName (chrom)

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

chromNames()

Return a list of the names of all chromosomes.

chromType (chrom)

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

chromTypes()

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

numChrom()

Return the number of chromosomes.

absLocusIndex (chrom, locus)

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

chromLocusPair (locus)

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

lociByNames (names)

Return the indexes of loci with names names. Raise a ValueError if any of the loci cannot be found.

lociDist (loc1, loc2)

Return the distance between loci loc1 and loc2 on the same chromosome. A negative value will be returned if loc1 is after loc2.

lociNames()

Return the names of all loci specified by the *lociNames* parameter of the population function.

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.

locusName(loc)

Return the name of locus *loc* specified by the *lociNames* parameter of the population function. Default to locX-Y where X and Y are 1-based chromosome and locus indexes (loc1-1, loc1-2, ... etc)

locusPos(loc)

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

numLoci (chrom)

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

numLoci()

Return the number of loci on all chromosomes.

totNumLoci()

Return the total number of loci on all chromosomes.

alleleName(allele)

Return the name of allele *allele* specified by the *alleleNames* parameter of the population function. If the name of an allele is not specified, its index ('0', '1', '2', etc) is returned. An IndexError will be raised if *allele* is larger than the maximum allowed allele state of this module (MaxAllele()).

alleleNames()

Return a list of allele names given by the *alleleNames* parameter of the population function. This list does not have to cover all possible allele states of a population so alleleNames() [allele] might fail (use alleleNames (allele) instead).

infoField(idx)

Return the name of information field idx.

infoFields()

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

infoIdx (name)

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

1.1.2 Class individual

A population consists of individuals with the same genotypic structure. An individual object cannot be created independently, but 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, are not restricted.

class individual()

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

allele(idx)

Return the current allele at a locus, using its absolute index *idx*.

allele(idx, p)

Return the current allele at locus *idx* on the *p*-th set of homologous chromosomes.

allele(idx, p, chrom)

Return the current allele at locus *idx* on chromosome *chrom* of the *p*-th set of homologous chromosomes.

setAllele (allele, idx)

Set allele *allele* to a locus, using its absolute index *idx*.

setAllele (allele, idx, p)

Set allele *allele* to locus *idx* on the *p*-th homologous set of chromosomes.

setAllele (allele, idx, p, chrom)

Set allele *allele* to locus *idx* on chromosome *chrom* of the *p*-th homologous set of chromosomes.

genotype()

Return an editable array (a carray of length totNumLoci()*ploidy()) that represents all alleles of an individual.

genotype(p)

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

genotype (p, chrom)

Return an editable array (a carrary of legnth numLoci (*chrom*)) that represents all alleles on chromosome *chrom* of the *p*-th homologous set of chromosomes.

setGenotype (geno)

Fill the genotype of an individual using a list of alleles *geno*. geno will be reused if its length is less than totNumLoci()*ploidy().

setGenotype (geno, p)

Fill the genotype of the p-th homologous set of chromosomes using a list of alleles geno. geno will be reused if its length is less than totNumLoci().

setGenotype (geno, p, chrom)

Fill the genotype of chromosome *chrom* on the p-th homologous set of chromosomes using a list of alleles *geno*. geno will be reused if its length is less than mumLoci (*chrom*).

setSex (sex)

Set individual sex to Male or Female.

sex(

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

sexChar()

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

affected()

Return True if this individual is affected.

affectedChar()

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

setAffected (affected)

Set affection status to affected (True or False).

info(idx)

Return the value of an information field *idx* (an index).

info(name)

Return the value of an information field *name*.

intInfo(idx)

Return the value of an information field idx (an index) as an integer number.

intInfo(name)

Return the value of an information field *name* as an integer number.

setInfo(value, idx)

Set the value of an information field *idx* (an index) to *value*.

setInfo(value, name)

Set the value of an information field name to value.

1.1.3 Class population

A simuPOP population consists of individuals of the same genotypic structure, organized by generations, subpopulations and virtual subpopulations. It also contains a Python dictionary that is used to store arbitrary population variables. In addition to genotypic structured related functions provided by the genoStruTrait class, the population class provides a large number of member functions that can be used to

- Create, copy and compare populations.
- Manipulate subpopulations. A population can be divided into several subpopulations. Because individuals only
 mate with individuals within the same subpopulation, exchange of genetic information across subpopulations
 can only be done through migration. A number of functions are provided to access subpopulation structure
 information, and to merge and split subpopulations.
- Define and access virtual subpopulations. A virtual subpopulation splitter can be assigned to a population, which defines groups of individuals called virtual subpopulations (VSP) within each subpopulation.
- Access individuals individually, or through iterators that iterate through individuals in (virtual) subpopulations.
- Access genotype and information fields of individuals at the population level. From a population point of view, all genotypes are arranged sequentially individual by individual. Please refer to class individual for an introduction to genotype arrangement of each individual.
- Store and access ancestral generations. A population can save arbitrary number of ancestral generations. It is
 possible to directly access an ancestor, or make an ancestral generation the current generation for more efficient
 access.
- Insert or remove loci, resize (shrink or expand) a population, sample from a population, or merge with other populations.
- Manipulate population variables and evaluate expressions in this *local namespace*.
- Save and load a population.

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

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

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

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

- *lociPos:* Positions of all loci on all chromosome, as a list of float numbers. Default to 1, 2, ... etc on each chromosome. Positions on the same chromosome should be ordered. A nested list that specifies positions of loci on each chromosome is also acceptable.
- 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 chrom1, chrom2, ... etc.
- alleleNames: A list of allele names for all markers. For example, alleleNames = ('A', 'C', 'T', 'G') names allele 0 3'A', 'C', 'T', and 'G' respectively. Note that simuPOP does not yet support locus-specific allele names.
- *lociNames:* A list or a matrix (separated by chromosomes) of names for each locus. Default to "locX-Y" where X and Y are 1-based chromosome and locus indexes, respectively.
- subPopNames: A list of subpopulation names. All subpopulations will have name " if this parameter is not specified.
- infoFields: Names of information fields (named float number) that will be attached to each individual.

absIndIndex (idx, subPop)

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

numSubPop()

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

subPopBegin (subPop)

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

subPopEnd(subPop)

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

subPopIndPair(idx)

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

setSubPopName (name, subPop)

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

subPopByName (name)

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

subPopName (subPop)

Return the name of a subpopulation *subPop*, and 'unnamed' if no name is assigned to *subPop*. If *subPop* is a virtual subpopulation (specified by a (sp, vsp) pair), a combined name such as subPop1 - Male is returned.

subPopNames()

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

popSize()

Return the total number of individuals in all subpopulations.

subPopSize(subPop)

Return the size of a subpopulation (subPopSize(sp)) or a virtual subpopulation (subPopSize([sp, vsp])).

subPopSizes()

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

numVirtualSubPop()

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

setVirtualSplitter(splitter)

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

individual (idx)

Return a refernce to individual *ind* in the population.

individual (idx, subPop)

Return a refernce to individual ind in subpopulation subPop.

individuals()

Return a Python iterator that can be used to iterate through all individuals in a population.

individuals (subPop)

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

genotype()

Return an editable array of the genotype of all individuals in this population.

genotype (subPop)

Return an editable array of the genotype of all individuals in subpopulation *subPop*. Virtual subpopulation is unsupported.

setGenotype (geno)

Fill the genotype of all individuals of a population using a list of alleles *geno*. *geno* will be reused if its length is less than popSize()*totNumLoci()*ploidy().

setGenotype (geno, subPop)

Fill the genotype of all individuals of in (virtual) subpopulation *subPop* using a list of alleles *geno*. *geno* will be reused if its length is less than subPopSize(subPop) *totNumLoci()*ploidy().

ancestor(idx, gen)

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).

ancestor (ind, subPop, gen)

Return a reference to individual idx of subpopulation *subPop* in ancestral generation gen.

ancestralGens()

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

push (pop)

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

setAncestralDepth (depth)

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

useAncestralGen(idx)

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

addChrom(lociPos, lociNames=[], chromName="", 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. If they are not specified, simuPOP will try to assign default names, and raise a ValueError if the default names have been used.

addChromFrom(pop)

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

addIndFrom(pop)

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

addLoci (chrom, pos, names=[])

Insert loci *names* at positions *pos* on chromosome *chrom*. These parameters should be lists of the same length, although *names* may be ignored, in which case random names will be given. 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. This function returns indexes of the inserted loci.

addLociFrom(pop)

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

extract (field=None, loci=None, infoFields=None, ancGen=-1)

Extract subsets of individuals, loci and/or information fields from the current population and create a new one. If information field field is not None, individuals with negative values at this information field will be removed, and others are put into subpopulations specified by this field. If loci is not None, only genotypes at loci are extracted. If infoFields is not None, only these information fields will be extracted. If ancGen is not -1 (default, meaing all ancestral generations), only ancGen ancestral generations will be kept. As an advanced feature, field can be information field of a pedigree object ped. This allows extraction of individuals according to pedigrees identified in a pedigree object. This pedigree should have the same number of individuals in all generations.

mergeSubPops (subPops=[])

Merge subpopulations *subPops*. If *subPops* is empty (default), all subpopulations will be merged. *subPops* do not have to be adjacent to each other. They will all be merged to the subpopulation with the smallest subpopulation ID. Indexes of the rest of the subpopulation may be changed.

removeIndividuals (inds)

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

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

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

removeSubPops (subPops)

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

resize (newSubPopSizes, propagate=False)

Resize population by giving new subpopulation sizes *newSubPopSizes*. Individuals at the end of some subpopulations will be removed if the new subpopulation size is smaller than the old one. New individuals will be appended to a subpopulation if the new size is larger. Their genotypes will be set to zero (default), or be copied from existing individuals if *propagate* is set to True. More specifically, if a subpopulation with 3 individuals is expanded to 7, the added individuals will copy genotypes from individual 1, 2, 3, and 1 respectively. Note that this function only resizes the current generation.

setSubPopByIndInfo(field)

Rearrange individuals to their new subpopulations according to their integer values at information field *field* (value returned by individual::indInfo(field)). Individuals with negative values at this *field* will be removed. Existing subpopulation names are unchanged but new subpopulations will not assign a name ('unnamed').

splitSubPop (subPop, sizes)

Split subpopulation *subPop* into subpopulations of given *sizes*, which should add up to the size of subpopulation *subPop*. Alternatively, *sizes* can be a list of proportions (add up to 1) from which the sizes of new subpopulations are determined. 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 split subpopulations.

addInfoField (field, init=0)

Add an information field *field* to a population and initialize its values to *init*.

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.

indInfo(idx)

Return the information field idx (an index) of all individuals as a list.

indInfo(name)

Return the information field name of all individuals as a list.

indInfo(idx, subPop)

Return the information field idx (an index) of all individuals in (virtual) subpopulation subPop as a list.

indInfo(name, subPop)

Return the information field name of all individuals in (virtual) subpopulation subPop as a list.

setIndInfo(values, idx)

Set information field idx (an index) of the current population to *values*. *values* will be reused if its length is smaller than popSize().

setIndInfo(values, name)

Set information field name of the current population to values. values will be reused if its length is smaller than popSize ().

setIndInfo(values, idx, subPop)

Set information field idx (an index) of a subpopulation (subPop=sp) or a virtual subpopulation (subPop=[sp, vsp]) to values. values will be reused if its length is smaller than subPopSize(subPop).

setIndInfo(values, name, subPop)

Set information field name of a subpopulation (subPop=sp) or a virtual subpopulation (subPop=[sp, vsp]) to values. values will be reused if its length is smaller than subPopSize (subPop).

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

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

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

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

clone()

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

save (filename)

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

vars()

Return variables of a population as a Python dictionary.

vars (subPop)

Return a dictionary vars () ["subPop"] [subPop]. subPop can be a number (subPop=spID), or a pair of numbers (subPop=(spID, vspID)). A ValueError will be raised if key 'subPop' does not exist in vars (), or if key subPop does not exist in vars () ["subPop"].

dvars()

Return a wrapper of Python dictionary returned by vars() so that dictionary keys can be accessed as attributes. For example pop.dvars().alleleFreq is equivalent to pop.vars()["alleleFreq"].

dvars (subPop)

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

1.1.4 Class simulator

A simuPOP simulator is responsible for evolving one or more replicates of a *population* forward in time, subject to various *operators*. Populations in a simulator are created as identical copies of a population and will become different after evolution. A *mating scheme* needs to be specified, which will be used to generate offspring generations during evolution. A number of functions are provided to access simulator properties, access populations and their variables, copy, save and load a simulator.

The most important member function of a simulator is evolve, which evolves populations forward in time, subject to various *operators*. Because populations in a simulator have to keep the same genotypic structure, several functions are provided to change ancestral depth and information fields of all populations. These functions cannot be replaced by similar calls to all populations in a simulator because the genotypic structure of the simulator itself needs to be updated.

class simulator (pop, matingScheme, rep=1)

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

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.

save (filename)

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

gen()

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

setGen (gen)

Set the current generation number of a simulator to gen.

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

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

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

Parameter *gen* can be set to a positive number, which is the number of generations to evolve. If *gen* is negative (default), the evolution will continue indefinitely, until all replicates are stopped by a special kind of operators called *terminators*. At the end of the evolution, the generations that each replicates have evolved are returned.

extract (rep)

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

numRep()

Return the number of replicates.

population (rep)

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

populations()

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

addInfoField (field, init=0)

Add an information field *field* to all populations in a simulator, and update the genotypic structure of the simulator itself. The information field will be initialized by value *init*.

addInfoFields (fields, init=0)

Add information fields *fields* to all populations in a simulator, and update the genotypic structure of the simulator itself. The information field will be initialized by value *init*.

setAncestralDepth(depth)

Set ancestral depth of all populations in a simulator.

setMatingScheme (matingScheme)

Set a new mating scheme matingScheme to a simulator.

vars (rep)

Return the local namespace of the *rep-th* population, equivalent to x.population(rep). vars().

vars (rep, subPop)

Return a dictionary of subpopulation variables in the local namespace of the rep-th population, equivalent to x.population(rep).vars(subPop).

dvars (rep)

Return a wrapper of Python dictionary returned by vars(rep) so that dictionary keys can be accessed as attributes. For example simu.dvars(1).alleleFreq is equivalent to simu.vars(1)["alleleFreq"].

dvars (rep, subPop)

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

1.1.5 Class pedigree

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

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

class pedigree (pop, loci=[], infoFields=[], ancGen=-1, parentFields=["father_idx", "mother_idx"])

Create a pedigree object from a population, using a subset of loci (parameter *loci*, default to no loci), information fields (parameter *infoFields*, default to no information field), and ancestral generations (parameter *ancGen*, default to all ancestral generations). By default, information field father_idx and mother_idx will be used to locate parents. If individuals in a pedigree has only one parent, one of *fatherField* and *motherField* should be set to an empty string.

father (idx, subPop)

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

mother (idx, subPop)

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

locateRelatives (relType, relFields, gen=-1, relSex=AnySex, parentFields=[])

This function locates relatives (of type <code>relType</code>, and sex <code>relSex</code>) of each individual and store their indexes in specified information fields <code>relFields</code>. The indexes of parents in the parental generation should be available in information fields <code>parentFields</code> (default to <code>['father_idx', 'mother_idx']</code> which are the information fields used by operator <code>parentsTagger</code>. This function currently only work for diploid populations.

relType: Relative type, which can be

- •Self set indexes of individual themselves.
- •Spouse locate spouses of individuals in the current generation. A spouse is defined as two individuals having an offspring with shared parentFields. If more than one infoFields is given, multiple spouses can be identified.
- •Offspring index of offspring in the offspring generation. If only one parent is given, only paternal or maternal relationship is considered. For example, parentFields=['father_idx'] will locate offspring for all fathers.

- •FullSibling all siblings with the same parents
- •Sibling all sibs with at least one shared parent

relFields: Information fields to hold relatives. The number of these fields limits the number of relatives to locate.

gen: Find relatives for individuals for how many generations. Default to -1, meaning for all generations. If a non-negative number is given, up till generation gen will be processed.

relSex: Whether or not only locate relative or certain sex. It can be AnySex (do not care, default), Male-Only, FemaleOnly, or OppositeSex (only locate relatives of opposite sex.

setIndexesOfRelatives (pathGen, pathFields, pathSex=[], resultFields=[])

```
Trace a relative path in a population and record the result in the given information fields. For example, setInfoWithRelatives(pathGen = [0, 1, 1, 0], pathFields = [['father_idx', 'mother_idx'], ['sib1', 'sib2'], ['off1', 'off2']], pathSex = [AnySex, MaleOnly, FemaleOnly], resultFields = ['cousin1', 'cousin2']) This function will 1. locate father_idx and mother_idx for each individual at generation 0 (pathGen[0]) 2. find AnySex individuals referred by father_idx and mother_idx at generation 1 (pathGen[1]) 3. find information fields sib1 and sib2 from these parents 4. locate MaleOnly individuals referred by sib1 and sib2 from generation 1 (pathGen[2]) 5. find information fields off1 and off2 from these individuals, and 6. locate FemaleOnly individuals referred by off1 and from geneartion 0 (pathGen[3]) 7. Save index of these individuals to information fields cousin1 and cousin2 at genearation pathGen[0]. In short, this function locates father or mother's brother's daughters.
```

pathGen: A list of generations that form a relative path. This array is one element longer than pathFields, with gen_i, gen_i+1 indicating the current and destinating generation of information fields path_i.

pathFields: A list of list of information fields forming a path to trace a certain type of relative.

resultFields: Where to store located relatives. Note that the result will be saved in the starting generation specified in pathGen[0], which is usually 0.

pathSex: (Optional) A list of sex choices, AnySex, Male, Female or OppositeSex, that is used to choose individuals at each step. Default to AnySex.

1.2 Virtual subpopulation splitters

1.2.1 Class vspSplitter

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

```
class vspSplitter()
```

This is a virtual class that cannot be instantiated.

```
clone()
```

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

name(vsp)

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

numVirtualSubPop()

Return the number of VSPs defined by this splitter.

1.2.2 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()
    Create a sex splitter that defines male and female VSPs.
    name (vsp)
        Return "Male" if vsp=0 and "Female" otherwise.
    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.

```
class affectionSplitter()
    Create a splitter that defined two VSPs by affection status.
name(vsp)
    Return "Unaffected" if vsp=0 and "Affected" if vsp=1.
numVirtualSubPop()
    Return 2.
```

1.2.4 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=[])
```

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 = 1 is the value of an individual at information field *field*. Of course, only one of the parameters *values* and *cutoff* should be defined, values in *cutoff* should be distinct, and in an increasing order.

```
name (vsp)
```

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

```
numVirtualSubPop()
```

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

1.2.5 Class proportionSplitter

This splitter divides subpopulations into several VSPs by proportion.

class proportionSplitter (proportions=[])

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

name(vsp)

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

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)

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

name(vsp)

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

numVirtualSubPop()

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

1.2.7 Class genotypeSplitter

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

class genotypeSplitter (loci, alleles, phase=False)

Create a splitter that defines VSPs by individual genotype at *loci* (a locus index or a list of loci indexes). Each list in a list *allele* defines a VSP, which is a list of allowed alleles at these *loci*. If only one VSP is defined, the outer list of the nested list can be ignored. If phase 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] 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.

$\mathbf{name}\ (vsp)$

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

numVirtualSubPop()

Number of virtual subpops of subpopulation sp

1.2.8 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. This splitter is usually used to define different types of VSPs to a population.

class combinedSplitter (splitters=[])

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

name(vsp)

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

numVirtualSubPop()

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

1.3 Basic Mating Schemes

1.3.1 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=uintListFunc, subPop=[], weight=0)

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

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

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

clone()

Deep copy of a homogeneous mating scheme.

1.3.2 Class heteroMating

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

class heteroMating (matingSchemes, subPopSize=uintListFunc, shuffleOffspring=True)

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

Each mating scheme defined in *matingSchemes* should specify which (virtual) subpopulation it is applied to (parameter *subPop*), and optionally a weight (parameter *weight*) to determine how many offspring it will produce, if multiple mating schemes are applied to the same subpopulation.

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.

clone()

Deep copy of a heterogeneous mating scheme

1.3.3 Class pedigreeMating

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

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

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

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

clone()

Deep copy of a Python mating scheme

1.4 Parent Choosers and Offspring generators

1.4.1 Class sequentialParentChooser

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

class sequentialParentChooser()

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

clone()

Deep copy of a sequential parent chooser.

1.4.2 Class sequentialParentsChooser

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

class sequentialParentsChooser()

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

clone()

Deep copy of a sequential parents chooser.

1.4.3 Class randomParentChooser

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

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

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

clone()

Deep copy of a random parent chooser.

1.4.4 Class randomParentsChooser

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

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

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

clone()

Deep copy of a random parents chooser.

1.4.5 Class polyParentsChooser

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

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

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

clone()

Deep copy of a parent chooser.

1.4.6 Class alphaParentsChooser

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

${\bf class\ alphaParentsChooser}\ (alphaSex=Male,\ alphaNum=0,\ alphaField=string,\ selectionField="fitness")$

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

clone()

Deep copy of an alpha parents chooser.

1.4.7 Class infoParentsChooser

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

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

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

${\bf class\ infoParentsChooser}\ (infoFields=[], func=None,\ param=None,\ selectionField="fitness")$

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

clone()

Deep copy of a infomation parent chooser.

1.4.8 Class pyParentsChooser

This parents chooser accept a Python generator function that repeatedly yields an index (relative to each subpopulation)

of a parent, or indexes of two parents as a Python list of tuple. The parent chooser calls the generator function with parental population and a subpopulation index for each subpopulation and retrieves indexes of parents repeatedly using the iterator interface of the generator function.

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

class pyParentsChooser (parentsGenerator)

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

clone()

Deep copy of a python parent chooser.

1.4.9 Class offspringGenerator

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

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

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

A number of *genotype transmitters* can be used to transmit genotype from parents to offspring. Additional during-mating operators can be passed from the evolve() function of a *simulator*, but the *ops* operators will be applied before them. An exception is that if one of the passed operators is set to form offspring genotype (a flag setOffGenotype), operators in *ops* with the same flag will not be applied. For example, a recombinator will override a mendelianGenoTransmitter used in randomMating if it is used in the ops parameter of the evolve function. This general offspring generator does not use any genotype transmitter. A number of derived offspring generators are available with a default transmitter. For example, a mendelianOffspringGenerator uses a mendelianGenoTransmitter to transmit genotypes.

Parameter *numOffspring* is used to control the number of offspring per mating event, or in another word the number of offspring in each family. It can be a number, a function, or a mode parameter followed by some optional arguments. If a number is given, given number of offspring will be generated at each mating event. If a Python function is given, it will be called each time when a mating event happens. Current generation number will be passed to this function, and its return value will be considered the number of offspring. In the last case, a tuple (or a list) in one of the following forms: (GeometricDistribution, p), (PoissonDistribution, p), (BinomialDistribution, p, N), or (UniformDistribution, a, b) can be given. The number of offspring will be determined randomly following these statistical distributions. Please refer to the simuPOP user's guide for a detailed description of these distribution and their parameters.

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

clone (

Make a deep copy of this offspring generator.

1.4.10 Class controlledOffspringGenerator

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

Create an offspring generator that selects offspring so that allele frequency at specified loci in the offspring generation reaches specified allele frequency. At the beginning of each generation, expected allele frequency of *alleles* at *loci* is returned from a user-defined trajectory function *freqFunc*. If there are multiple subpopulations, *freqFunc* can return a list of allele frequencies for each subpopulation, or a list of allele frequencies in the whole population. 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 multi-nomial 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*.

clone()

Deep copy of a controlled random mating scheme.

mendelianOffspringGenerator(ops=[], *args, **kwargs)

An offspring generator that uses mendelianGenoTransmitter()

1.5 Pre-defined Mating schemes

randomMating (numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0)
A mating scheme of basic sexually random mating

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

 $\verb"randomSelection" (numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0) \\$

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

Unexpected indentation.

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

monogamousMating (numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0)

This mating scheme is identical to random mating except that parents are chosen without replacement. Under this mating scheme, offspring share the same mother must share the same father. In case that all parental pairs are exhausted, parameter c replenish=True allows for the replenishment of one or both sex groups.

 $\label{eq:polygamousMating} \begin{aligned} & \text{polySex=1, polyNum=1, numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], sub-Pop=(), weight=0)} \end{aligned}$

This mating scheme is composed of a random parents chooser that allows for polygamous mating, and a mendelian offspring generator. In this mating scheme, a male (or female) parent will have more than one sex partner (c numPartner). Parents returned from this parents chooser will yield the same male (or female) parents, each with varying partners.

- $\textbf{alphaMating} (alphaSex=1, \ alphaNum=0, \ alphaField=", \ numOffspring=1.0, \ sexMode=31, \ ops=[], \ subPop-Size=[], \ subPop=(), \ weight=0)$
- $\label{local_post_problem} \begin{tabular}{ll} haplodiploidMating (replacement=True, numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], sub-Pop=(), weight=0) \end{tabular}$

This mating scheme is composed of an alphaParentsChooser and a haplodiploidOffspringGenerator. The alphaParentChooser chooses a single Female randomly or from a given information field. This female will mate with random males from the colony. The offspring will have one of the two copies of chromosomes from the female parent, and the first copy of chromosomes from the male parent. Note that if a recombinator is used, it should disable recombination of male parent.

Chapter 2

Operator References

2.1 Common interface of 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 subpopulation an operator will be 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), or a filename prefixed by one or more '>' characters. 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 write 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.

class baseOperator (output, outputExpr, stage, begin, end, step, at, rep, subPop, 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), or 'filename' prefixed by one or more '>'.

outputExpr: An expression that determines the output parameter dynamically. This expression will be evaluated against a population's local namespace each time when an output filename is required. For example, "'>>out%s_%s.xml' % (gen, rep) " will output to >>out10_1.xml for replicate 1 at generation 10.

- stage: Stage(s) of a life cycle at which an operator will be applied. It can be PreMating, DuringMating, PostMating and any of their combined stages PrePostMating, PreDuringMatingDuringPostMating and PreDuringPostMating. Note that all operators have their default stage parameter and some of them ignores this parameter because they can only be applied at certain stage(s) of a life cycle.
- *begin:* The starting generation at which an operator will be applied. Default to 0. A negative number is interpreted as a generation counted from the end of an evolution (-1 being the last evolved generation).
- end: The last generation at which an operator will be applied. Default to -1, namely the last generation.
- step: The number of generations between applicable generations. Default to 1.
- at: A list of applicable generations. Parameters begin, end, and step will be ignored if this parameter is specified.
- rep: A list of applicable replicates. An empty list (default) 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].
- subPop: A list of applicable (virtual) subpopulations, such as subPop=[sp1, sp2, (sp2, vsp1)]. An empty list (default) is interpreted as all subpopulations. subPop=[sp1] can be simplied as subPop=sp1. Negative indexes are not supported. Suport for this parameter vary from operator to operator. Some operators do not support virtual subpopulations and some operators do not support this parameter 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.

initialize(pop)

FIXME: No document

2.2 During-mating genotype transmitters

2.2.1 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.

```
class cloneGenoTransmitter (begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[]) Create a cloneGenoTransmitter.
```

clone()

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

2.2.2 Class mendelianGenoTransmitter

Mendelian offspring generator accepts two parents and pass their genotype to a number of offspring following Mendelian's law. Basically, one of the paternal chromosomes is chosen randomly to form the paternal copy of the offspring, and one of the maternal chromosome is chosen randomly to form the maternal copy of the offspring. The number of offspring produced is controlled by parameters numOffspring, numOffspringFunc, maxNumOffspring and mode. Recombination will not happen unless a during-mating operator recombinator is used.

```
class mendelianGenoTransmitter (begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[])
    FIXME: No document
    clone()
        Return a cloned copy of an operator. This function is available to all operators.
    initialize(pop)
        FIXME: No document
    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.

2.2.3 Class selfingGenoTransmitter

Selfing offspring generator works similarly as a mendelian offspring generator but a single parent produces both the paternal and maternal copy of the offspring chromosomes. This offspring generator accepts a dipload parent. A random copy of the parental chromosomes is chosen randomly to form the parental copy of the offspring chromosome, and is chosen randomly again to form the maternal copy of the offspring chromosome.

```
class selfingGenoTransmitter (begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[])
    FIXME: No document
    clone()
        Return a cloned copy of an operator. This function is available to all operators.
```

2.2.4 Class haplodiploidGenoTransmitter

Haplodiploid offspring generator mimics sex-determination in honey bees. Given a female (queen) parent and a male parent, the female is considered as diploid with two set of chromosomes, and the male is condiered as haploid. Actually, the first set of male chromosomes are used. During mating, female produce eggs, subject to potential recombination and gene conversion, while male sperm is identical to the parental chromosome. Female offspring has two sets of chromosomes, one from mother and one from father. Male offspring has one set of chromosomes from his mother.

```
class haplodiploidGenoTransmitter (begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[])
    FIXME: No document
    clone ()
        Return a cloned copy of an operator. This function is available to all operators.
    initialize (pop)
        FIXME: No document
```

2.2.5 Class mitochondrialGenoTransmitter

This geno transmitter transmits some customized chromosomes as human mitochondrial chromosomes. It randomly inherit the first homologous copy of several customized chromosomes of the female parent.

$\verb"initialize"\,(pop)$

FIXME: No document

2.2.6 Class recombinator

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

- it only works for diploid (and for females in haplodiploid) populations.
- the recombination rate must be comprised between 0.0 and 0.5. A recombination rate of 0.0 means that the loci are completely linked, and thus behave together as a single linked locus. A recombination rate of 0.5 is equivalent to free of recombination. All other values between 0.0 and 0.5 will represent various linkage intensities between adjacent pairs of loci. The recombination rate is equivalent to 1-linkage and represents the probability that the allele at the next locus is randomly drawn.
- it works for selfing. I.e., when only one parent is provided, it will be recombined twice, producing both maternal and paternal chromosomes of the offspring.
- conversion is allowed. Note that conversion will nullify many recombination events, depending on the parameters chosen.

Recombine chromosomes from parents *convMode* can take the following forms NoConversion: no conversion (NumMarkers, prob, n): converts a fixed number of markers (GeometricDistribution, prob, p): An geometric distribution is used to determine how many markers will be converted. (TractLength, prob, n): converts a fixed length of tract. (ExponentialDistribution, prob, p): An exponential distribution with parameter convLen will be used to determine track length. The first number is that probability of conversion event among all recombination events. When a recombination event happens, it may become a recombination event if the Holliday junction is resolved/repaired successfully, or a conversion event if the junction is not resolved/repaired. The default convProb is 0, meaning no conversion event at all. Note that the ratio of conversion to recombination events 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 this parameter. When Note that

- •conversion tract length is usually short, and is estimated to be between 337 and 456 bp, with overall range between maybe 50 2500 bp.
- •simuPOP does not impose a unit for marker distance so your choice of convParam needs to be consistent with your unit. In the HapMap dataset, cM is usually assumed and marker distances are around 10kb (0.001cM ~ 1kb). Gene conversion can largely be ignored. This is important when you use distance based conversion mode such as CONVERT_TrackLength or CONVERT_ExponentialDistribution.
- After a track length is determined, if a second recombination event happens within this region, the track length will be shortened. Note that conversion is identical to double recombination under this context.
- *intensity:* Intensity of recombination. The actual recombination rate between two loci is determined by intensity*locus distance (between them).
- rate: Recombination rate regardless of locus distance after all afterLoci. It can also be an array of recombination rates. Should have the same length as afterLoci or totNumOfLoci(). The recombination rates are independent of locus distance.
- afterLoci: An array of locus indexes. Recombination will occur after these loci. If rate is also specified, they should have the same length. Default to all loci (but meaningless for those loci located at the end of a

chromosome). If this parameter is given, it should be ordered, and can not include loci at the end of a chromosome.

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

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

maleAfterLoci: If given, males will recombine at different locations.

haplodiploid: If set to true, the first copy of paternal chromosomes is copied directly as the paternal chromosomes of the offspring. This is because haplodiploid male has only one set of chromosome.

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

Deep copy of a recombinator

convCount (size)

Return the count of conversion of a certain size (only valid in standard modules)

convCounts()

Return the count of conversions of all sizes (only valid in standard modules)

initialize(pop)

FIXME: No document

recCount (idx)

Return recombination counts (only valid in standard modules)

recCounts()

Return recombination counts (only valid in standard modules)

transmitGenotype (parent, offspring, ploidy)

FIXME: No document

2.3 Initialization

2.3.1 Class initSex (Function InitSex)

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

```
class initSex (maleFreq=0.5, sex=[], stage=PreMating, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], in-
foFields=[])
```

Create an operator that initialize individual sex to Male or Female. By default, it assign sex to individuals randomly, with equal probability of having a male or a female. This probabability can be adjusted through parameter *maleFreq*. Alternatively, a fixed sequence of sexes can be assigned. For example, if sex=[Male, Female], individuals will be assigned Male and Female successively. Parameter *maleFreq* is ignored if *sex* is given. If a list of (virtual) subpopulation is specified in parameter *subPop*, only individuals in these subpopulations will be initialized.

```
apply(pop)
```

Apply this operator to population pop

clone()

Deep copy of an initSex

2.3. Initialization

2.3.2 Class initByFreq (Function InitByFreq)

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

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

```
apply (pop)
     Apply this operator to population pop
clone()
     Deep copy of the operator initByFreq
```

2.3.3 Class initByValue (Function InitByValue)

This operator initialize individuals by given values.

```
class initByValue (value=[], loci=[], ploidy=[], proportions=[], initSex=True, maleFreq=0.5, sex=[], stage=PreMating, begin=0, end=1, step=1, at=[], rep=[], subPop=[], infoFields=[])

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

```
apply (pop)
    Apply this operator to population pop
clone()
    Deep copy of the operator initByValue
```

2.4 Migration

2.4.1 Class migrator

Migrate individuals from (virtual) subpopulations to other subpopulations Migrator is the only way to mix genotypes of several subpopulations because mating is strictly within subpopulations in simuPOP. Migrators are quite flexible in simuPOP in the sense that

- migration can happen from and to a subset of subpopulations.
- migration can be done by probability, proportion or by counts. In the case of probability, if the migration rate from subpopulation a to b is r, then everyone in subpopulation a will have this probability to migrate to b.

In the case of proportion, exactly r*size_of_subPop_a individuals (chosen by random) will migrate to subpopulation b. In the last case, a given number of individuals will migrate.

• new subpopulation can be generated through migration. You simply need to migrate to a subpopulation with a new subpopulation number.

Create a migrator

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

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

fromSubPop: An array of 'from' subpopulations (a number) or virtual subpopulations (a pair of numbers). Default to all subpopulations. For example, if you define a virtual subpopulation by sex, you can use fromSubpop=[(0,0), 1] to choose migrants from the first virtual subpopulation of subpopulation 0, and from subpopulation 1. If a single number sp is given, it is intepretted as [sp]. Note that fromSubPop=(0, 1) (two subpopulation) is different from fromSubPop=[(0,1)] (a virtual subpopulation).

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

stage: Default to PreMating

Note

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

```
apply (pop)
```

Apply the migrator

clone()

Deep copy of a migrator

rate()

Return migration rate

setRates (rate, mode)

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

2.4.2 Class pyMigrator

A more flexible Python migrator This migrator can be used in two ways

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

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More specifically, func can be

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

Create a hybrid migrator

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

indFunc: A Python function that accepts an individual, optional genotypes and parameters, then returns a sub-population ID. This method can be used to separate a population according to individual genotype.

```
stage: Default to PreMating
apply (pop)
    Apply a pyMigrator
clone()
    Deep copy of a pyMigrator
```

2.4.3 Class splitSubPop (Function SplitSubPop)

Split a subpopulation

Split a subpopulation Split a subpopulation by sizes or proportions. Individuals are randomly (by default) assigned to the resulting subpopulations. Because mating schemes may introduce certain order to individuals, randomization ensures that split subpopulations have roughly even distribution of genotypes.

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

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

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

randomize: Whether or not randomize individuals before population split. Default to True.

```
apply (pop)
    Apply a splitSubPop operator

clone()
    Deep copy of a splitSubPop operator
```

2.4.4 Class mergeSubPops (Function MergeSubPops)

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

2.4.5 Class resizeSubPops (Function ResizeSubPops)

Resize subpopulations This operator resize subpopulations subPops to a another size. If subPops is ignored, all subpopulations will be resized. If the new size is smaller than the original one, the remaining individuals are discarded. If the new size if greater, individuals will be copied again if propagate is true, and be empty otherwise.

2.5 Mutation

2.5.1 Class mutator

Base class of all mutators. The base class of all functional mutators. It is not supposed to be called directly.

Every mutator can specify rate (equal rate or different rates for different loci) and a vector of applicable loci (default to all but should have the same length as rate if rate has length greater than one).

Maximum allele can be specified as well but more parameters, if needed, should be implemented by individual mutator classes.

There are numbers of possible allelic states. Most theoretical studies assume an infinite number of allelic states to avoid any homoplasy. If it facilitates any analysis, this is however extremely unrealistic.

```
 \textbf{class mutator} \ (rate=[],\ loci=[],\ maxAllele=0,\ output=">",\ outputExpr="",\ stage=PostMating,\ begin=0,\ end=-1,\ step=1,\ at=[],\ rep=[],\ subPop=[],\ infoFields=[])
```

Create a mutator, do not call this constructor directly All mutators have the following common parameters. However, the actual meaning of these parameters may vary according to different models. The only differences between the following mutators are the way they actually mutate an allele, and corresponding input parameters. The number of mutation events at each locus is recorded and can be accessed from the mutationCount or mutationCounts functions.

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

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

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

2.5.2 Class kamMutator (Function KamMutate)

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

2.5.3 Class smmMutator (Function SmmMutate)

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

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

Create a SMM mutator The SMM is developed for allozymes. It provides better description for these kinds of evolutionary processes.
```

```
Please see class mutator for the descriptions of other parameters. 
incProb: Probability to increase allele state. Default to 0.5.

clone()

Deep copy of a smmMutator
```

2.5.4 Class gsmMutator (Function GsmMutate)

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

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

2.5.5 Class pyMutator (Function PyMutate)

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

2.5.6 Class pointMutator (Function PointMutate)

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

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2.6 Selection

2.6.1 Class selector

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

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

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

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

Note:

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

```
subPop: A shortcut to subPops=[subPop]
subPops: Subpopulations that the selector will apply to. Default to all.
apply (pop)
    Set fitness to all individuals. No selection will happen!
clone()
    Deep copy of a selector
```

2.6.2 Class mapSelector (Function MapSelector)

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

2.6.3 Class maSelector (Function MaSelect)

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

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

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```
•maSelector only works for diploid populations.
```

•wildtype alleles at all loci are the same.

```
clone()
```

Deep copy of a maSelector

indFitness(ind, gen)

Calculate/return the fitness value, currently assuming diploid

2.6.4 Class mlSelector (Function MlSelect)

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

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

```
class mlSelector (selectors, mode=SEL\_Multiplicative, subPops=[], stage=PreMating, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=["fitness"])
```

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

selectors: A list of selectors

clone()

Deep copy of a mlSelector

2.6.5 Class pySelector (Function PySelect)

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

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

Create a Python hybrid selector

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

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

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

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

```
clone()
```

Deep copy of a pySelector

2.7 Penetrance

2.7.1 Class penetrance

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

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

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

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

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

2.7.2 Class mapPenetrance (Function MapPenetrance)

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

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```
phase: If True, a/b and b/a will have different penetrance values. Default to False.
output: And other parameters please refer to help(baseOperator.__init__)
clone()
Deep copy of a map penetrance operator
```

2.7.3 Class maPenetrance (Function MaPenetrance)

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

2.7.4 Class mlPenetrance (Function MlPenetrance)

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

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

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

2.7.5 Class pyPenetrance (Function PyPenetrance)

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

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

2.8 Quantitative Trait

2.8.1 Class quanTrait

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

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

2.8.2 Class mapQuanTrait (Function MapQuanTrait)

Quantitative trait according to genotype at one locus Assign quantitative trait using a table with keys 'X-Y' where X

2.8. Quantitative Trait 41

and Y are allele numbers. If parameter sigma is not zero, the return value is the sum of the trait plus $N\left(0,\sigma^2\right)$. This random part is usually considered as the environmental factor of the trait.

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

Create a map quantitative trait operator
```

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

loci: An array of locus indexes. The quantitative trait is determined by genotypes at these loci.

qtrait: A dictionary of quantitative traits. The genotype must be in the form of 'a-b'. This is the mean of the quantitative trait. The actual trait value will be $N\left(mean, \sigma^2\right)$. For multiple loci, the form is 'a-blc-dle-f' etc.

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

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

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

clone(

Deep copy of a map quantitative trait operator

2.8.3 Class maQuanTrait (Function MaQuanTrait)

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

2.8.4 Class mlQuanTrait (Function MlQuanTrait)

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

- QT_Multiplicative: the mean of the quantitative trait is calculated as $f = \prod f_i$.
- QT_Additive: the mean of the quantitative trait is calculated as $f = \sum f_i$.

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

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

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

2.8.5 Class pyQuanTrait (Function PyQuanTrait)

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

2.9 Statistics Calculation

2.9.1 Class stator

Base class of all the statistics calculator Operator stator calculates various basic statistics for the population and set variables in the local namespace. Other operators or functions can refer to the results from the namespace after stat is applied.

2.9.2 Class stat (Function Stat)

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

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

Create an stat operator

- popSize: Whether or not calculate population and virtual subpopulation sizes. This parameter will set the following variables:
 - •numSubPop the number of subpopulations.
 - •subPopSize an array of subpopulation sizes.
 - •virtualSubPopSize (optional) an array of virtual subpopulation sizes. If a subpopulation does not have any virtual subpopulation, the subpopulation size is returned.
 - •popSize, subPop[sp]['popSize'] the population/subpopulation size.
- *numOfMale*: Whether or not count the numbers or proportions of males and females. This parameter can set the following variables by user's specification:
 - •numOfMale, subPop[sp]['numOfMale'] the number of males in the population/subpopulation.
 - •numOfFemale, subPop[sp]['numOfFemale'] the number of females in the population/subpopulation.
 - •propOfMale, subPop[sp]['propOfMale'] the proportion of males in the population/subpopulation.
 - •propOfFemale, subPop[sp]['propOfFemale'] the proportion of females in the population/subpopulation.
- numOfMale_param: A dictionary of parameters of numOfMale statistics. Can be one or more items choosen from the following options: numOfMale, propOfMale, numOfFemale, and propOfFemale.
- *numOfAffected:* Whether or not count the numbers or proportions of affected and unaffected individuals. This parameter can set the following variables by user's specification:
 - •numOfAffected, subPop[sp]['numOfAffected'] the number of affected individuals in the population.
 - •numOfUnaffected, subPop[sp]['numOfUnAffected'] the number of unaffected individuals in the population/subpopulation.
 - •propOfAffected, subPop[sp]['propOfAffected'] the proportion of affected individuals in the population/subpopulation.
 - •propOfUnaffected, subPop[sp]['propOfUnAffected'] the proportion of unaffected individuals in the population/subpopulation.
- numOfAffected_param: A dictionary of parameters of numOfAffected statistics. Can be one or more items choosen from the following options: numOfAffected, propOfAffected, numOfUnaffected, propOfUnaffected.
- numOfAlleles: An array of loci at which the numbers of distinct alleles will be counted (numOfAlleles=[loc1, loc2, ...] where loc1 etc. are absolute locus indexes). This is done through the calculation of allele frequencies. Therefore, allele frequencies will also be calculated if this statistics is requested. This parameter will set the following variables (carray objects of the numbers of alleles for all loci). Unrequested loci will have 0 distinct alleles.
 - •numOfAlleles, subPop[sp]['numOfAlleles'] the number of distinct alleles at each locus. (Calculated only at requested loci.)

- numOfAlleles_param: A dictionary of parameters of numOfAlleles statistics. Can be one or more items choosen from the following options: numOfAffected, propOfAffected, numOfUnaffected, propOfUnaffected.
- - •alleleNum[a], subPop[sp]['alleleNum'][a]
 - •alleleFreq[a], subPop[sp]['alleleFreq'][a].
- *alleleFreq_param:* A dictionary of parameters of alleleFreq statistics. Can be one or more items choosen from the following options: numOfAlleles, alleleNum, and alleleFreq.
- genoFreq: An array of loci at which all genotype frequencies will be calculated (genoFreq=[loc1, loc2, ...]. You may use parameter genoFreq_param to control if a/b and b/a are the same genotype. This parameter will set the following dictionary variables. Note that unlike list used for alleleFreq etc., the indexes a, b of genoFreq[loc][a][b] are dictionary keys, so you will get a *KeyError* when you used a wrong key. You can get around this problem by using expressions like genoNum[loc].setDefault(a, {}).
 - •genoNum[loc][allele1][allele2] and subPop[sp]['genoNum'][loc][allele1][allele2], the number of genotype allele1-allele2 at locus loc.
 - •genoFreq[loc][allele1][allele2] and subPop[sp]['genoFreq'][loc][allele1][allele2], the frequency of genotype allele1-allele2 at locus loc.
 - •genoFreq_param a dictionary of parameters of phase = 0 or 1.
- heteroFreq: An array of loci at which observed heterozygosities will be calculated (heteroFreq=[loc1, loc2, ...]). For each locus, the number and frequency of allele specific and overall heterozygotes will be calculated and stored in four population variables. For example, heteroNum[loc][1] stores number of heterozygotes at locus loc, with respect to allele 1, which is the number of all genotype 1x or x1 where does not equal to 1. All other genotypes such as 02 are considered as homozygotes when heteroFreq[loc][1] is calculated. The overall number of heterozygotes (HeteroNum[loc]) is the number of genotype xy if x does not equal to y.
 - •HeteroNum[loc], subPop[sp]['HeteroNum'][loc], the overall heterozygote count.
 - •HeteroFreq[loc], subPop[sp]['HeteroFreq'][loc], the overall heterozygote frequency.
 - •heteroNum[loc][allele], subPop[sp]['heteroNum'][loc][allele], allele-specific heterozygote counts.
 - •heteroFreq[loc][allele], subPop[sp]['heteroFreq'][loc][allele], allele-specific heterozygote frequency.
- homoFreq: An array of loci to calculate observed homozygosities and expected homozygosities (homoFreq=[loc1, loc2, ...]). This parameter will calculate the numbers and frequencies of homozygotes **xx** and set the following variables:
 - •homoNum[loc], subPop[sp]['homoNum'][loc].
 - •homoFreq[loc], subPop[sp]['homoFreq'][loc].
- *expHetero*: An array of loci at which the expected heterozygosities will be calculated (expHetero=[loc1, loc2, ...]). The expected heterozygosity is calculated by

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

where p_i is the allele frequency of allele i. The following variables will be set:

- •expHetero[loc], subPop[sp]['expHetero'][loc].
- expHetero_param: A dictionary of parameters of expHetero statistics. Can be one or more items choosen from the following options: subpop and midValues.
- haploFreq: A matrix of haplotypes (allele sequences on different loci) to count. For example, haploFreq = [[0,1,2], [1,2]] will count all haplotypes on loci 0, 1 and 2; and all haplotypes on loci 1, 2. If only one haplotype is specified, the outer [] can be omitted. I.e., haploFreq=[0,1] is acceptable. The following dictionary variables will be set with keys 0-1-2 etc. For example, haploNum['1-2']['5-6'] is the number of allele pair 5, 6 (on loci 1 and 2 respectively) in the population.
 - •haploNum[haplo] and subPop[sp]['haploNum'][haplo], the number of allele sequencies on loci haplo.
 - •haploFreq[haplo], subPop[sp]['haploFreq'][haplo], the frequency of allele sequencies on loci haplo.
- LD: Calculate linkage disequilibria LD, LD' and r^2 , given $LD=[\ [loc1,\ loc2],\ [\ loc1,\ loc2],$ allele1, allele2], ...]. For each item $[loc1,\ loc2,\ allele1,\ allele2], D, D'$ and r^2 will be calculated based on allele1 at loc1 and allele2 at loc2. If only two loci are given, the LD values are averaged over all allele pairs. For example, for allele A at locus 1 and allele B at locus 2,

$$D = P_{AB} - P_A P_B$$
$$D' = D/D_{max}$$

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

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

If only one item is specified, the outer [] can be ignored. I.e., LD=[loc1, loc2] is acceptable. This parameter will set the following variables. Please note that the difference between the data structures used for ld and LD.

- •ld['loc1-loc2']['allele1-allele2'], subPop[sp]['ld']['loc1-loc2']['allele1-allele2']
- •ld_prime['loc1-loc2']['allele1-allele2'], subPop[sp]['ld_prime']['loc1-loc2']['allel
- •r2['loc1-loc2']['allele1-allele2'], subPop[sp]['r2']['loc1-loc2']['allele1-allele2']
- •LD[loc1][loc2], subPop[sp]['LD'][loc1][loc2].
- •LD_prime[loc1][loc2], subPop[sp]['LD_prime'][loc1][loc2].
- •R2[loc1][loc2], subPop[sp]['R2'][loc1][loc2].
- LD_param: A dictionary of parameters of LD statistics. Can have key stat which is a list of statistics to calculate. Default to all. If any statistics is specified, only those specified will be calculated. For example, you may use LD_param={LD_prime} to calculate D' only, where LD_prime is a shortcut for 'stat':['LD_prime']. Other parameters that you may use are:
 - •subPop whether or not calculate statistics for subpopulations.
 - •midValues whether or not keep intermediate results.

association: Association measures

- association_param: A dictionary of parameters of association statistics. Can be one or more items choosen from the following options: ChiSq_P, UC_U, and CramerV.
- Fst: Calculate F_{st} , F_{is} , F_{it} . For example, Fst = [0,1,2] will calculate F_{st} , F_{is} , F_{it} based on alleles at loci 0, 1, 2. The locus-specific values will be used to calculate AvgFst, which is an average value over all alleles (Weir & Cockerham, 1984). Terms and values that match Weir & Cockerham are:

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

This parameter will set the following variables:

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

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

relMethod: Method used to calculate relatedness. Can be either REL_Queller or REL_Lynch. The relatedness values between two individuals, or two groups of individuals are calculated according to Queller & Goodnight (1989) (method=REL_Queller) and Lynch et al. (1999) (method=REL_Lynch). The results are pairwise relatedness values, in the form of a matrix. Original group or subpopulation numbers are discarded. There is no subpopulation level relatedness value.

relGroups: Calculate pairwise relatedness between groups. Can be in the form of either [[1,2,3],[5,6,7],[8,9]] or [2,3,4]. The first one specifies groups of individuals, while the second specifies subpopulations. By default, relatedness between subpopulations is calculated.

relLoci: Loci on which relatedness values are calculated

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

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

midValues: Whether or not post intermediate results. Default to False. For example, Fst will need to calculate allele frequencies. If midValues is set to True, allele frequencies will be posted as well. This will be helpful in debugging and sometimes in deriving statistics.

```
apply (pop)
    Apply the stat operator
clone()
    Deep copy of a stat operator
```

2.10 Expression and Statements

2.10.1 Class dumper

Dump the content of a population.

```
    subPop: Only display subpopulation(s)
    indRange: Range(s) of individuals to display
    max: The maximum number of individuals to display. Default to 100. This is to avoid careless dump of huge populations.
    output: Output file. Default to the standard output.
    outputExpr: And other parameters: refer to help(baseOperator.__init__)
    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.
```

2.10.2 Class savePopulation

Save population to a file

2.10.3 Class pyOutput

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

2.10.4 Class pyEval (Function PyEval)

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

```
class pyEval (expr="", stmts="", preStmts="", postStmts="", exposePop=False, name="", output=">", output=", outp
                                            Expr="", stage=PostMating, begin=0, end=-1, <math>step=1, at=[], rep=[], subPop=[], infoFields=[])
                 Evaluate expressions/statments in the local namespace of a replicate
                 expr: The expression to be evaluated. The result will be sent to output.
                 stmts: The statement that will be executed before the expression
                 preStmts: The statement that will be executed when the operator is constructed
                 postStmts: The statement that will be executed when the operator is destroyed
                 exposePop: If True, expose the current population as a variable named pop
                 name: Used to let pure Python operator to identify themselves
                 output: Default to >. I.e., output to standard output.
                 apply(pop)
                                Apply the pyEval operator
                 clone()
                                Deep copy of a pyEval operator
                 name()
                                Return the name of an expression The name of a pyEval operator is given by an optional parameter name.
                                It can be used to identify this pyEval operator in debug output, or in the dryrun mode of simulator::evolve.
```

2.10.5 Class pyExec (Function PyExec)

Execute a Python statement This operator takes a list of statements and executes them. No value will be returned or outputted.

2.10.6 Class infoEval (Function infoEval)

Unlike operator pyEval and pyExec that work at the population level, in its local namespace, infoEval works at the individual level, working with individual information fields. is statement can change the value of existing information fields. Optionally, variables in population's local namespace can be used in the statement, but this should be used with caution.

Evaluate Python statements with variables being an individual's information fields The expression and statements will be executed for each individual, in a Python namespace (dictionary) where individual information

fields are made available as variables. Population dictionary can be made available with option usePopVars. Changes to these variables will change the corresponding information fields of individuals. Please note that, 1. If population variables are used, and there are name conflicts between information fields and variables, population variables will be overridden by information fields, without any warning. 2. Information fields are float numbers. An exceptions will raise if an information field can not be converted to a float number. 3. This operator can be used in all stages. When it is used during-mating, it will act on each offspring.

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

stmts: The statement that will be executed before the expression

subPop: A shortcut to subPops=[subPop]

subPops: Subpopulations this operator will apply to. Default to all.

usePopVars: If True, import variables from expose the current population as a variable named pop

exposePop: If True, expose the current population as a variable named pop

name: Used to let pure Python operator to identify themselves

output: Default to >. I.e., output to standard output. Note that because the expression will be executed for each individual, the output can be large.

```
apply(pop)
```

Apply the infoEval operator

clone()

Deep copy of a infoEval operator

name()

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

2.10.7 Class infoExec (Function infoExec)

Execute a Python statement for each individual, using information fields This operator takes a list of statements and executes them. No value will be returned or outputted.

```
class infoExec (stmts="", subPops=[], usePopVars=False, exposePop=False, name="", output=">", output=">", output=">", output=">", output=">", stage=PostMating, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[]) Fields, optionally with variable in population's local namespace Please refer to class infoEval for parameter descriptions.
```

```
clone()
```

Deep copy of a infoExec operator

2.11 Tagging (used for pedigree tracking)

2.11.1 Class tagger

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

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

2.11.2 Class inheritTagger

Inherite tag from parents This during-mating operator will copy the tag (information field) from his/her parents. Depending on mode parameter, this tagger will obtain tag, value of the first specified information fields, from his/her father or mother (two tag fields), or both (first tag field from father, and second tag field from mother).

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

2.11.3 Class parentTagger

Tagging according to parental indexes This during-mating operator set tag() each individual with indexes of his/her parent in the parental population. Because only one parent is recorded, this is recommended to be used for mating schemes that requires only one parent (such as selfMating). This tagger record indexes to information field parent_idx, and/or a given file. The usage is similar to parentsTagger.

2.11.4 Class parents Tagger

Tagging according to parents' indexes This during-mating operator set tag(), currently a pair of numbers, of each individual with indexes of his/her parents in the parental population. This information will be used by pedigree-related operators like affectedSibpairSample to track the pedigree information. Because parental population will be discarded or stored after mating, these index will not be affected by post-mating operators. This tagger record parental index to one or both

• one or two information fields. Default to father_idx and mother_idx. If only one parent is passed in a mating scheme (such as selfing), only the first information field is used. If two parents are passed, the first information field records paternal index, and the second records maternal index.

• a file. Indexes will be written to this file. This tagger will also act as a post-mating operator to add a new-line to this file.

2.11.5 Class pedigreeTagger

Pedigree tagger is used to save a complete pedigree to a pedigree file during an evolution process. Because is destroyed of record individuals involved in an evolutioary process. This is a simple post-mating tagger that write given information fields to a file (or standard output).

2.11.6 Class pyTagger

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

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

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

2.12 Terminator

2.12.1 Class terminateIf

This operator evaluates an expression in a population's local namespace and terminate the evolution of this population, or the whole simulator, if the return value of this expression is True. Termination caused by an operator will stop the execution of all operators after it. Because a life-cycle is considered to be complete if mating is complete, the *evolved generations* (return value from simulator::evolve) of a terminated replicate is determined by when the last evolution cycle is terminated.

class terminateIf (condition="", stopAll=False, message="", output="", outputExpr="", stage=PostMating, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], 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* or *outputExpr* (both default to ""), the generation number, preceded with an optional *message* will be written to it.

```
apply(pop)
```

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

clone()

Deep copy of a terminateIf terminator

2.13 The Python operator

2.13.1 Class pyOperator

A python operator that directly operate a population. This operator accepts a function that can take the form of

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

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

class pyOperator (func, param=None, stage=PostMating, formOffGenotype=False, offspringOnly=False, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[])

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

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

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

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

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

Note

- •Output to output or outputExpr is not supported. That is to say, you have to open/close/append to files explicitly in the Python function. Because files specified by output or outputExpr are controlled (opened/closed) by simulators, they should not be manipulated in a pyOperator operator.
- •This operator can be applied Pre-, During- or Post- Mating and is applied PostMating by default. For example, if you would like to examine the fitness values set by a selector, a PreMating Python operator should be used.

```
apply (pop)
```

Apply the pyOperator operator to one population

2.14 Miscellaneous

2.14.1 Class if Else

Conditional operator This operator accepts

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

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

2.14.2 Class turnOnDebug (Function TurnOnDebug)

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

- set environment variable SIMUDEBUG.
- use simuOpt.setOptions(debug) function.
- use TurnOnDebug or TurnOnDebugByName function.
- use this turnOnDebug operator

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

class turnOnDebug (code, stage=PreMating, begin=0, end=-1, step=1, at=[], rep=[], subPop=[], infoFields=[])

Create a turnOnDebug operator

2.14.3 Class turnOffDebug (Function TurnOffDebug)

Set debug off Turn off debug.

2.14.4 Class noneOp

None operator This operator does nothing.

2.14.5 Class pause

Pause a simulator This operator pauses the evolution of a simulator at given generations or at a key stroke, using stopOnKeyStroke=True option. Users can use 'q' to stop an evolution. When a simulator is stopped, press any other key to resume the simulation or escape to a Python shell to examine the status of the simulation by pressing 's'.

There are two ways to use this operator, the first one is to pause the simulation at specified generations, using the usual operator parameters such as at. Another way is to pause a simulation with any key stroke, using the stopOnKeyStroke parameter. This feature is useful for a presentation or an interactive simulation. When 's' is pressed, this operator expose the current population to the main Python dictionary as variable pop and enter an interactive Python session. The way current population is exposed can be controlled by parameter exposePop and popName. This feature is useful when you want to examine the properties of a population during evolution.

2.14.6 Class ticToc (Function TicToc)

Timer operator 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.

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2.14.7 Class setAncestralDepth

Set ancestral depth This operator set the number of ancestral generations to keep in a population. It is usually called like setAncestral(at=[-2]) to start recording ancestral generations to a population at the end of the evolution. This is useful when constructing pedigree trees from a population.

Chapter 3

Global and Python Utility functions

3.1 Global functions

AlleleType()

Return the allele type of the current module. Can be binary, short, or long.

AvailableRNGs()

List the names of all available random number generators

Limits()

Print out system limits

ListDebugCode()

List all debug codes

LoadPopulation (file)

Load a population from a file.

LoadSimulator (file, matingScheme)

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

MaxAllele()

Return the maximum allowed allele state of the current simuPOP module, which is 1 for binary modules, 255 for short modules and 65535 for long modules.

ModuleCompiler()

Return the compiler used to compile this simuPOP module

ModuleDate()

Return the date when this simuPOP module is compiled

ModulePlatForm()

Return the platform on which this simuPOP module is compiled

ModulePyVersion()

Return the Python version this simuPOP module is compiled for

Optimized()

Return True if this simuPOP module is optimized

SetRNG (rng="", seed=0)

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

TurnOffDebug(code=DBG_ALL)

Turn off debug information. Default to turn off all debug codes. Only available in non-optimized modules.

TurnOnDebug (code=DBG ALL)

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

rng()

Return the currently used random number generator

simuRev()

Return the revision number of this simuPOP module. Can be used to test if a feature is available.

simuVer()

Return the version of this simuPOP module

3.2 Module simuPOP

3.3 Module simuOpt

3.4 Module simuUtil

3.5 Module simuRPy

3.5.1 Class varPlotter

This class defines a Python operator that uses R to plot a simuPOP express. During the evolution, this express is evaluated in each replicate's local namespace. How this expression is plotted depends on the dimension of the return value (if a sequence is returned), number of replicates, whether or not historical values (collected over several generations) are plotted, and plot type (lines or images).

The default behavior of this operator is to plot the history of an expression. For example, when operator

```
varPlotter(var='expr')
```

is used in simulator::evolve, the value of expr will be recorded each time when this operator is applied. A line will be draw in a figure with x-axis being the generation number. Parameters ylim can be used to specify the range of y-axis.

If the return value of expression expr is a sequence (tuple or list), parameter varDim has to be used to indicate the dimension of this expression. For example,

```
varPlotter(var='expr', varDim=3)
```

will plot three lines, corresponding to the histories of each item in the array.

If the expression returns a number and there are several replicates, parameter numRep' should be used. In this case, each line will correspond to a replicate.

If the expression returns a vector and there are several replicates, several subplots will be used. Parameter by Rep or by Var should be used to tell varPlotter whether the subplots should be divided by replicate or by variable. For example,

```
varPlotter(var='expr', varDim=8, numRep=5, byRep=1)
```

will use an appropriate layout for your subplots, which is, in this case, 2x3 for 5 replicates. Each subplot will have 8 lines. If by Val is True, there will be 3x3 subplots for 8 items in an array, and each subplot will have 5 lines. Note that by Rep or by Val can also be used when there is only one replicate or if the dimension of the expression is one.

When history=False, histories of each variable will be discarded so the figure will always plot the current value of the expression.

expr: expression that will be evaluate at each replicate's local namespace when the operator is applied.

history: whether or not record and plot the history of an expression. Default to True.

varDim: If the return value of expr is a sequence, varDim should be set to the length of this sequence.
Default to 1.

numRep: Number of replicates of the simulator. Default to 1.

win: Window of generations. I.e., how many generations to keep in a figure. This is useful when you want to keep track of only recent changes of an expression. The default value is 0, which will keep all histories.

ylim: The range of y-axis.

update: Update figure after update generations. This is used when you do not want to update the figure every time when this operator is applied.

title, xlab, ylab: Title, label at x and y axes of your figure(s). xtitle is defaulted to 'generation'.

axes: Whether or not plot axes. Default to True.

lty: A list of line type for each line in the figure.

col: A list of colors for each line in the figure.

level: level of image colors (default to 20).

saveAs: save figures in files saveAs#gen.eps. For example, if saveAs='demo', you will get files demo1.eps, demo2.eps etc.

separate: plot data lines in separate panels.

image: use R image function to plot image, instead of lines.

leaveOpen: whether or not leave the plot open when plotting is done. Default to True.

3.6 Utility Classes

3.6.1 Class RNG

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

```
class RNG (rng=None, seed=0)
    RNG used by simuPOP.

max()
    Maximum value of this RNG.

maxSeed()
    Return the maximum allowed seed value
name()
    Return RNG name
```

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pvalChiSq(chisq, df)

Right hand side (single side) p-value for ChiSq value

randBinomial(n, p)

Binomial distribution B(n, p).

randBit()

FIXME: No document

randExponential(v)

FIXME: No document

randGeometric(p)

Geometric distribution.

randGet()

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

randInt(n)

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

randMultinomial(N, p, n)

Multinomial distribution.

randMultinomialVal(N, p)

FIXME: No document

randNormal (m, v)

Normal distribution.

randPoisson(p)

Poisson distribution.

randUniform01()

Uniform distribution [0,1).

seed()

Return the seed of this RNG

setRNG (rng=None, seed=0)

Choose an random number generator, or set seed to the current RNG

rng: Name of the RNG. If rng is not given, environmental variable GSL_RNG_TYPE will be used if it is available. Otherwise, RNGmt19937 will be used.

seed: Random seed. If not given, /dev/urandom, /dev/random, system time will be used, depending on availability, in that order. Note that windows system does not have /dev so system time is used.

setSeed(seed)

If seed is 0, method described in setRNG is used.

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