# 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.

# **Contents**

1	simu		mponents	1		
	1.1	Individu	ual, population and simulator	1		
		1.1.1	Class GenoStruTrait	1		
		1.1.2	Class individual	3		
		1.1.3	Class population	4		
		1.1.4	Class simulator	9		
		1.1.5	Class pedigree	11		
		1.1.6	Class vspSplitter	12		
		1.1.7	Class sexSplitter	12		
		1.1.8	Class affectionSplitter	13		
		1.1.9	Class infoSplitter	13		
		1.1.10	Class proportionSplitter	13		
		1.1.11	Class rangeSplitter	14		
		1.1.12	Class genotypeSplitter	14		
		1.1.13	Class combinedSplitter	14		
	1.2	Mating	Schemes	15		
		1.2.1	Class homoMating	15		
		1.2.2	Class heteroMating	15		
		1.2.3	Class pedigreeMating	16		
		1.2.4	Class sequentialParentChooser	16		
		1.2.5	Class sequentialParentsChooser	16		
		1.2.6	Class randomParentChooser	17		
		1.2.7	Class randomParentsChooser	17		
		1.2.8	Class polyParentsChooser	17		
		1.2.9	Class alphaParentsChooser	18		
		1.2.10	Class infoParentsChooser	18		
		1.2.11	Class pyParentsChooser	18		
		1.2.12	Class offspringGenerator	19		
		1.2.13	Class controlledOffspringGenerator	19		
		1.2.14	Pre-defined mating schemes	20		
		1.2.15	Pre-defined offspring generators	22		
	1.3	Utility (	Classes	22		
		1.3.1		22		
	1.4	Global	functions	23		
2	Oper	rator References (under revision)				
	2.1	Base cla	ass for all operators	25		
		2.1.1	Class baseOperator	25		
	2.2	Initializ	ation	26		
		2.2.1		26		
		2.2.2	2 1 1	27		
		2.2.3	Class initByValue (Function InitByValue)	27		

2.3	Express	ion and Statements
	2.3.1	Class pyOutput 27
	2.3.2	Class pyEval (Function PyEval) 28
	2.3.3	Class pyExec (Function PyExec) 28
	2.3.4	Class infoEval (Function InfoEval)
	2.3.5	Class infoExec (Function InfoExec)
2.4		raphic models
	2.4.1	Class migrator 30
	2.4.2	Class splitSubPops (Function SplitSubPops)
	2.4.3	Class mergeSubPops (Function MergeSubPops)
	2.4.4	Class resizeSubPops (Function ResizeSubPops)
2.5		be transmitters
	2.5.1	Class genoTransmitter
	2.5.2	Class cloneGenoTransmitter
	2.5.3	Class mendelianGenoTransmitter
	2.5.4	Class selfingGenoTransmitter 34
	2.5.5	Class haplodiploidGenoTransmitter 34
	2.5.6	Class mitochondrialGenoTransmitter 34
2.6	2.5.7	Class recombinator
2.6		n
	2.6.1	Class mutator
	2.6.2	Class matrixMutator (Function MatrixMutate)
	2.6.3	Class kamMutator (Function KamMutate) 37
	2.6.4	Class smmMutator (Function SmmMutate) 38
	2.6.5	Class pyMutator (Function PyMutate) 38
	2.6.6	Class mixedMutator (Function MixedMutate) 39
	2.6.7	Class contextMutator (Function ContextMutate) 39
	2.6.8	Class pointMutator (Function PointMutate) 39
2.5	2.6.9	Derived mutation operators
2.7		n
	2.7.1	Class selector
	2.7.2	Class mapSelector (Function MapSelector)
	2.7.3	Class maSelector (Function MaSelect) 41
	2.7.4	Class mlSelector (Function MlSelect) 42
2.0	2.7.5	Class pySelector (Function PySelect) 42
2.8		nce
	2.8.1	Class basePenetrance
		Class mapPenetrance (Function MapPenetrance)
	2.8.3	Class maPenetrance (Function MaPenetrance)
	2.8.4	Class mlPenetrance (Function MlPenetrance)
2.0	2.8.5	Class pyPenetrance (Function PyPenetrance)
2.9	-	ative Trait
	2.9.1	Class quanTrait
	2.9.2	Class mapQuanTrait (Function MapQuanTrait)
	2.9.3	Class maQuanTrait (Function MaQuanTrait)
	2.9.4	Class mlQuanTrait (Function MlQuanTrait)
2.10	2.9.5	Class pyQuanTrait (Function PyQuanTrait)
2.10		s Calculation
0.11	2.10.1	Class stat (Function Stat)
2.11		(used for pedigree tracking)
	2.11.1	Class tagger
	2.11.2	Class inheritTagger 53
	2.11.3	Class parentTagger
	2.11.4	Class parents Tagger 53

		2.11.5	Class pedigreeTagger	54
		2.11.6	Class pyTagger	54
	2.12	Termina	ator	54
		2.12.1	Class terminateIf	54
	2.13	The Pyt	thon operator	55
		2.13.1	Class pyOperator	55
	2.14	Ascerta	inment operators	55
		2.14.1		56
		2.14.2	Class caseControlSample	56
		2.14.3	Class affectedSibpairSample	56
2.15		Miscell	aneous operators	57
		2.15.1	Class noneOp	57
		2.15.2	Class dumper	57
		2.15.3	Class savePopulation	58
		2.15.4	Class setAncestralDepth	58
		2.15.5		58
		2.15.6	Class pause	58
		2.15.7	Class turnOnDebug (Function TurnOnDebug)	59
		2.15.8		59
		2.15.9	Class ticToc	59
	2.16	Functio	on form of operators	60
2	TT. •11•	36.3		-1
3		y Modu		61
	3.1			61
		3.1.1		61
		3.1.2	$\epsilon$	62 63
	2.2	3.1.3	Class simuOpt	<b>1</b> 3
		3 / 1 1		
	3.2		esimuUtil (under revision)	65
	3.2	3.2.1	e simuUtil (under revision)	65 67
	3.2	3.2.1 3.2.2	c simuUtil (under revision)       0         Class simuProgress       0         Class trajectory       0	65 67 67
		3.2.1 3.2.2 3.2.3	Class simuProgress       Class trajectory         Class trajectory       Class trajectory	65 67 67 68
	3.2	3.2.1 3.2.2 3.2.3 Module	c simuUtil (under revision) Class simuProgress   Class trajectory Class trajectorySimulator   c simuRPy Class trajectorySimulator	65 67 67 68 69
		3.2.1 3.2.2 3.2.3 Module 3.3.1	c simuUtil (under revision) Class simuProgress   Class trajectory Class trajectorySimulator   c simuRPy Class derivedArgs	65 67 67 68 69 70
		3.2.1 3.2.2 3.2.3 Module 3.3.1 3.3.2	Class simuProgress Class trajectory Class trajectory Class trajectory Class trajectory Class trajectory Class trajectory Class derivedArgs Class varPlotter	65 67 68 69 70
		3.2.1 3.2.2 3.2.3 Module 3.3.1 3.3.2 3.3.3	Class simuProgress Class trajectory Class trajectorySimulator Class derivedArgs Class varPlotter Class scatterPlotter	65 67 68 69 70 72
		3.2.1 3.2.2 3.2.3 Module 3.3.1 3.3.2 3.3.3 3.3.4	Class simuProgress Class trajectory Class trajectorySimulator SimuRPy Class derivedArgs Class varPlotter Class scatterPlotter Class infoPlotter	65 67 68 69 70 72 73
		3.2.1 3.2.2 3.2.3 Module 3.3.1 3.3.2 3.3.3	Class simuProgress Class trajectory Class trajectorySimulator SimuRPy Class derivedArgs Class varPlotter Class scatterPlotter Class infoPlotter	65 67 68 69 70 72

# **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. An empty list will be returned if *lociNames* was not specified.

#### lociPos()

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

## locusByName (name)

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

## locusName(loc)

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

## 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 refences 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, ploidy=-1, chrom=-1)

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

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

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

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

Return an editable array (a carray of length totNumLoci()) that represents all alleles on the p-th homologous set of chromosomes. If ploidy or chrom is given, only alleles on the chrom-th chromosome (or all chromosomes if chrom = -1) of ploidy-th homologous copy of chromosomes will be returned.

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

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

```
setSex (sex)
    Set individual sex to Male or Female.

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

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

affected()
    Return True if this individual is affected.

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

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

info (field)
    Return the value of an information field filed (by index or name).
intInfo (field)
```

# 1.1.3 Class population

setInfo(value, field)

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.

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

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

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

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

- Insert or remove loci, resize (shrink or expand) a population, sample from a population, or merge with other populations.
- Manipulate population variables and evaluate expressions in this *local namespace*.
- Save and load a population.

class population (size=[], ploidy=2, loci=[], chromTypes=[], lociPos=[], ancGen=0, chromNames=""List, alleleNames=""List, lociNames=""List, subPopNames=""List, infoFields=""List)
The following parameters are used to create a population object:

- size: A list of subpopulation sizes. The length of this list determines the number of subpopulations of this population. If there is no subpopulation, size=[popSize] can be written as size=popSize.
- ploidy: Number of homologous sets of chromosomes. Default to 2 (diploid). For efficiency considerations, all chromosomes have the same number of homologous sets, even if some customized chromosomes or some individuals (e.g. males in a haplodiploid population) have different numbers of homologous sets. The first case is handled by setting *chromTypes* of each chromosome. Only the haplodiploid populations are handled for the second case, for which ploidy=Haplodiploid should be used.
- *loci:* A list of numbers of loci on each chromosome. The length of this parameter determines the number of chromosomes. Default to [1], meaning one chromosome with a single locus.
- chromTypes: A list that specifies the type of each chromosome, which can be Autosome, ChromosomeX, ChromosomeY, or Customized. All chromosomes are assumed to be autosomes if this parameter is ignored. Sex chromosome can only be specified in a diploid population where the sex of an individual is determined by the existence of these chromosomes using the XX (Female) and XY (Male) convention. Both sex chromosomes have to be available and be specified only once. Because chromosomes X and Y are treated as two chromosomes, recombination on the pseudo-autosomal regions of the sex chromosomes is not supported. Customized chromosomes are special chromosomes whose inheritance patterns are undefined. They rely on user-defined functions and operators to be passed from parents to offspring. Multiple customized chromosomes have to be arranged consecutively.
- *lociPos:* Positions of all loci on all chromosome, as a list of float numbers. Default to 1, 2, ... etc on each chromosome. *lociPos* should be arranged chromosome by chromosome. If lociPos are not in order within a chromosome, they will be re-arranged along with corresponding *lociNames* (if specified).
- ancGen: Number of the most recent ancestral generations to keep during evolution. Default to 0, which means only the current generation will be kept. If it is set to -1, all ancestral generations will be kept in this population (and exhaust your computer RAM quickly).
- chromNames: A list of chromosome names. Default to chrom1, chrom2, ... etc.
- alleleNames: A list of allele names for all markers. For example, alleleNames = ('A','C','T','G') gives names A, C, T, and G to alleles 0, 1, 2, and 3 respectively.
- *lociNames*: A list of names for each locus. It can be empty or a list of unique names for each locus. If loci are not specified in order, loci names will be rearranged according to their position on the chromosome.
- subPopNames: A list of subpopulation names. All subpopulations will have name " if this parameter is not specified.
- infoFields: Names of information fields (named float number) that will be attached to each individual.

**Note** simuPOP does not yet support locus-specific allele names. If this information is very important, you can save allele names in the local namespace of a population.

absIndIndex (idx, subPop)

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

#### numSubPop()

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

#### subPopBegin (subPop)

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

#### subPopEnd(subPop)

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

## subPopIndPair(idx)

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

#### setSubPopName (name, subPop)

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

#### subPopByName (name)

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

## subPopName (subPop)

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

#### subPopNames()

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

#### popSize()

Return the total number of individuals in all subpopulations.

#### subPopSize(subPop=[])

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

## subPopSizes()

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

## numVirtualSubPop()

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

## setVirtualSplitter(splitter)

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

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

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

#### individuals (subPop=[])

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

## genotype (subPop=[])

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

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

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

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

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

## ancestralGens()

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

#### push (pop)

Push population *pop* into the current population. Both populations should have the same genotypic structure. The current population is discarded if *ancestralDepth* (maximum number of ancestral generations to hold) is zero so no ancestral generation can be kept. 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. Empty loci names will be used if *lociNames* is not specified.

## addChromFrom(pop)

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

#### addIndFrom(pop)

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

#### addLoci (chrom, pos, 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 empty strings will be assumed. Single-value input is allowed for parameter *chrom* and *pos* if only one locus is added. Alleles at inserted loci are initialized with zero alleles. Note that loci have to be added to existing chromosomes. If loci on a new chromosome need to be added, function addChrom should be used. This function returns indexes of the inserted loci.

## $\verb"addLociFrom"\,(pop)$

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)

## mergeSubPops (subPops=[], name=UnnamedSubPop)

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

#### removeIndividuals(inds)

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

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

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

## removeSubPops (subPops)

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

## resize (sizes, propagate=False)

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

## setSubPopByIndInfo(field)

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

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

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

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

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

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

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

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

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

## setInfoFields (fields, init=0)

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

## updateInfoFieldsFrom (fields, pop, fromFields=""List, ancGen=-1)

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

#### clone()

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

## save (filename)

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

#### vars (subPop=[])

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

#### dvars (subPop)

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

## 1.1.4 Class simulator

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

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

## class simulator (pop, matingScheme, rep=1)

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

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

## clone()

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

# save (filename)

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

#### gen()

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

#### setGen (gen)

Set the current generation number of a simulator to gen.

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

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

Operators *ops* are applied during the life cycle of each generation. Depending on the stage of these operators, they can be applied before-, during-, and/or post-mating. These operators can be applied at all or some of the generations, depending the *begin*, *end*, *step*, and *at* parameters of these operators. Populations in a simulator are evolved one by one. At each generation, the applicability of these operators are determined. Pre-mating operators are applied to a population first. A mating scheme is then used to populate an offspring generation, 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. If not all replicates are stopped at the same generation, the negative replicate numbers are calculated according to *active* replicates, meaning replicate -1 will refer to the last active replicate even if the last replicate has stopped. In addition, *postOps* are applied to all replicates, including those that stopped before other replicates.

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

#### extract(rep)

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

## numRep()

Return the number of replicates.

## population (rep)

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

## add(pop)

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

# populations()

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

## setMatingScheme (matingScheme)

Set a new mating scheme matingScheme to a simulator.

#### vars (rep, subPop=[])

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

#### dvars (rep, subPop)

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

## 1.1.5 Class pedigree

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

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

```
 \textbf{class pedigree} \ (pop, \quad loci=[], \quad infoFields=""List, \quad ancGen=-1, \quad fatherField="father\_idx", \quad mother-Field="mother\_idx")
```

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

#### clone()

Create a cloned copy of a pedigree.

# numParents()

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

## father (idx, subPop)

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

## mother (idx, subPop)

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

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

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

Parameter relType specifies what type of relative to locate. It can be Self, Spouse (having at least one common offspring), Offspring, FullSibling (having common father and mother), Sibling (having at least one common parent) or SpouseAndOffspring (One spouse and their common offspring). Optionally, you can specify the sex of relatives you would like to locate, in the form of relType=(type, sexChoice). sexChoice can be AnySex (default), MaleOnly, FemaleOnly, SameSex or OppositeSex. sexChoice for SpouseAndOffspring only refer to sex of offspring. This function will by default go through all ancestral generations and locate relatives for all individuals. This can be changed by setting parameter ancGen to the greatest ancestral generation you would like to process.

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

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

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

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

# 1.1.6 Class vspSplitter

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

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

```
class vspSplitter()
    This is a virtual class that cannot be instantiated.
    clone()
        All VSP splitter defines a clone() function to create an identical copy of itself.
    name(vsp)
        Return the name of VSP vsp (an index between 0 and numVirtualSubPop()).
    numVirtualSubPop()
        Return the number of VSPs defined by this splitter.
```

# 1.1.7 Class sexSplitter

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

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

#### numVirtualSubPop()

Return 2.

## 1.1.8 Class affectionSplitter

This class defines two VSPs according individual affection status. The first VSP consists of unaffected 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.

# 1.1.9 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 (vsn)

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

#### numVirtualSubPop()

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

# 1.1.10 Class proportionSplitter

This splitter divides subpopulations into several VSPs by proportion.

# class proportionSplitter (proportions=[])

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

```
name(vsp)
```

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

#### numVirtualSubPop()

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

## 1.1.11 Class rangeSplitter

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

## class rangeSplitter (ranges)

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

#### name(vsp)

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

#### numVirtualSubPop()

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

## 1.1.12 Class genotypeSplitter

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

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

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

#### name(vsp)

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

## numVirtualSubPop()

Number of virtual subpops of subpopulation sp

## 1.1.13 Class combinedSplitter

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

## class combinedSplitter (splitters=[])

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

#### name(vsp)

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

#### numVirtualSubPop()

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

# 1.2 Mating Schemes

# 1.2.1 Class homoMating

A homogeneous mating scheme that uses a parent chooser to choose parents from a 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=[], 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.

## 1.2.2 Class heteroMating

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

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

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

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

If multiple mating schemes are applied to the same subpopulation, a weight (parameter *weight*) can be given to each mating scheme to determine how many offspring it will produce. The default for all mating schemes are 0. In this case, the number of offspring each mating scheme produces is proportional to the size of its parental (virtual) subpopulation. If all weights are negative, the numbers of offspring are determined by the multiplication of the absolute values of the weights and their respective parental (virtual) subpopulation sizes.

If all weights are positive, the number of offspring produced by each mating scheme is proportional to these weights. Mating schemes with zero weight in this case will produce no offspring. If both negative and positive weights are present, negative weights are processed before positive ones.

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

clone()

Deep copy of a heterogeneous mating scheme

# 1.2.3 Class pedigreeMating

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

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

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

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

clone()

Deep copy of a Python mating scheme

## 1.2.4 Class sequentialParentChooser

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

#### class sequentialParentChooser()

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

clone()

Deep copy of a sequential parent chooser.

## 1.2.5 Class sequentialParentsChooser

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

#### class sequentialParentsChooser()

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

clone()

Deep copy of a sequential parents chooser.

#### 1.2.6 Class randomParentChooser

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

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

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

clone()

Deep copy of a random parent chooser.

## 1.2.7 Class randomParentsChooser

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

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

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

clone()

Deep copy of a random parents chooser.

## 1.2.8 Class polyParentsChooser

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

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

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

clone()

Deep copy of a parent chooser.

# 1.2.9 Class alphaParentsChooser

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

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

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

clone()

Deep copy of an alpha parents chooser.

### 1.2.10 Class infoParentsChooser

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

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

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

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

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

clone()

Deep copy of a infomation parent chooser.

## 1.2.11 Class pyParentsChooser

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

This parent chooser does not support virtual subpopulation directly. A ValueError will be raised if this parent chooser is applied to a virtual subpopulation. However, because virtual subpopulations are defined in the passed

parental population, it is easy to return parents from a particular virtual subpopulation using virtual subpopulation related functions.

## class pyParentsChooser (parentsGenerator)

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

clone()

Deep copy of a python parent chooser.

# 1.2.12 Class offspringGenerator

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

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

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

A number of *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 distributions 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.

## 1.2.13 Class controlledOffspringGenerator

This offspring generator populates an offspring population and controls allele frequencies at specified loci. At each generation, expected allele frequencies at these loci are passed from a user defined allele frequency *trajectory* function.

The offspring population is populated in two steps. At the first step, only families with disease alleles are accepted until until the expected number of disease alleles are met. At the second step, only families with wide type alleles are accepted to populate the rest of the offspring generation. This method is described in detail in "Peng et al, (2007) Forward-time simulations of populations with complex human diseases, PLoS Genetics".

class controlledOffspringGenerator (loci, alleles, freqFunc, ops=[], numOffspring=1, sex-Mode=RandomSex)

Create an offspring generator that selects offspring so that allele frequency at specified loci in the offspring generation reaches specified allele frequency. At the beginning of each generation, expected allele frequency of *alleles* at *loci* is returned from a user-defined trajectory function *freqFunc*. If there is no subpopulation, this function should return a list of frequencies for each locus. If there are multiple subpopulations, *freqFunc* can return a list of allele frequencies for all subpopulations or combined frequencies that ignore population structure. In the former case, allele frequencies should be arranged by loc0\_sp0, loc0\_sp1, ... loc1\_sp0, loc1\_sp1, ..., and so on. In the latter case, overall expected number of alleles are scattered to each subpopulation in proportion to existing number of alleles in each subpopulation, using a multinomial distribution.

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

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

clone()

Deep copy of a controlled random mating scheme.

## 1.2.14 Pre-defined mating schemes

cloneMating (numOffspring=1, sexMode=None, ops=[], subPopSize=[], subPop=(), weight=0, selection-field=None)

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

randomSelection (numOffspring=1, sexMode=None, ops=[], subPopSize=[], subPop=(), weight=0, selection-Field='fitness')

A homogeneous mating scheme that uses a random single-parent parent chooser with replacement, and a clone offspring generator. This mating scheme is usually used to simulate the basic haploid Wright-Fisher model but it can also be applied to diploid populations. Please refer to class randomParentChooser for parameter selectionField, to class offspringGenerator for parameters ops and numOffspring, and to class homoMating for parameters subPopSize, subPop and weight. Parameter sexMode is ignored because cloneOffspringGenerator copies sex from parents to offspring.

 $\begin{tabular}{ll} {\bf randomMating} (numOffspring=1, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0, selection-field='fitness') \\ \end{tabular}$ 

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

 $\begin{tabular}{ll} \textbf{monogamousMating} (numOffspring=1, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0, selection-field=None) \\ \end{tabular}$ 

A homogeneous mating scheme that uses a random parents chooser without replacement and a Mendelian offspring generator. It differs from the basic random mating scheme in that each parent can mate only once so there is no half-sibling in the population. Please refer to class offspringGenerator for parameters

ops, sexMode and numOffspring, and to class homoMating for parameters subPopSize, subPop and weight. Parameter selectionField is ignored because this mating scheme does not support natural selection.

polygamousMating (polySex=1, polyNum=1, numOffspring=1, sexMode=31, ops=[], subPopSize=[], sub-Pop=(), weight=0, selectionField='fitness')

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

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

haplodiploidMating (numOffspring=1.0, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0, selectionField='fitness')

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

selfMating (replacement=True, numOffspring=1, sexMode=31, ops=[], subPopSize=[], subPop=(), weight=0, selectionField='fitness')

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

**consanguineousMating** (infoFields=[], func=None, param=None, replacement=False, numOffspring=1.0, sex-Mode=31, ops=[], subPopSize=[], subPop=(), weight=0, selectionField='fitness')

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

controlledRandomMating (loci=[], alleles=[], freqFunc=None, numOffspring=1, sexMode=31, ops=[], sub-PopSize=[], subPop=(), weight=0, selectionField='fitness')

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

# 1.2.15 Pre-defined offspring generators

## cloneOffspringGenerator(ops=[], \*args, \*\*kwargs)

An offspring generator that uses cloneGenoTransmitter() as a default genotype transmitter. Additional during mating operators can be specified using the *ops* parameter. Other parameters are passed directly to offspringGenerator.

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

An offspring generator that uses mendelianGenoTransmitter() as a default genotype transmitter. Additional during mating operators can be specified using the *ops* parameter. Other parameters are passed directly to offspringGenerator.

## haplodiploidOffspringGenerator(ops=[], \*args, \*\*kwargs)

An offspring generator that uses haplodiploidGenoTransmitter() as a default genotype transmitter. Additional during mating operators can be specified using the *ops* parameter. Other parameters are passed directly to offspringGenerator.

## selfingOffspringGenerator(ops=[], \*args, \*\*kwargs)

An offspring generator that uses selfingGenoTransmitter() as a default genotype transmitter. Additional during mating operators can be specified using the *ops* parameter. Other parameters are passed directly to offspringGenerator.

# 1.3 Utility Classes

## 1.3.1 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 GetRNG() 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
     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.

# 1.4 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

## CloseOutput (output="")

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

#### Limits()

Print out system limits

#### DebugCodes()

Return names of all debug codes

## LoadPopulation (file)

Load a population from a file.

#### LoadSimulator (file, matingScheme)

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

#### 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

1.4. Global functions

#### 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.

# ${\tt TurnOnDebug}\,(code)$

Set debug code code. Name of available codes are available from DebugCodes.

## $TurnOffDebug(code=DBG\_ALL)$

Turn off debug code code. Default to turn off all debug codes.

## GetRNG()

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

# Chapter 2

# **Operator References (under revision)**

# 2.1 Base class for all operators

# 2.1.1 Class baseOperator

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

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

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

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

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

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

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

- mark ('!expr'). Alternatively, a Python function can be given to handle outputs.
- stage: Stage(s) of a life cycle at which an operator will be applied. It can be PreMating, DuringMating, PostMating or any of their combined stages PrePostMating, PreDuringMating, DuringPostMating and PreDuringPostMating. Note that all operators have their default stage parameter and some of them ignore this parameter because they can only be applied at certain stage(s) of a life cycle.
- *begin:* The starting generation at which an operator will be applied. Default to 0. A negative number is interpreted as a generation counted from the end of an evolution (-1 being the last evolved generation).
- end: The last generation at which an operator will be applied. Default to -1, namely the last generation.
- step: The number of generations between applicable generations. Default to 1.
- at: A list of applicable generations. Parameters begin, end, and step will be ignored if this parameter is specified. A single generation number is also acceptable.
- reps: A list of applicable replicates. A default value AllReps is interpreted as all replicates in a simulator. Negative indexes such as -1 (last replicate) is acceptable. rep=idx can be used as a shortcut for rep=[idx].
- subPops: A list of applicable (virtual) subpopulations, such as subPops=[sp1, sp2, (sp2, vsp1)].
  subPops=[sp1] can be simplied as subPops=sp1. Negative indexes are not supported. The default value of this parameter is usually AllSubPops which reprents all subpopulations of the population being aplied. Suport for this parameter vary from operator to operator and some operators do not support virtual subpopulations at all. Please refer to the reference manual of individual operators for their support for this parameter.
- *infoFields:* A list of information fields that will be used by an operator. You usually do not need to specify this parameter because operators that use information fields usually have default values for this parameter.

## apply (pop)

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

#### clone()

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

## 2.2 Initialization

## **2.2.1** Class initSex (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=[], reps=AllReps, sub-Pops=AllSubPops, infoFields=""List)

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 operator.

# 2.2.2 Class initByFreq (Function InitByFreq)

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

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

## **2.2.3 Class initByValue (Function** InitByValue)

This operator initialize individuals by given values.

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

# 2.3 Expression and Statements

# 2.3.1 Class pyOutput

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

```
 \textbf{class pyOutput} \ (msg="", output=">", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllReps, sub-Pops=AllSubPops, infoFields=""List)
```

Creates a pyoutput operator that outputs a string msg to output (default to standard terminal output) when it

is applied to a population. Please refer to class baseOperator for a detailed description of common operator parameters such as *stage*, *begin* and *output*.

```
apply (pop)
    Simply output some info
clone()
    Deep copy of a pyOutput operator.
```

# **2.3.2 Class pyEval (Function PyEval)**

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

```
class pyEval (expr="", stmts="", exposePop="", output=">", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List)
```

Crete a pyÉval operator that evaluates a Python expression *expr* in a population's local namespace when it is applied to this population. If Python statements *stmts* is given (a single or multi-line string), the statement will be executed before *expr*. If *exposePop* is set to an non-empty string, the current population will be exposed in its own local namespace as a variable with this name. This allows the execution of expressions such as 'pop.individual(0).allele(0)'. The result of *expr* will be sent to an output stream specified by parameter output. The exposed population variable will be removed after *expr* is evaluated. Please refer to class baseOperator for other parameters.

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

```
apply(pop)
```

Apply the pyEval operator to population *pop*.

clone()

Deep copy of a pyEval operator

evaluate(pop)

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

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

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

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

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

```
clone()
```

Deep copy of a pyExec operator

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

Unlike operator pyEval and pyExec that work at the population level, in a population's local namespace, operator

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

#### Note:

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

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

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

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

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

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

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

### 2.3.5 Class infoExec (Function InfoExec)

Operator infoExec is similar to infoEval in that it works at the individual level, using individual information fields as variables. The difference is that instead of evaluating an expression and outputing its result, this operator execute one or more statements and **update individual information fields** from the namespace after the specified statements are executed.

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

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

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

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

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

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

# 2.4 Demographic models

### 2.4.1 Class migrator

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

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

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

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

If migration is applied by probability, the row of the migration matrix corresponding to a source subpopulation is intepreted as probabilities to migrate to each destination subpopulation. Each individual's detination subpopulation is assigned randomly according to these probabilities. Note that the probability of staying at the present subpopulation is automatically calculated so the corresponding matrix elements are ignored.

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

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

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

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

Depending on the value of parameter mode, elements in the migration matrix (rate) are interpreted as either the probabilities to migrate from source to destination subpopulations (mode = ByProbability), proportions of

individuals in the source (virtual) subpopulations to the destination subpopulations (mode = ByProportion), numbers of migrants in the source (virtual) subpopulations (mode = ByPounts), or ignored completely (mode = ByIndInfo). In the last case, parameter subPops is respected (only individuals in specified (virtual) subpopulations will migrate) but toSubPops is ignored.

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

```
apply (pop)
    Apply the migrator to populaiton pop.
clone()
    Deep copy of a migrator
rate()
    Return migration rate
```

# **2.4.2 Class splitSubPops (Function SplitSubPops)**

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

```
class splitSubPops (subPops=AllSubPops, sizes=[], proportions=[], names=""List, randomize=True, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllReps, infoFields=""List)
Split a list of subpopulations subPops into finer subpopulations. A single subpopulation is acceptable but virtual subpopulations are not allowed. All subpopulations will be split if subPops is not specified.
```

The subpopulations can be split in three ways:

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

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

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

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

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

apply (pop)
Apply a splitSubPops operator

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

# **2.4.3 Class mergeSubPops (Function MergeSubPops)**

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

```
class mergeSubPops (subPops=AllSubPops, name="", stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllReps, infoFields=""List)
```

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

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

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

# **2.4.4 Class resizeSubPops (Function ResizeSubPops)**

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

```
class resizeSubPops (subPops=AllSubPops, sizes=[], proportions=[], propagate=True, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllReps, infoFields=""List"
```

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

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

```
apply (pop)
    Apply a resizeSubPops operator

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

# 2.5 Genotype transmitters

# 2.5.1 Class genoTransmitter

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

```
class genoTransmitter (begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List")

Create a base genotype transmitter.
```

#### clearChromosome (ind, ploidy, chrom)

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

#### clone()

Deep copy of a base genotype transmitter.

### copyChromosome (parent, parPloidy, offspring, ploidy, chrom)

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

### copyChromosomes (parent, parPloidy, offspring, ploidy)

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

### initialize(pop)

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

### 2.5.2 Class cloneGenoTransmitter

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

class cloneGenoTransmitter (begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List")

Create a clone genotype transmitter (a during-mating operator) that copies genotypes from parents to offspring. If two parents are specified, genotypes are copied maternally. Parameters *subPops*, and *infoFields* are ignored.

### clone()

Deep copy of a clone genotype transmitter.

### 2.5.3 Class mendelianGenoTransmitter

This Mendelian offspring generator accepts two parents and pass their genotypes to an offspring following Mendel's laws. Sex chromosomes are handled according to the sex of the offspring, which is usually determined in advance by an offspring generator. Customized chromosomes are not handled.

class mendelianGenoTransmitter (begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List)

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

#### clone()

Deep copy of a Mendelian genotype transmitter.

### initialize(pop)

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

### transmitGenotype (parent, offspring, ploidy)

Transmit genotype from parent to offspring, and fill the ploidy homologous set of chromosomes. This

function does not set genotypes of customized chromosomes and handles sex chromosomes properly, according to offspring sex and ploidy.

### 2.5.4 Class selfingGenoTransmitter

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

class selfingGenoTransmitter (begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, in-foFields=""List")

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

clone()

Deep copy of a selfing genotype transmitter.

# 2.5.5 Class haplodiploidGenoTransmitter

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

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

clone()

Deep copy of a haplodiploid transmitter.

#### 2.5.6 Class mitochondrialGenoTransmitter

This geno transmitter assumes that the first homologous copy of several (or all) Customized chromosomes are copies of mitochondrial chromosomes. It transmits these chromosomes randomly from the female parent to offspring. If this transmitter is applied to populations with more than one homologous copies of chromosomes, it transmits the first homologous copy of chromosomes and clears alleles (set to zero) on other homologous copies.

 $\textbf{class mitochondrialGenoTransmitter} (\textit{chroms} = [], \ \textit{begin} = 0, \ \textit{end} = -1, \ \textit{step} = 1, \ \textit{at} = [], \ \textit{reps} = AllReps, \ \textit{sub-Pops} = AllSubPops, \ \textit{infoFields} = ""List)$ 

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

**Note** The 'form offspring genotype' flag of this operator is set to False so this operator will not be the promary genotype transmitter. Please refer to the simuPOP user's guide for the implication of this setting. **clone**()

Deep copy of a mitochondrial genotype transmitter.

### 2.5.7 Class recombinator

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

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

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

#### Note:

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

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

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

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

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

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

Gene conversion is controlled using parameter convMode, which can be

- •NoConversion: no gene conversion (default).
- (NumMarkers, prob, n): With probability *prob*, convert a fixed number (n) of markers if a recombination event happens.
- (Geometric Distribution, prob, p): With probability prob, convert a random number of markers if a recombination event happens. The number of markes converted follows a geometric distribution with probability p.
- (TractLength, prob, n): With probability *prob*, convert a region of fixed tract length (n) if a recombination event happens. The actual number of markers converted depends on loci positions of surrounding loci. The starting position of this tract is the middle of two adjacent markers. For example, if four loci are located at 0, 1, 2, 3 respectively, a conversion event happens between 0 and 1, with a tract length 2 will start at 0.5 and end at 2.5, covering the second and third loci.
- (ExponentialDistribution, prob, p): With probability *prob*, convert a region of random tract length if a recombination event happens. The distribution of tract length follows a exponential distri-

bution with probability p. The actual number of markers converted depends on loci positions of surrounding loci.

simuPOP uses this probabilistic model of gene conversion because when a recombination event happens, it may become a recombination event if the Holliday junction is resolved/repaired successfully, or a conversion event if the junction is not resolved/repaired. The probability, however, is more commonly denoted by the ratio of conversion to recombination events in the literature. This ratio varies greatly from study to study, ranging from 0.1 to 15 (Chen et al, Nature Review Genetics, 2007). This translate to 0.1/0.90.1 to 15/160.94 of the gene conversion probability.

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

#### clone()

Deep copy of a recombinator

#### initialize(pop)

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

### transmitGenotype (parent, offspring, ploidy)

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

# 2.6 Mutation

### 2.6.1 Class mutator

Class mutator is the base class of all mutators. It handles all the work of picking an allele at specified loci from certain (virtual) subpopulation with certain probability, and calling a derived mutator to mutate the allele. Alleles can be changed before and after mutation if existing allele numbers do not match those of a mutation model.

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

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

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

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

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

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

```
apply (pop)
    Apply a mutator.

clone()
    Deep copy of a mutator

fillContext (pop, ptr, locus)
    A rarely used feature, performance should be a secondary consideration.
```

### **2.6.2** Class matrixMutator (Function MatrixMutate)

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

Create a mutator that mutates alleles 0, 1, ..., n-1 using a n by n matrix rate. Item (i, j) of this matrix specifies the probability at which allele i mutates to allele j. Diagnal items (i, i) are ignored because they are automatically determined by other probabilities. Only one mutation rate matrix can be specified which will be used for all loci in the applied population, or loci specified by parameter *loci*. Please refer to classes mutator and baseOperator for detailed explanation of other parameters.

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

### **2.6.3 Class kamMutator (Function KamMutate)**

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

```
class kamMutator (k=0, rates=[], loci=[], mapIn=[], mapOut=[], output=">", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List)
```

Create a k-allele mutator that mutates alleles to one of the other k-1 alleles with equal probability. If parameter k is unspecified, it will be assumed to be the number of allowed allelic states of the current simuPOP module. This mutator by default applies to all loci unless parameter loci is specified. A single mutation rate will be used for all loci if a single value of parameter rates is given. Otherwise, a list of mutation rates can be specified for each locus in parameter loci. Please refer to classes mutator and baseOperator for descriptions of other parameters.

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

2.6. Mutation 37

### **2.6.4 Class smmMutator (Function SmmMutate)**

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

```
 \begin{array}{lll} \textbf{class smmMutator} \ (rates=[], \ loci=[], \ incProb=0.5, \ maxAllele=0, \ mutStep=[], \ mapIn=[], \ mapOut=[], \ output=">", \ stage=PostMating, \ begin=0, \ end=-1, \ step=1, \ at=[], \ reps=AllReps, \ sub-Pops=AllSubPops, infoFields=""List) \end{array}
```

Create a stepwise mutation mutator that mutates an allele by increasing or decreasing it. This mutator by default applies to all loci unless parameter *loci* is specified. A single mutation rate will be used for all loci if a single value of parameter *rates* is given. Otherwise, a list of mutation rates can be specified for each locus in parameter *loci*.

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

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

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

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

```
clone()
```

Deep copy of a smmMutator

# **2.6.5** Class pyMutator (Function PyMutate)

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

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

```
clone()
```

Deep copy of a pyMutator

### **2.6.6 Class mixedMutator (Function MixedMutate)**

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

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

```
clone()
```

Deep copy of a mixedMutator

### **2.6.7 Class contextMutator (Function** ContextMutate)

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

Create a mutator that choose one of the specified *mutators* to mutate an allele when a mutation event happens. The mutators are choosen according to the context of the mutated allele, which is specified as a list of alleles to the left and right of an allele ( *contexts*). For example, contexts=[(0,0), (0,1), (1,1)] indicates which mutators should be used to mutate allele X in the context of 0X0, 0X1, and 1X1. A context can include more than one alleles at both left and right sides of a mutated allele but all contexts should have the same (even) number of alleles. If an allele does not have full context (e.g. when a locus is the first locus on a chromosome), unavailable alleles will be marked as -1. There should be a mutator for each context but an additional mutator can be specified as the default mutator for unmatched contexts. If parameters *mapIn* is specified, both mutated allele and its context alleles will be mapped. Most parameters, including *loci*, *mapIn*, *mapOut*, *rep*, and *subPops* of mutators specified in parameter *mutators* are ignored. This mutator by default applies to all loci unless parameter *loci* is specified. Please refer to classes mutator and baseOperator for descriptions of other parameters.

```
clone()
```

Deep copy of a context-dependent Mutator

### **2.6.8 Class pointMutator (Function PointMutate)**

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

Create a point mutator that mutates alleles at specified *loci* to a given *allele* of individuals *inds*. If there are multiple alleles at a locus (e.g. individuals in a diploid population), only the first allele is mutated unless indexes of alleles are listed in parameter *ploidy*. Please refer to class baseOperator for detailed descriptions of other parameters.

2.6. Mutation 39

```
apply (pop)
    Apply a pointMutator
clone()
    Deep copy of a pointMutator
```

### 2.6.9 Derived mutation operators

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

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

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

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

### 2.7 Selection

### 2.7.1 Class selector

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

- PreMating selectors assign fitness values to each individual, and mark part or all subpopulations as under selection.
- during sexless mating (e.g. binomialSelection mating scheme), individuals are chosen at probabilities that are proportional to their fitness values. If there are N individuals with fitness values  $f_i, i = 1, ..., N$ , 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.

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

#### 2.7.2 Class mapSelector (Function MapSelector)

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

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

### 2.7.3 Class maSelector (Function MaSelect)

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

This selector accepts an array of fitness values:

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

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

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

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

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

2.7. Selection 41

Calculate/return the fitness value, currently assuming diploid

### 2.7.4 Class mlSelector (Function MlSelect)

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

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

# **2.7.5** Class pySelector (Function PySelect)

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

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

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

clone()

Deep copy of a pySelector

### 2.8 Penetrance

### 2.8.1 Class basePenetrance

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

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

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

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

Penetrance functions can be applied to the current, all, or certain number of ancestral generations. This is controlled by the 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.

```
 \textbf{class basePenetrance} \ (ancestralGen=-1, \ stage=DuringMating, \ begin=0, \ end=-1, \ step=1, \ at=[], \ reps=AllReps, \\ subPops=AllSubPops, \ infoFields=""List)
```

Create a penetrance operator

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

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

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

 $\mathtt{apply}\,(pop)$ 

Set penetrance to all individuals and record penetrance if requested

clone (

Deep copy of a penetrance operator

### **2.8.2** Class mapPenetrance (Function MapPenetrance)

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

2.8. Penetrance 43

### 2.8.3 Class maPenetrance (Function MaPenetrance)

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

### **2.8.4** 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.

### **2.8.5** Class pyPenetrance (Function PyPenetrance)

Assign penetrance values by calling a user provided function For each individual, the penetrance is determined by a user-defined penetrance function func. This function takes 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.

# 2.9 Quantitative Trait

### 2.9.1 Class quanTrait

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

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

```
 \begin{array}{c} \textbf{class quanTrait} \ (ancGen=-1, \quad stage=PostMating, \quad begin=0, \quad end=-1, \quad step=1, \quad at=[], \quad reps=AllReps, \quad sub-Pops=AllSubPops, \quad infoFields=""List") \\ \textbf{Create a quantitative trait operator} \end{array}
```

2.9. Quantitative Trait 45

```
apply (pop)
    Set qtrait to all individual
clone()
    Deep copy of a quantitative trait operator
```

### **2.9.2 Class mapQuanTrait (Function** MapQuanTrait)

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

```
class mapQuanTrait (loci, qtrait, sigma=0, phase=False, ancGen=-1, stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List")

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\left(0,\sigma^2\right). phase: If True, a/b and b/a will have different quantitative trait values. Default to False. output: And other parameters please refer to help (baseOperator.__init__) clone()

Deep copy of a map quantitative trait operator
```

### **2.9.3 Class maQuanTrait (Function** MaQuanTrait)

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

### 2.9.4 Class mlQuanTrait (Function MlQuanTrait)

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

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

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

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

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

Create a multiple locus quantitative trait operator Please refer to quantitative for other parameter descriptions.

qtraits: A list of quantitative traits

mode: Can be one of Multiplicative and Additive

clone()

Deep copy of a multiple loci quantitative trait operator

qtrait (ind)

Currently assuming diploid

### **2.9.5** Class pyQuanTrait (Function PyQuanTrait)

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

Create a Python quantitative trait operator Please refer to quanTrait for other parameter descriptions.

loci: The genotypes at these loci will be passed to func.

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

output: And other parameters please refer to help(baseOperator.\_\_init\_\_)

clone()

Deep copy of a Python quantitative trait operator

### 2.10 Statistics Calculation

### **2.10.1 Class stat (Function Stat)**

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

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

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

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

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

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

Operator stat supports the following statistics:

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

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

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

- •numOfMale (default): Total number of male individuals in all or specified (virtual) subpopulations.
- •numOfMale (default): Total number of female individuals in all or specified (virtual) subpopulations.
- •propOfMale: Proportion of male individuals.
- •propOfFemale: Proportion of female individuals.
- •numOfMale\_sp: Number of male individuals in each (virtual) subpopulation.
- •numOfFemale\_sp: Number of female individuals in each (virtual) subpopulation.

- •propOfMale\_sp: Proportion of male individuals in each (virtual) subpopulation.
- •propOfFemale\_sp: Proportion of female individuals in each (virtual) subpopulation.

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

- •numOfAffected (default): Total number of affected individuals in all or specified (virtual) subpopulations.
- •numOfAffected (default): Total number of unaffected individuals in all or specified (virtual) subpopulations.
- •propOfAffected: Proportion of affected individuals.
- •propOfUnaffected: Proportion of unaffected individuals.
- •numOfAffected\_sp: Number of affected individuals in each (virtual) subpopulation.
- •numOfUnaffected\_sp: Number of unaffected individuals in each (virtual) subpopulation.
- •propOfAffected\_sp: Proportion of affected individuals in each (virtual) subpopulation.
- •propOfUnaffected\_sp: Proportion of unaffected individuals in each (virtual) subpopulation.

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

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

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

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

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

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

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

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

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

- •sumOfInfo (default for *sumOfInfo*): A dictionary of the sum of specified information fields of individuals in all or specified (virtual) subpopulations. This dictionary is indexed by names of information fields.
- •meanOfInfo (default for *meanOfInfo*): A dictionary of the mean of information fields of all individuals.
- •varOfInfo (default for *varOfInfo*): A dictionary of the sample variance of information fields of all individuals.
- •maxOfInfo (default for *maxOfInfo*): A dictionary of the maximum value of information fields of all individuals.
- •minOfInfo (default for *minOfInfo*): A dictionary of the minimal value of information fields of all individuals.
- •sumOfInfo\_sp: A dictionary of the sum of information fields of individuals in each subpopulation.
- •meanOfInfo\_sp: A dictionary of the mean of information fields of individuals in each subpopulation.
- •varOfInfo\_sp: A dictionary of the sample variance of information fields of individuals in each subpopulation.
- •maxOfInfo\_sp: A dictionary of the maximum value of information fields of individuals in each subpopulation.
- •minOfInfo\_sp: A dictionary of the minimal value of information fields of individuals in each subpopulation.
- **LD**: Parameter LD accepts one or a list of loci pairs (e.g. LD=[[0,1], [2,3]]) with optional primary alleles at both loci (e.g. LD=[0,1,0,0]). For each pair of loci, this operator calculates linkage disequilibrium

and optional association statistics between two loci. When primary alleles are specified, signed linkage disequilibrium values are calculated with non-primary alleles are combined. Otherwise, absolute values of diallelic measures are combined to yield positive measure of LD. Association measures are calculated from a m by n contigency of haplotype counts (m=n=2 if primary alleles are specified). Please refer to the simuPOP user's guide for detailed information. This statistic sets the following variables:

- LD (default) Basic LD measure for haplotypes in all or specified (virtual) subpopulations. Signed if primary alleles are specified.
- •LD\_prime (default) Lewontin's D' measure for haplotypes in all or specified (virtual) subpopulations. Signed if primary alleles are specified.
- •R2 (default) Correlation LD measure for haplotypes in all or specified (virtual) subpopulations.
- •LD\_ChiSq ChiSq statistics for a contigency table with frequencies of haplotypes in all or specified (virtual) subpopulations.
- •LD\_ChiSq\_p Single side p-value for the ChiSq statistic. Degrees of freedom is determined by number of alleles at both loci and the specification of primary alleles.
- •CramerV Normalized ChiSq statistics.
- •LD\_sp Basic LD measure for haplotypes in each (virtual) subpopulation.
- •LD\_prime\_sp Lewontin's D' measure for haplotypes in each (virtual) subpopulation.
- •R2\_sp R2 measure for haplotypes in each (virtual) subpopulation.
- •LD\_ChiSq\_sp ChiSq statistics for each (virtual) subpopulation.
- •LD\_ChiSq\_p\_sp p value for the ChiSq statistics for each (virtual) subpopulation.
- •CramerV\_sp Cramer V statistics for each (virtual) subpopulation.

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

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

This statistic sets the following variables:

- •Allele\_ChiSq A dictionary of allele-based Chi-Square statistics for each locus, using cases and controls in all or specified (virtual) subpopulations.
- •Allele\_ChiSq\_p (default) A dictionary of *p-values* of the corresponding Chi-square statistics.
- •Geno\_ChiSq A dictionary of genotype-based Chi-Square statistics for each locus, using cases and controls in all or specified (virtual) subpopulations.
- •Geno\_ChiSq\_p A dictionary of *p-values* of the corresponding genotype-based Chi-square test.
- •Armitage\_p A dictionary of *p-values* of the Cochran-Armitage tests, using cases and controls in all or specified (virtual) subpopulations.
- •Allele\_ChiSq\_sp A dictionary of allele-based Chi-Square statistics for each locus, using cases and controls from each subpopulation.
- •Allele\_ChiSq\_p\_sp A dictionary of p-values of allele-based Chi-square tests, using cases and controls from each (virtual) subpopulation.

- •Geno\_ChiSq\_sp A dictionary of genotype-based Chi-Square tests for each locus, using cases and controls from each subpopulation.
- •Geno\_ChiSq\_p\_sp A dictionary of p-values of genotype-based Chi-Square tests, using cases and controls from each subpopulation.
- •Armitage\_p\_sp A dictionary of *p-values* of the Cochran- Armitage tests, using cases and controls from each subpopulation.

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

- •Pi Mean pairwise difference between all sequences from all or specified (virtual) subpopulations.
- •Pi\_sp Mean paiewise difference between all sequences in each (virtual) subpopulation.

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

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

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

- •HWE (default) A dictionary of p-values of HWE tests using genotypes in all or specified (virtual) subpopulations
- •HWE\_sp A dictionary of p-values of HWS tests using genotypes in each (virtual) subpopulation.

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

# 2.11 Tagging (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

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

list even if only one field is given.

### 2.12 Terminator

### 2.12.1 Class terminateIf

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

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

```
apply (pop)
```

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

clone()

Deep copy of a terminateIf terminator

# 2.13 The Python operator

# 2.13.1 Class pyOperator

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

**class pyOperator** (func, param=None, stage=PostMating, isTransmitter=False, offspringOnly=False, begin=0, end=-1, step=1, at=[], reps=AllReps, subPops=AllSubPops, infoFields=""List)

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

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

where pop is the population to which the operator is applied, off is the offspring of dad and mom, and param is the parameter *param* specified when the operator is created. When this operator is applied during mating, it can become a *genotype transmitter* if parameter *isTransmitter* is set to True. That is to say, the genotype transmitter defined in a mating scheme will not be applied when this operator is active. Please refer to the simuPOP user's guide for a detailed explanation about *genotype transmitters*.

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

### apply(pop)

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

# 2.14 Ascertainment operators

# 2.14.1 Class randomSample

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

### class randomSample (size, \*args, \*\*kwargs)

Draw *size* random samples from a population *times* times. *size* can be a number or a list of numbers. In the former case, individuals are drawn from the whole population and the samples has only one subpopulation. In the latter case, a given number of individuals are drawn from each subpopulation and the result sample has the same number of subpopulation as the population from which samples are drawn. The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

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

Function version of operator randomSample.

# 2.14.2 Class caseControlSample

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

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

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

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

Function version of operator caseControlSample whose \_\_init\_\_function is

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

### 2.14.3 Class affectedSibpairSample

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

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

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

Draw *size* families, including two affected siblings and their parents from a population repeatedly. The population to be sampled must have at least one ancestral generation. It should also have two information fields specified by parameter *infoFields* (Default to ['father\_idx', 'mother\_idx']. Parameter *size* can be

a number or a list of numbers. In the former case, affected sibpairs are drawn from the whole population. In the latter case, a given number of affected sibpairs are drawn from each subpopulation. In both cases, affected sibpairs in the resulting sample form their own subpopulations (of size two). The samples are saved in the population's local namespace if *name* or *nameExpr* is given, and are saved as diskfiles if *saveAs* or *saveAsExpr* is given.

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

Function version of operator affectedSibpairSample whose \_\_init\_\_function is

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

# 2.15 Miscellaneous operators

### 2.15.1 Class noneOp

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

### 2.15.2 Class dumper

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

Create a operator that dumps the genotype structure (if *structure* is True) and genotype (if *genotype* is True) to an *output* (default to standard terminal output). Because a population can be large, this operator will only output the first 100 (parameter *max*) individuals of the present generation (parameter *ancGen*). All loci will be outputed unless parameter *loci* are used to specify a subset of loci. If a list of (virtual) subpopulations are specified, this operator will only output individuals in these outputs. Please refer to class baseOperator for a detailed explanation for common parameters such as *output* and *stage*.

```
apply (pop)
          Apply a dumper operator to population pop.
clone()
          Deep copy of a dumper operator.
```

### 2.15.3 Class savePopulation

An operator that save populations to specified files.

**class savePopulation** (output="", stage=PostMating, begin=0, end=-1, step=1, at=[], reps=AllReps, sub-Pops=AllSubPops, infoFields=""List)

Create an operator that saves a population to *output* when it is applied to the population. This operator supports all output specifications (", 'filename', 'filename' prefixed by one or more '>' characters, and '!expr') but output from different operators will always replace existing files (effectively ignore '>' specification). Parameter *subPops* is ignored. Please refer to class baseOperator for a detailed description about common operator parameters such as *stage* and *begin*.

```
\mathtt{apply}\left(pop\right)
```

Apply operator to population pop.

clone()

Deep copy of a savePopulation operator.

### 2.15.4 Class setAncestralDepth

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

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

apply(pop)

Apply the setAncestralDepth operator to population pop.

### 2.15.5 Class if Else

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

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

apply (pop)

Apply the ifElse operator to population *pop*.

### 2.15.6 Class pause

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

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

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

After a population has been paused, a message will be displayed (unless *prompt* is set to False) and tells you how to proceed. You can press 's' to stop the evolution of this population, 'S' to stop the evolution of all populations, or 'p' to enter a Python shell. The current population will be available in this Python shell as "pop\_X\_Y" when X is generation number and Y is replicate number. The evolution will continue after you exit this interactive Python shell.

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

Apply the pause operator to one population

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

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

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

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

 $\begin{array}{c} \textbf{class turnOnDebug} \ (code, \quad stage = PreMating, \quad begin = 0, \quad end = -1, \quad step = 1, \quad at = [], \quad reps = AllReps, \quad sub-Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\ \hline \\ Pops = AllSubPops, \quad infoFields = ""List) \\$ 

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

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

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

class turnOffDebug (code, stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllReps, sub-Pops=AllSubPops, infoFields=""List")

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

# 2.15.9 Class ticToc

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

class ticToc (output=">", stage=PreMating, begin=0, end=-1, step=1, at=[], reps=AllReps, sub-Pops=AllSubPops, infoFields=""List)

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

# 2.16 Function form of operators

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

Apply operator dumper to population pop.

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

Apply operator initSex to population pop.

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

Apply operator initByFreq to population pop.

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

Apply operator initByValue to population pop.

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

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

### **Note**

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

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

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

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

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

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

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

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

Function form of operator migrator.

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

Function form of operator matrixMutator

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

Function form of operator snpMutator

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

Function form of operator acgtMutator

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

Function form of operator kamMutator

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

Function form of operator smmMutator

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

Function form of operator pyMutator

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

Function form of operator mixedMutator

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

Function form of operator contextMutator

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

Function form of operator pointMutator

# **Chapter 3**

# **Utility Modules**

# 3.1 Module simuOpt

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

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

"-optimized" Load the optimized version of a simuPOP module.

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

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

"-h" or "-help" Print usage message.

be loaded.

"-config=configFile" Read parameters from a configuration file \*configFile\*.

### 3.1.1 Loadding a simuPOP module

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

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

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

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

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

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

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

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

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

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

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

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

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

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

### 3.1.2 Parameter handling

#### valueNot (t)

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

#### valueOr(t1, t2)

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

#### valueAnd(t1, t2)

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

#### valueOneOf(t)

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

#### valueTrueFalse()

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

#### valueBetween(a, b)

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

#### valueGT(a)

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

### valueGE(a)

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

#### valueLT(a)

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

### valueLE(a)

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

#### valueEqual(a)

Return a function that returns true if passed option equals a

#### valueNotEqual(a)

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

#### valueIsNum()

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

#### valueIsList()

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

#### valueValidDir()

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

#### valueValidFile()

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

### 3.1.3 Class simuOpt

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

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

- arg: Short command line option name. For example 'c' checks the presence of argument -c. If a value is expected, a comma should be appened to the option name. For example, 'p:' matches command line option -p=100 or -p 100. An options that does not expect a value is displayed in the parameter input dialog as an on/off switch.
- longarg: Long command line option name. For example 'version' checks the presence of argument --version. A equal character should be appended to the option name if a value is expected. For example, 'mu=' matches command line option --mu=0.001 or --mu 0.001. This item defines the name of an option and cannot be ignored. An options that does not expect a value is displayed in the parameter input dialog as an on/off switch.
- *label:* The label of the input field in a parameter input dialog. It will also be used as the prompt for this option during interactive parameter input. **Options without a label will not be displayed in the parameter input dialog and will not be saved to a configuration file.** A typical example of such an option is --version.
- default: Default value for this parameter. It is used as the default value in the parameter input dialog, and as the option value when a user presses Enter directly during interactive parameter input. A default value is required for all options.
- useDefault: Use default value without asking, if the value can not be determined from GUI, command line option or config file. This is usually used for options that rarely need to be changed. Setting useDefault to such options simplifies user input.
- description: A long description of this parameter. This description will be put into the usage information, and as parameter tooltip in the parameter input dialog. This string will be reformatted when it is written to a usage string (remove newlines and extra spaces and re-indent), with the exception that lines with 'l' as the first non-space/tab character will be outputed as is without the leading 'l' symbol.
- allowedTypes: A list of acceptable types of this option. class simuOpt will try to convert user input to these types. For example, if allowedTypes is types.ListType or types.TupleType and the user's input is a scalar, the input will be converted to a list automatically. An option will not be accepted if such conversion fails. If this item is not specified, the type of the default value will be used.
- validate: A function to validate the parameter. The function will be applied to user input. The option will not be accepted if this function returns False. This module defines a large number of such validation functions but user defined functions are also acceptable.

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

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

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

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

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

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

### class simuOpt (options=[], doc=", details=", \*\*kwargs)

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

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

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

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

#### asDict()

Return parameters as a dictionary.

#### asList()

Return parameters as a list.

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

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

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

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

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

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

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

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

Get parameter from a Tkinter or wxPython dialog. The parameter will try to arrange parameters optimally but you can also set the number of columns using parameter nCol. If both GUI toolkits are

available, wxPython will be used unless *gui* is set to Tkinter. If none of the toolkits are available, this function will raise an ImportError.

#### Note

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

#### loadConfig (file, params=[])

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

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

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

```
saveConfig (file, params=[])
```

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

#### termGetParam (params=[])

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

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

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

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

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

# 3.2 Module simuUtil (under revision)

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

#### ViewVars (var, gui=None)

list a variable in tree format, either in text format or in a: wxPython window.

var: A dictionary variable to be viewed. Dictionary wrapper objects returned by population.dvars() and simulator.dvars() are also acceptable.

gui: If gui is False or 'Tkinter', a text presentation (use the pprint module) of the variable will be printed to the screen. If gui is 'wxPython' and wxPython is available, a wxPython windows will be used. The default mode is determined by the global gui mode (see also simuOpt.setOptions).

### MigrIslandRates(r, n)

migration rate matrix

```
x m/(n-1) m/(n-1) \dots m/(n-1) x \dots
```

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

#### MigrHierarchicalIslandRates (r1, r2, n)

Return the migration rate matrix for a hierarchical island model where there are different migration rate within and across groups of islands.

- r1: Within group migration rates. It can be a number or a list of numbers for each group of the islands.
- *r2:* Across group migration rates which is the probability that someone will migrate to a subpopulation outside of his group. A list of r2 could be specified for each group of the islands.
- n: Number of islands in each group. E.g. n=[5, 4] specifies two groups of islands with 5 and 4 islands each.

For individuals in an island, the probability that it remains in the same island is 1-r1-r2 (r1, r2 might vary by island groups), that it migrates to another island in the same group is r1 and migrates to another island outside of the group is r2. Migrate rate to a specific island depends on the size of group.

### MigrSteppingStoneRates (r, n, circular=False)

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

or non-circular

SaveCSV (pop, filename=", fields=[], loci=[], header=True, shift=1, sexCode={1: '1', 2: '2'}, affection-Code={False: '2', True: '1'}, \*\*kwargs)

Save a simuPOP population pop in csv format.

pop: A simuPOP population object. If a string is given, it will be loaded.

filename: Output filename.

fileds: Information fields to be outputted.

loci: If a list of loci is given, only genotype at these loci will be written.

header: Whether or not a header should be written. These headers will include information fields, sex (if sexCode is not None), affection status (if affectionCode is not None) and loci names. If genotype at a locus needs more than one column, \_1, \_2 etc will be appended to locus names.

genotype: list of loci to output, default to all.

combine: how to combine the markers. Default to None. A function can be specified, that takes the form:

```
def func(markers):
    return markers[0]+markers[1]
```

*shift:* since alleles in simuPOP is 0-based, shift=1 is usually needed to output alleles starting from allele 1. This parameter is ignored if combine is used.

# 3.2.1 Class simuProgress

The simuProgress class defines a progress bar. This class will use a text-based progress bar that outputs progressing dots (.) with intermediate numbers (e.g. 5 for 50%) under a non-GUI mode (gui=False). In the GUI mode, a Tkinter or wxPython progress dialog will be used (gui=Tkinter or gui=wxPython). The default mode is determined by the global gui mode of simuPOP (see also simuOpt.setOptions).

This class is usually used as follows:

```
progress = simuProgress("Start simulation", 500)
for i in range (500):
     progress.update(i+1)
# if you would like to make sure the done message is displayed.
progress.done()
class simuProgress (message, totalCount, progressChar='.', block=2, done=' Done.
                      n', gui=None)
     message: Title of the progress bar.
totalCount: Total expected steps.
progressChar: Character to be displayed for each progress. This is only used for text-based progress bars.
block: Intervals at which progresses will be displayed. Default to 2 (percent).
done: Message displayed when the job is finished.
done()
     Finish progressbar, print 'done' message if in text-mode.
update(count)
     Update the progreebar.
```

# 3.2.2 Class trajectory

A trajectory object returned by trajectory simulation class trajectorySimulator(...) with several user- friendly built-in functions. Function func() could refer to allele frequencies in any simulated generation in cases of single/multiple loci with single population/multiple subpopulations. Function printTraj() shows allele frequencies of all generations from the simulation. Function plot() illustrates allele frequencies of all generations based on numbers of loci and variable number of subpopulations. For example, at generation i, if there are x loci and y subpopulations, x \* y dots showing corresponded allele frequencies at any different locus or subpopulation will appear in the plot for i.

```
class trajectory (endGen, nLoci, beginGen=None)
```

beginGen and endGen are inclusive. (frequency for endGen exists) parameters description:

*traj:* built-in dictionary which records allele frequencies at multiple loci within all subpopulations and has generation numbers as keys.

*beginGen:* passed in value which represents the beginning generation number in the forward trajectory. Default None in backward trajectory.

*endGen:* passed in value which is the ending generation number in forward trajectory and namely the current generation number in backward trajectory where simulations begin.

*nLoci:* passed in value of number of loci

```
freq(gen)
```

Return frequencies at generation gen. If the trajectory is empty, it returns a list of 0s for n Loci.

#### func()

Return a Python function that returns allele frequencies for each locus. If there are multiple subpopulations, allele frequencies are arranged in the order of loc0\_sp0, loc0\_sp1, ..., loc1\_sp0, loc1\_sp1, ... and so on.

```
plot (r, **kwargs)
```

Plot current trajectory.

r: The R object defined in a rpy module.

kwargs: Additional keyword arguments that will be passed to the plot function.

#### printTraj()

Print allele frequencies for all generations.

```
setFreq(freq, gen, nSubPop)
```

This function sets passed in frequencies for generation gen to the global dictionary object traj.

## 3.2.3 Class trajectorySimulator

Simulate trajectories of disease susceptibility loci using an extension of the backward method described in Slatkin 2001 or forward algorithms.

Tracking allele frequencies of alleles on all loci.

Class trajectory(...) takes four arguments, at least three (N, fitness, nLoci) need to be specified by the user:

*N*: population size, which may be passed in as a constant number or an array of subpop sizes or a user defined function, NtFunc(gen), which returns population size at each generation.

fitness: selection pressure for all loci, which can be passed in as a constant array showing fitness for [AA, Aa, aa, BB, Bb, bb,...] or a user defined function, fitnessFunc(gen), which returns selection pressure at each generation.

*nLoci:* number of Loci, which should be passed in as a constant integer number with its value equal to or larger than 1.

logger: Logged messages have levels of importance associated with them. The default levels provided are DEBUG, INFO, WARNING, ERROR and CRITICAL. User should indicate the importance of a logged message. Default value for logger is None.

#### class trajectorySimulator (N, fitness, nLoci, logger=None)

Initialization of global parameters.

Parameter description:

N: pass in population size "N" to global variable self.N, which may be a number, a list of subpop sizes or a user-defined function.

fitness: pass in selection pressure "fitness" to global variable self.fitness, which may take forms such as, a list of three values in the case of single locus or same fitness for any locus within multiple loci, a list of 3 \* nLoci values in the case of multi-loci without interaction, a list of 3\*\*nLoci values when multi-loci and interaction situation are both considered.

*nLoci:* pass in number of loci "nLoci" to global variable self.nLoci.

*logger:* pass in level of importance "logger" to global variable self.logger, which is a logging object that can be used to record warnings and error messages.

*errorCount:* define global dictionary object self.errorCount as the variable to record counts of distinct forms of errors that occur during the simulation.

Simulate trajectories of multiple disease susceptibility loci using an extension of the backward method described in Slatkin 2001.

parameter description:

*genEnd:* generation number in the end, namely the current generation number in the backward trajectory. *freq:* expected allele frequencies of alleles of multiple unlinked loci. It may take forms of a single value or a list of values with number of elements equal to nLoci. In the case of single value, such freq will

be shared by all loci. FIXME: There are multiple subpopultions and only one frequency is given, the same frequency will be used for all subpopulations. Users can specify different allele frequencies for each subpopulation using the long form...

minMutAge: minimum generation number. The process will restart if the trajectory is less than it. Default to 0.

maxMutAge: maximum generation number. The process will terminate or restart if it can not reach allele zero after T generations. Default to 100,000, roughly 2,000,000 years which is longer than human history.

ploidy: number of chromosomes will be N \* ploidy

*restartIfFail:* If the process can not finish after T generations, restart if restartIfFail = True, otherwise return. Default to False.

maxAttempts: How many times to try to get a valid path? Default to 1000.

logger: return potential problems if not None. Default to None.

Return the trajectory for each locus at each subpopulation. In the order of LOC0: sp0, sp1, sp2,..., LOC1: sp0, sp1, sp2,...

**simuForward** (*freq*, *destFreq*, *genBegin=0*, *genEnd=0*, *ploidy=2*, *maxAttempts=10000*, *logger=None*) Simulate trajectories of multiple disease susceptibility loci using a forward time approach

Return the trajectory for each locus at each subpopulation. In the order of LOC0: sp0, sp1, sp2, ..., LOC1: sp0, sp1, sp2,... Each trajectory will have length genEnd - genBegin + 1

parameter description:

genBegin: starting generation number

genEnd: ending generation number

freq: allele frequencies of alleles of multiple unlinked loci at the beginning generation.

destFreq: expected range of allele frequencies of alleles of multiple unlinked loci, at generation genEnd, with all subpopulation combined. If there are two loci, it can be [[0.08, 0.12], [0.19, 0.21]]

ploidy: number of chromosomes will be N\*ploidy

maxAttempts: How many times to try to get a valid path? Default 10,000

ForwardTrajectory (N, fitness, nLoci, freq, destFreq, genBegin=0, genEnd=0, ploidy=2, maxAttempts=10000, logger=None)

Return an object to class trajectory in forward simulation.

 $\label{eq:backwardTrajectory} \textbf{Exact N}, \textit{fitness}, \textit{nLoci}, \textit{genEnd}, \textit{freq}, \textit{minMutAge=0}, \textit{maxMutAge=100000}, \textit{ploidy=2}, \textit{restartIfFail=False}, \textit{maxAttempts=1000}, \textit{logger=None})$ 

Return an object to class trajectory in backward simulation.

# 3.3 Module simuRPy

This module defines several utility functions and Python operators that make use of the Python rpy module (http://rpy.sourceforge.net) to plot expressions and information fields of evolving populations using a popular statistical analysis language R (http://www.r-project.org). Note that rpy2, the successor of rpy, is currently not supported.

Each operator calls a sequence of R functions to draw and save figures. A special parameter passing mechanism is used so that you can specify arbitrary parameters to these functions. For example, you can use parameter "par\_mfrow=[2,2]" to pass "mfrow=[2,2]" to function "par", and use "lty\_rep=[1,2]" to pass "lty=1" and "lty=2" to specify different line types for different replicates. The help message of each class will describe which and in what sequence these R functions are called to help you figure out which parameters are allowed.

#### newDevice()

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

saveFigure (file=None, \*\*kwargs)

Save current figure into file. File format and graphics device are determined by file extension. Supported file

formats include pdf, png, bmp, jpg (jpeg), tif (tiff), and eps, which correspond to R devices pdf, png, bmp, jpeg, tiff and postscript. A postscript device will be used if there is no file extension or the file extension is not recognizable. Additional keyword parameters will be passed to the underlying dev.print function.

## 3.3.1 Class derivedArgs

This class implements the derived keyword argument handling mechanism that is used by all classes defined in this module. It is provided for users who would like to use this mechanism for their own rpy-related operators.

An derived keyword argument is an argument that is prefixed with a function name and/or suffixed by an iterator name. The former specifies to which underlying R function this parameter will be passed to; the latter allows the users to specify a list of values that will be passed, for example, to lines representing different replicates. For example, parameter  $par_mar=[1]*4$  will pass mar=[1]\*4 to R function par, and  $lty_rep=[1, 2, 3]$  will pass lty=1, lty=2 and lty=3 to different replicates.

Values provided to derived arguments are usually passed unchanged, but with one exception: string value with a leading! mark will be evaluated against the current population before it is returned. For example, main='!"Allele frequency at generation %d" % gen' will return main="Allele frequency at generation 100" at generation 100.

```
class derivedArgs (defaultFuncs=[], allFuncs=[], suffixes=[], defaultParams={}, **kwargs) defaultFunc: Default functions. Parameters without a prefix will be passed to these functions.
```

allFuncs: Allowed functions. This should be all the R functions called in your class.

suffixes: A list of allowed suffixes.

defaultParams: Default parameters in a dictionary. E.g. {'plot\_type': 'l'} will pass type='l' to the plot function unless users provides another value.

kwargs: User specified parameters. These parameters will overwide default values in defaultParams.

```
addDefault (**kwargs)
```

Add keyword parameters kwargs if they have not been defined.

```
getArgs (func, pop, **kwargs)
```

Get all single format parameters from keyword parameters. Additional keyword arguments can be used to specify suffix and its index. (e.g. rep=1 will return the second element of par\_rep). Unrecognized keyword arguments are handled as default value that will be used if a parameter is not defined. E.g. getArgs('line', pop, rep=1, pch=4) will get parameters for replicate 1 and add pch=4 if pch is not defined.

```
getLegendArgs (func, pop, args, keys, values, **kwargs)
```

Get argument values for legend drawing purposes. For example,

```
getMultiArgs('lines', pop, ['lty', 'pch'], 'rep', [0,1,2])
```

will get parameter for lty and pch for all rep. If there are more keys (e.g. ['rep', 'dim']), values should be a list of of lists (e.g., [(0, 0), (0, 1), (0, 2), (1, 0), (1, 1), (1, 2)]). Default values could be passed as additional keyword arguments.

# 3.3.2 Class varPlotter

This class defines a Python operator that uses R to plot the current and historical values of a Python expression (expr), which are evaluated (against each population's local namespace) and saved during evolution. The return value of the expression can be a number or a sequence, but should have the same type and length across all replicates and generations. Histories of each value (or each item in the returned sequence) of each replicate form a line, with generation numbers as its x-axis. Number of lines will be the number of replicates multiplied by dimension of the

expression. Although complete histories are usually saved, you can use parameter win to save histories only within the last win generations.

A figure will be draw at the end of the last replicate (except for the first generation where no line could be drawn) unless the current generation is less than update generations away from the last generation at which a figure has been drawn. Lines for multiple replicates or dimensions could be plotted in the same figure (by default), or be separated to subplots by replicates (byRep), by each dimention of the results (byDim), or by both. These figure could be saved to files in various formats if parameter saveAs is specified. File format is determined by file extension. After the evolution, the graphic device could be left open (leaveOpen).

Besides parameters mentioned above, arbitrary keyword parameters could be specified and be passed to the underlying R drawing functions plot and lines. These parameters could be used to specify line type (lty), color (col), title (main), limit of x and y axes (xlim and ylim) and many other options (see R manual for details). As a special case, multiple values can be passed to each replicate and/or dimension if the name of a parameter ends with \_rep, \_dim, or \_repdim For example, lty\_rep=range(1, 5) will pass parameters lty=1, ... lty=4 to four replicates. You can also pass parameters to specific R functions such as par, plot, lines, legend, dev\_print by prefixing parameter names with a function name. For example, dev\_print\_width=300 will pass width=300 to function dev.print() when you save your figures using this function. In addition, if the value of a parameter is a string starting with!, the evaluated result of the remaining string will be used as parameter value. Further customization of your figures could be achieved by writing your own hook functions that will be called before and after a figure is drawn, and after each plot call.

This opertor calls R functions par, plot, lines, legend, and dev.print. Functions plot and lines are the default destination for keyword arguments and the ones that accept list parameters to customize lines by replicate and/or dimension.

*expr:* expression that will be evaluated at each replicate's local namespace when the operator is applied. Its value can be a number or a list (or tuple) but the type and length of the return value should be consistent for all replicates and at all generations.

win: Window of generations. If given, only values from generation -win to -1 will be plotted.

update: Update the figure after specified generations. For example, you can evalulate an expression and save its values at every 10 generations (parameter step=10) but only draw a figure after every 50 generations (parameter update=50.

byRep: Separate values at different replicates to different subplots.

byDim: Separate items from sequence results of expr to different subplots. If both byRep and byDim are True, the subplots will be arranged by variable and then replicates.

saveAs: Save figures in files saveAs\_gen.ext (e.g. figure\_10.eps if saveAs='figure.eps'). If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used. Currently supported formats include .pdf, .png, .bmp, .jpg, and .tif. The default filename could be overridden by derived argument dev\_print\_file.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to False functions.
If this option is set to True, you will have to close the graphic device explicitly using function rpy.r.dev\_off(). Note that leaving the device open allows further manipuation of the figures outside of this operator.

*legend:* labels of the lines. This operator will look for keyword parameters such as col, lty, lwd, and pch and call the legend function to draw a legend. If figure has multiple lines for both replicates and dimensions, legends should be given to each dimension, and then each replicate.

*preHook:* A function that, if given, will be called before the figure is draw. The r object from the rpy module will be passed to this function.

- postHook: A function that, if given, will be called after the figure is drawn. The r object from the rpy module will be passed to this function.
- plotHook: A function that, if given, will be called after each plot function. The r object from the rpy module, generation list, data being plotted, replicate number (if applicable) and dimension index (if applicable) will be passed as keyword arguments r, gen, data, rep (optional) and dim (optional).
- kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) plot\_, lines\_, par\_, legend\_ and dev\_print\_, and suffixes (list parameters) \_rep, \_dim, and \_repdim. Arguments without prefixes are sent to functions plot and lines. String values with a leading! will be replaced by its evaluated result against the current population.

#### 3.3.3 Class scatterPlotter

This class defines a Python operator that uses R to plot individuals in a population, using values at two information fields as their x- and y-axis.

Arbitrary keyword parameters could be specified and be passed to the underlying R drawing functions plot and points. These parameters could be used to specify point type (pch), color (col), title (main), limit of x and y axes (xlim and ylim) and many other options (see R manual for details). You can also pass parameters to specific R functions such as par, plot, points, legend, pdf by prefixing parameter names with a function name. For example, par\_mar=[1]\*4 will pass par=[1]\*4 to function par() which is called before a figure is drawn. (Note that the function to save a figure is dev.print so parameters such as dev\_print\_width should be used.) Further customization of your figures could be achieved by writing your own hook functions that will be called before and after a figure is drawn.

The power of this operator lies in its ability to differentiate individuals from different (virtual) subpopulations. If you specify IDs of (virtual) subpopulations (VSPs) in parameter <code>subPops</code>, only individuals from these VSPs will be displayed. Points from these subpopulations will be drawn with different shapes and colors. You can also customize these points using list parameters with suffix <code>\_sp</code>. For example, if you have defined two VSPs by sex and set <code>subPops=[(0, 0), (0, 1)], col\_sp=['blue', 'red']</code> will color male individuals with blue and female individuals with red. In addition, if the value of a parameter is a string starting with!, the evaluated result of the remaining string will be used as parameter value.

This opertor calls R functions par, plot, points, legend, and dev.print. Functions plot and points are the default destination for keyword arguments and the ones that accept list parameters to customize lines by (virtual) subpopulation.

*infoFields*: Two information fields whose values will be the x- and y-axis of each point (individual) in the plot.

- *subPops:* A list of subpopulations and virtual subpopulations. Only individuals from these subpopulations will be plotted. Default to subpopulation indexes.
- saveAs: Save figures in files saveAs\_gen\_rep.ext (e.g. figure\_10\_0.eps if saveAs='figure.eps').
  If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used.
  Currently supported formats include .pdf, .png, .bmp, .jpg, and .tif. The default filename could be overriden by derived argument dev\_print\_file.
- *leaveOpen:* Whether or not leave the plot open when plotting is done. Default to False functions. If this option is set to True, you will have to close the graphic device explicitly using function rpy.r.dev\_off(). Note that leaving the device open allows further manipuation of the figures outside of this operator.

*legend:* labels of the points. It must match the specified subpopulations.

*preHook:* A function that, if given, will be called before the figure is draw. The r object from the rpy module will be passed to this function.

postHook: A function that, if given, will be called after the figure is drawn. The r object from the rpy module will be passed to this function.

kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) plot\_, points\_, par\_, legend\_ and dev\_print\_, and suffixes (list parameters)\_sp. Arguments without prefixes are sent to functions plot and points. String values with a leading! will be replaced by its evaluated result against the current population.

#### 3.3.4 Class infoPlotter

This operator uses a R function such as hist and qqplot to plot properties of one or more information fields of individuals in one or more (virtual) subpopulations. Separate subplots are used for different information fields and subpopulations.

This operator essentially gets values of information fields and sends them to a R function such as hist. The resulting figures could be customized by additional keyword parameters and various hook functions. For example, a qqline function could be called in a plotHook function to add a QQ line to a qqnorm plot. The plotHook can be used to draw the whole (sub)plot if no R function is specified for parameter func.

Besides regular keyword parameters, keyword parameters ending in \_sp, \_fld or \_spfld are expected to have multiple values which will be used for differnt subpopulations, information fields, and their combinations. You can also specify which function the keyword should be sent by prefixing a function name to the parameter name. For example, pch\_fld=[1, 2] will use different symbols for different information fields, and par\_mar=[1] \*4 will send parameter mar=[1] \*4 to function par. In addition, if the value of a parameter is a string starting with !, the evaluated result of the remaining string will be used as parameter value.

This opertor calls R functions par, dev.print, and a user-specified function. Additional keyword arguments without function prefix will be sent to this function.

class infoPlotter (func=None, infoFields=[], saveAs=", leaveOpen=False, preHook=None, postHook=None, plotHook=None, stage=4, begin=0, end=-1, step=1, at=[], reps=<simuPOP\_std.repList; proxy of <Swig Object of type 'simuPOP::repList \*' at 0x2aed305c2490> >, sub-Pops=<simuPOP\_std.subPopList; proxy of <Swig Object of type 'simuPOP::subPopList \*' at 0x2aed305c2490> >, \*\*kwargs)

func: Name of the R function that will be called to draw figures from values of given information fields. No R function will be called if it is not specified. In this case, a plotHook can be used to plot passed values.

infoFields: Information fields whose values will be sent to the specified plotting function.

*subPops:* A list of subpopulations and virtual subpopulations. Each subpopulation will be plotted in a separate subplot.

saveAs: Save figures in files saveAs\_gen\_rep.ext (e.g. figure\_10\_0.eps if saveAs=' figure.eps').
If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used.
Currently supported formats include .pdf, .png, .bmp, .jpg, and .tif. The default filename could be overriden by derived argument dev\_print\_file.

leaveOpen: Whether or not leave the plot open when plotting is done. Default to False functions. If this option is set to True, you will have to close the graphic device explicitly using function rpy.r.dev\_off(). Note that leaving the device open allows further manipuation of the figures outside of this operator.

*preHook:* A function that, if given, will be called before the figure is draw. The r object from the rpy module will be passed to this function.

3.3. Module simuRPy

- postHook: A function that, if given, will be called after the figure is drawn. The r object from the rpy module will be passed to this function.
- plotHook: A function that, if given, will be called after each specified plot function. The r object from the rpy module, data being plotted, name of the information field and index of subpopulation (in parameter subPops, if applicable) will be passed with keywords r, data, field and subPop (optional) respectively.
- kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) par\_, dev\_print\_ and the function you specify (parameter func), and suffixes (list parameters) \_sp, \_fld, and \_spfld. Arguments without prefixes are sent to the user specified function. String values with a leading! will be replaced by its evaluated result against the current population.

#### histPlotter(\*args, \*\*kwargs)

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

#### qqPlotter(\*args, \*\*kwargs)

A infoPlotter that uses R function <code>qqnorm</code> to draw qq plot of individual information fields of specified (virtual) subpopulations. Please see <code>infoPlotter</code> for details.

#### 3.3.5 Class boxPlotter

This operator draws boxplots of one or more information fields of individuals in one or more (virtual) subpopulations of a population. Although a infoPlotter with func=boxplot could be used to plot boxplots for each information field and/or subpopulation, this class allows multiple whiskers to share one plot. How the whiskers are oraganized is controlled by parameters byField and bySubPop.

This operator essentially gets values of information fields and sends them to boxplots. Individual ownerships (subpopulation or field) are also passed so that multiple whiskers could be drawn in the same plot. The resulting figures could be customized by additional keyword parameters and various hook functions.

Besides regular keyword parameters, keyword parameters ending in \_sp, \_fld or \_spfld are expected to have multiple values which will be used for differnt subpopulations, information fields, and their combinations. You can also specify which function the keyword should be sent by prefixing a function name to the parameter name. For example, pch\_fld=[1, 2] will use different symbols for different information fields, and par\_mar=[1] \*4 will send parameter mar=[1] \*4 to function par. In addition, if the value of a parameter is a string starting with!, the evaluated result of the remaining string will be used as parameter value.

This opertor calls R functions par, boxplot and dev.print. Keyword parameters without function prefix will be passed to boxplot.

- class boxPlotter (infoFields=[], byField=False, bySubPop=False, saveAs=", leaveOpen=False, pre-Hook=None, postHook=None, plotHook=None, stage=4, begin=0, end=-1, step=1, at=[], reps=<simuPOP\_std.repList; proxy of <Swig Object of type 'simuPOP::repList \*' at 0x2aed305c2490> >, subPops=<simuPOP\_std.subPopList; proxy of <Swig Object of type 'simuPOP::subPopList \*' at 0x2aed305c2490> >, \*\*kwargs)
  - infoFields: Information fields whose values will be sent to R function boxplot.
- *subPops:* A list of subpopulations and virtual subpopulations. Separate whiskers will be drawn for individuals in these subpopulations.
- *byField:* If multiple information fields are specified, separate the whiskers different subplots if this parameter is True.
- *bySubPop:* If multiple (virtual) subpopulations are specified, separate the whiskers to different subplots if this parameter is True.
- saveAs: Save figures in files saveAs\_gen\_rep.ext (e.g. figure\_10\_0.eps if saveAs=' figure.eps').

  If ext is given, a corresponding device will be used. Otherwise, a default postscript driver will be used.

- Currently supported formats include .pdf, .png, .bmp, .jpg, and .tif. The default filename could be overriden by derived argument dev\_print\_file.
- leaveOpen: Whether or not leave the plot open when plotting is done. Default to False functions. If this option is set to True, you will have to close the graphic device explicitly using function rpy.r.dev\_off(). Note that leaving the device open allows further manipuation of the figures outside of this operator.
- *preHook:* A function that, if given, will be called before the figure is draw. The r object from the rpy module will be passed to this function.
- *postHook:* A function that, if given, will be called after the figure is drawn. The r object from the rpy module will be passed to this function.
- plotHook: A function that, if given, will be called after each specified plot function. The r object from the rpy module, current field and subpopulation will be passed with keywords r, field and subpopulation if applicable.
- kwargs: Additional keyword arguments that will be interpreted and sent to underlying R functions. These arguments could have prefixes (destination function names) plot\_, boxplot\_, par\_, and dev\_print\_, and suffixes (list parameters) \_sp, \_fld and \_spfld. Arguments without prefixes are sent to function boxplot. String values with a leading! will be replaced by its evaluated result against the current population.

3.3. Module simuRPy 75

absIndIndex() (population method), 5	apply() (pyOutput method), 28
absLocusIndex() (GenoStruTrait method), 2	apply () (quanTrait method), 46
AcgtMutate() (in module), 60	apply () (resizeSubPops method), 32
acgtMutator() (in module), 40	apply() (savePopulation method), 58
add() (simulator method), 10	apply() (selector method), 41
addChrom() (population method), 7	apply () (setAncestralDepth method), 58
addChromFrom() (population method), 7	apply() (splitSubPops method), 31
addDefault () (derivedArgs method), 70	apply() (stat method), 52
addIndFrom() (population method), 7	apply () (terminateIf method), 55
addInfoFields() (population method), 8	asDict () (simuOpt method), 64
addLoci() (population method), 7	asList() (simuOpt method), 64
addLociFrom() (population method), 7	AvailableRNGs () (in module), 23
addOption() (simuOpt method), 64	
affected() (individual method), 4	BackwardTrajectory() (in module),69
affectedChar() (individual method), 4	baseOperator (class in ), 25
AffectedSibpairSample() (in module), 57	basePenetrance (class in ), 43
affectedSibpairSample (class in ), 56	boxPlotter (class in ), 74
affectionSplitter(class in), 13	
allele() (individual method), 3	CaseControlSample() (in module), 56
alleleName() (GenoStruTrait method), 3	caseControlSample (class in ), 56
alleleNames() (GenoStruTrait method), 3	chromBegin() (GenoStruTrait method), 2
AlleleType() (in module), 23	chromByName() (GenoStruTrait method), 2
alphaMating() (in module), 21	chromEnd() (GenoStruTrait method), 2
alphaParentsChooser (class in ), 18	chromLocusPair() (GenoStruTrait method), 2
ancestor() (population method), 7	chromName () (GenoStruTrait method), 2
ancestralGens() (population method), 7	chromNames () (GenoStruTrait method), 2
apply () (baseOperator method), 26	chromType() (GenoStruTrait method), 2
apply () (basePenetrance method), 43	chromTypes() (GenoStruTrait method), 2
apply() (dumper method), 57	class
apply () (ifElse method), 58	affectionSplitter, 13
apply () (infoEval method), 29	alphaParentsChooser, 18
apply () (infoExec method), 30	baseOperator, 25
apply () (initByFreq method), 27	basePenetrance, 43
apply () (initByValue method), 27	cloneGenoTransmitter, 33
apply () (initSex method), 26	combinedSplitter, 14
apply () (mergeSubPops method), 32	contextMutator, 39
apply () (migrator method), 31	controlledOffspringGenerator, 19
apply () (mutator method), 37	dumper, 57
apply() (noneOp method), 57	GenoStruTrait, 1
apply() (parentTagger method), 53	genoTransmitter, 32
apply () (parentsTagger method), 54	genotypeSplitter, 14
apply() (pause method), 59	haplodiploidGenoTransmitter, 34
apply() (pointMutator method), 40	heteroMating, 15 homoMating, 15
apply() (pyEval method), 28	ifElse, 58
apply() (pyOperator method), 55	HEISE, JO

individual, 3	RNG, 22
infoEval, 28	savePopulation, 58
infoExec, 29	selector, 40
infoParentsChooser, 18	selfingGenoTransmitter, 34
infoSplitter, 13	sequentialParentChooser, 16
inheritTagger, 53	sequentialParentsChooser, 16
initByFreq, 27	setAncestralDepth, 58
initByValue, 27	sexSplitter, 12
initSex, 26	simulator, 9
kamMutator, 37	smmMutator, 38
maPenetrance, 44	splitSubPops, 31
mapPenetrance, 43	stat, 47
mapQuanTrait, 46	
* -	tagger, 52
mapSelector, 41	terminateIf, 54
maQuanTrait, 46	ticToc, 59
maSelector, 41	turnOffDebug, 59
matrixMutator, 37	turnOnDebug, 59
mendelianGenoTransmitter, 33	vspSplitter, 12
mergeSubPops, 32	clearChromosome() (genoTransmitter method), 32
migrator, 30	clone() (alphaParentsChooser method), 18
mitochondrialGenoTransmitter, 34	clone() (baseOperator method), 26
mixedMutator, 39	clone() (basePenetrance method), 43
mlPenetrance, 44	clone() (cloneGenoTransmitter method), 33
mlQuanTrait, 47	clone() (contextMutator method), 39
mlSelector, 42	clone () (controlledOffspringGenerator method), 20
mutator, 36	clone() (dumper method), 57
noneOp, 57	clone() (genoTransmitter method), 33
offspringGenerator, 19	clone() (haplodiploidGenoTransmitter method), 34
parentsTagger, 53	clone() (heteroMating method), 16
parentTagger, 53	clone() (homoMating method), 15
pause, 58	clone() (infoEval method), 29
pedigree, 11	clone() (infoExec method), 30
pedigreeMating, 16	clone() (infoParentsChooser method), 18
pedigreeTagger, 54	clone() (inheritTagger method), 53
pointMutator, 39	clone () (initByFreq method), 27
polyParentsChooser, 17	clone () (initByValue method), 27
population, 4	clone () (initSex method), 26
proportionSplitter, 13	clone() (kamMutator method), 37
pyEval, 28	clone () (maPenetrance method), 44
pyExec, 28	clone () (maQuanTrait method), 46
pyMutator, 38	clone () (maSelector method), 42
pyOperator, 55	clone () (mapPenetrance method), 44
pyOutput, 27	clone() (mapQuanTrait method), 46
pyParentsChooser, 18	clone() (mapSelector method), 41
pyPenetrance, 45	clone() (matrixMutator method), 37
pyQuanTrait, 47	clone() (mendelianGenoTransmitter method), 33
pySelector, 42	clone() (mergeSubPops method), 32
pyTagger, 54	clone() (migrator method), 31
quanTrait, 45	clone() (mitochondrialGenoTransmitter method), 34
randomParentChooser, 17	clone() (mixedMutator method), 39
randomParentsChooser, 17	clone() (mlPenetrance method), 45
rangeSplitter, 14	clone() (mlQuanTrait method), 47
recombinator, 35	clone() (mlSelector method), 42
resizeSubPops, 32	clone() (mutator method), 37

clone () (offspringGenerator method), 19	evaluate() (pyEval method), 28
clone() (parentTagger method), 53	evolve() (simulator method), 10
clone () (parentsTagger method), 54	extract() (population method), 8
clone() (pedigreeMating method), 16	extract() (simulator method), 10
clone() (pedigree method), 11	
clone () (pointMutator method), 40	father() (pedigree method), 11
clone () (polyParentsChooser method), 18	fillContext() (mutator method), 37
clone () (population method), 9	ForwardTrajectory()(in module),69
clone () (pyEval method), 28	freq() (trajectory method), 67
clone() (pyExec method), 28	func() (trajectory method), 67
clone () (pyMutator method), 38	function
clone () (pyOutput method), 28	ContextMutate, 39
clone () (pyParentsChooser method), 19	InfoEval, 28
clone () (pyPenetrance method), 45	InfoExec, 29
clone () (pyQuanTrait method), 47	InitByFreq, 27
clone() (pySelector method), 43	InitByValue, 27
clone() (pyTagger method), 54	InitSex, 26
clone() (quanTrait method), 46	KamMutate, 37
clone() (randomParentChooser method), 17	MaPenetrance, 44
clone() (randomParentsChooser method), 17	MaQuanTrait, 46
clone () (recombinator method), 36	MaSelect,41
clone() (resizeSubPops method), 32	MapPenetrance, 43
clone () (savePopulation method), 58	MapQuanTrait,46
clone () (selector method), 41	MapSelector, 41
clone () (selfingGenoTransmitter method), 34	MatrixMutate, 37
clone () (sequentialParentChooser method), 16	MergeSubPops, 32
clone () (sequential Parents Chooser method), 17	MixedMutate, 39
clone() (simulator method), 9	MlPenetrance, 44
clone() (smmMutator method), 38	MlQuanTrait,47
clone() (splitSubPops method), 31	MlSelect, 42
clone() (stat method), 52	PointMutate, 39
clone() (tagger method), 53	PyEval, 28
clone() (tagger method), 55	PyExec, 28
clone() (vspSplitter method), 12	PyMutate, 38
cloneGenoTransmitter (class in ), 33	PyPenetrance, 45
	PyQuanTrait, 47
cloneMating() (in module), 20 cloneOffspringGenerator() (in module), 22	PySelect, 42
CloseOutput() (in module), 23	ResizeSubPops, 32
	SmmMutate, 38
combinedSplitter (class in), 14	SplitSubPops, 31
consanguineousMating() (in module), 21	Stat, 47
ContextMutate() (in module), 60	TurnOffDebug, 59
contextMutator (class in ), 39	TurnOnDebug, 59
controlledOffspringGenerator(class in), 20	Turnonbebug, 39
controlledRandomMating() (in module), 21	gen () (simulator method), 10
copyChromosome () (genoTransmitter method), 33	GenoStruTrait (class in ), 1
copyChromosomes() (genoTransmitter method), 33	genoTransmitter (class in ), 32
DebugGedes () (in modula) 23	genotype() (individual method), 3
DebugCodes () (in module), 23 derivedArgs (class in), 70	genotype () (population method), 6
done() (simuProgress method), 67	genotypeSplitter(class in), 14
	getArgs () (derivedArgs method), 70
Dump () (in module), 60	getLegendArgs() (derivedArgs method), 70
dumper (class in), 57	getParam() (simuOpt method), 64
dvars () (population method), 9	GetRNG() (in module), 24
dvars() (simulator method), 11	3331113 ( / (III III 0 0 0 II ), 2 I

<pre>guiGetParam() (simuOpt method), 64</pre>	locusName() (GenoStruTrait method), 2 locusPos() (GenoStruTrait method), 2
haplodiploidGenoTransmitter (class in), 34	
haplodiploidMating() (in module), 21	maPenetrance (class in ), 44
$\verb haplodiploidOffspringGenerator()  (in mod-$	mapPenetrance (class in ), 44
ule ), 22	mapQuanTrait (class in ), 46
heteroMating (class in ), 15	mapSelector(class in),41
histPlotter() (in module), 74	maQuanTrait (class in ), 46
homoMating (class in ), 15	maSelector (class in ), 41
	mating scheme, 15
ifElse (class in ), 58	MatrixMutate() (in module),60
indFitness() (maSelector method), 42	matrixMutator (class in ), 37
indInfo() (population method), 8	max() (RNG method), 22
individual, 1	MaxAllele() (in module), 23
individual() (population method), 6	maxSeed() (RNG method), 22
individual (class in ), 3	mendelianGenoTransmitter (class in), 33
individuals () (population method), 6	<pre>mendelianOffspringGenerator() (in module),</pre>
info() (individual method), 4	22
InfoEval() (in module), 60	mergeSubPops() (population method), 8
infoEval (class in ), 29	mergeSubPops (class in ), 32
InfoExec() (in module), 60	Migrate() (in module), 60
infoExec (class in ), 29	migrator, 30
infoField() (GenoStruTrait method), 3	migrator (class in ), 30
<pre>infoFields() (GenoStruTrait method), 3</pre>	MigrHierarchicalIslandRates() (in module),
infoldx() (GenoStruTrait method), 3	66
infoParentsChooser (class in ), 18	MigrIslandRates() (in module), 65
infoPlotter (class in ), 73	MigrSteppingStoneRates() (in module), 66
infoSplitter (class in ), 13	mitochondrialGenoTransmitter (class in), 34
inheritTagger (class in ), 53	MixedMutate() (in module), 60
<pre>InitByFreq() (in module), 60</pre>	mixedMutator(class in), 39
initByFreq(class in), 27	mlPenetrance (class in ), 45
<pre>InitByValue() (in module), 60</pre>	mlQuanTrait (class in ), 47
initByValue(class in), 27	mlSelector (class in), 42
initialize() (genoTransmitter method), 33	module
$\verb initialize()  (mendelian Geno Transmitter method),\\$	affectedSibpairSample, 56
33	boxPlotter, 74
initialize() (recombinator method), 36	caseControlSample, 56
initializer, 26	derivedArgs, 70
InitSex() (in module), 60	infoPlotter, 73
initSex (class in ), 26	randomSample, 56
intInfo() (individual method), 4	scatterPlotter, 72
4.4.	simuOpt, 63
KamMutate() (in module), 60	simuProgress, 67
kamMutator (class in ), 37	trajectory, 67
T 1 11 () (2	trajectorySimulator, 68
Limits() (in module), 23	varPlotter, 70
loadConfig() (simuOpt method), 65	ModuleCompiler() (in module), 23
LoadPopulation() (in module), 23	ModuleDate() (in module), 24
LoadSimulator() (in module), 23	ModulePlatForm() (in module), 24
locateRelatives () (pedigree method), 11	ModulePyVersion() (in module), 24
lociByNames () (GenoStruTrait method), 2	monogamousMating() (in module), 20
lociDist() (GenoStruTrait method), 2	mother() (pedigree method), 11
lociNames () (GenoStruTrait method), 2	Mutation, 36
lociPos() (GenoStruTrait method), 2	mutator (class in ), 36
locusByName() (GenoStruTrait method), 2	

name () (RNG method), 22	PyEval() (in module), 60
name () (affectionSplitter method), 13	pyEval (class in ), 28
name () (combinedSplitter method), 15	PyExec() (in module), 60
name () (genotypeSplitter method), 14	pyExec (class in ), 28
name () (infoSplitter method), 13	PyMutate() (in module), 60
name () (proportionSplitter method), 13	pyMutator (class in ), 38
name () (rangeSplitter method), 14	pyOperator(class in),55
name () (sexSplitter method), 12	pyOutput (class in ), 27
name() (vspSplitter method), 12	pyParentsChooser (class in ), 19
newDevice() (in module), 69	pyPenetrance (class in ), 45
noneOp (class in ), 57	pyQuanTrait (class in ), 47
numChrom() (GenoStruTrait method), 2	pySelector (class in ), 42
numLoci() (GenoStruTrait method), 2	pyTagger (class in ), 54
numParents() (pedigree method), 11	
numRep() (simulator method), 10	qqPlotter() (in module), 74
numSubPop() (population method), 5	qtrait() (mlQuanTrait method), 47
numVirtualSubPop() (affectionSplitter method), 13	quantitative trait, 45
numVirtualSubPop() (combinedSplitter method), 15	quanTrait (class in ), 45
<pre>numVirtualSubPop() (genotypeSplitter method), 14</pre>	randBinomial() (RNG method), 22
numVirtualSubPop() (infoSplitter method), 13	randBit () (RNG method), 22
numVirtualSubPop() (population method), 6	randExponential() (RNG method), 22
<pre>numVirtualSubPop() (proportionSplitter method),</pre>	randGeometric() (RNG method), 22
13	randGet () (RNG method), 22
numVirtualSubPop() (rangeSplitter method), 14	randInt() (RNG method), 22
numVirtualSubPop() (sexSplitter method), 13	randMultinomial() (RNG method), 23
numVirtualSubPop() (vspSplitter method), 12	randMultinomialVal() (RNG method), 23
	randNormal() (RNG method), 23 randomMating() (in module), 20
offspringGenerator (class in ), 19	randomParentChooser (class in ), 17
Optimized() (in module), 24	randomParentsChooser (class in), 17
parentsTagger (class in ), 54	RandomSample() (in module), 56
parentTagger (class in ), 53	randomSample (class in), 56
pause (class in ), 59	randomSelection() (in module), 20
pedigree (class in ), 11	randPoisson() (RNG method), 23
pedigreeMating (class in ), 16	randUniform01() (RNG method), 23
pedigreeTagger (class in ), 76	rangeSplitter (class in ), 14
penetrance, 43	rate() (migrator method), 31
ploidy() (GenoStruTrait method), 1	recombinator (class in), 35
ploidyName() (GenoStruTrait method), 1	removeIndividuals() (population method), 8
plot () (trajectory method), 68	removeLoci() (population method), 8
PointMutate() (in module), 60	removeSubPops() (population method), 8
pointMutator (class in ), 39	resize() (population method), 8
polygamousMating() (in module), 21	resizeSubPops (class in), 32
polyParentsChooser (class in ), 17	RNG (class in ), 22
popSize() (population method), 6	•
population, 1	save() (population method), 9
population() (simulator method), 10	save() (simulator method), 9
population (class in ), 5	saveConfig() (simuOpt method), 65
populations () (simulator method), 10	SaveCSV() (in module), 66
printTraj() (trajectory method), 68	saveFigure() (in module), 69
processArgs() (simuOpt method), 65	savePopulation (class in ), 58
proportionSplitter (class in ), 13	scatterPlotter (class in ),72
push () (population method), 7	seed() (RNG method), 23
* *	selection, 40

selector (class in ), 41	acgtMutator, 40
selfingGenoTransmitter(class in), 34	AffectedSibpairSample, 57
<pre>selfingOffspringGenerator() (in module), 22</pre>	alphaMating, 21
selfMating() (in module), 21	CaseControlSample, 56
sequentialParentChooser (class in), 16	cloneMating, 20
sequentialParentsChooser (class in ), 17	cloneOffspringGenerator, 22
setAffected() (individual method), 4	consanguineousMating, 21
setAllele() (individual method), 3	ContextMutate, 60
setAncestralDepth() (population method), 7	controlledRandomMating, 21
setAncestralDepth (class in ), 58	DebugCodes, 23
setFreq() (trajectory method), 68	Dump, 60
setGen() (simulator method), 10	haplodiploidMating, 21
setGenotype() (individual method), 4	haplodiploidOffspringGenerator, 22
setGenotype() (population method), 7	InfoEval, 60
setIndInfo() (population method), 9	InfoEvat, 60
setInfo() (individual method), 4	InitByFreq, 60
setInfoFields() (population method), 9	InitByValue, 60
setMatingScheme() (simulator method), 10	InitSex, 60
	KamMutate, 60
setOptions() (in module), 61	
SetRNG() (in module), 24	MatrixMutate, 60
setRNG() (RNG method), 23	mendelianOffspringGenerator, 22
setSeed() (RNG method), 23	Migrate, 60
setSex() (individual method), 4	MixedMutate, 60
setSubPopByIndInfo() (population method), 8	monogamousMating, 20
setSubPopName() (population method), 6	PointMutate, 60
setVirtualSplitter() (population method), 6	polygamousMating, 21
sex() (individual method), 4	PyEval, 60
sexChar() (individual method), 4	PyExec, 60
sexSplitter (class in ), 12	PyMutate, 60
simuBackward() (trajectorySimulator method), 68	randomMating, 20
simuForward() (trajectorySimulator method), 69	RandomSample, 56
Simulator, 1	randomSelection, 20
simulator (class in ), 9	selfingOffspringGenerator, 22
simuOpt, 61	selfMating, 21
setOptions, 61	SmmMutate, 60
valueAnd, 62	SnpMutate, 60
valueBetween, 62	snpMutator, 40
valueEqual, 62	simuProgress(classin),67
valueGE, 62	simuRev() (in module), 24
valueGT, 62	simuRPy, 69
valueIsList, 63	histPlotter, 74
valueIsNum, 63	newDevice, 69
valueLE, 62	qqPlotter, 74
valueLT, 62	saveFigure, 69
valueNot, 62	simuUtil, 65
valueNotEqual, 62	BackwardTrajectory, 69
valueOneOf, 62	ForwardTrajectory, 69
valueOr, 62	MigrHierarchicalIslandRates, 66
valueTrueFalse, 62	MigrIslandRates, 65
value Valid Dir, 63	MigrSteppingStoneRates, 66
value ValidFile, 63	SaveCSV, 66
simuOpt (class in ), 64	ViewVars, 65
simuPOP	simuVer() (in module), 24
AcgtMutate, 60	SmmMutate() (in module), 60
110501100000	ommutacace () (in inoduic ), oo

```
smmMutator (class in), 38
                                                  ViewVars() (in module), 65
SnpMutate() (in module), 60
                                                  vspSplitter (class in), 12
snpMutator() (in module), 40
splitSubPop() (population method), 8
splitSubPops (class in), 31
stat (class in), 48
subPopBegin() (population method), 6
subPopByName () (population method), 6
subPopEnd() (population method), 6
subPopIndPair() (population method), 6
subPopName() (population method), 6
subPopNames () (population method), 6
subPopSize() (population method), 6
subPopSizes() (population method), 6
tagger (class in), 53
termGetParam() (simuOpt method), 65
terminateIf (class in), 55
ticToc (class in), 59
totNumLoci() (GenoStruTrait method), 3
traceRelatives() (pedigree method), 12
trajectory (class in), 67
trajectorySimulator (class in), 68
transmitGenotype() (mendelianGenoTransmitter
        method), 33
transmitGenotype() (recombinator method), 36
TurnOffDebug() (in module), 24
turnOffDebug (class in), 59
TurnOnDebug() (in module), 24
turnOnDebug (class in), 59
update() (simuProgress method), 67
updateInfoFieldsFrom() (population method), 9
usage() (simuOpt method), 65
useAncestralGen() (population method), 7
valueAnd() (in module), 62
valueBetween () (in module), 62
valueEqual() (in module), 62
valueGE() (in module), 62
valueGT() (in module), 62
valueIsList() (in module), 63
valueIsNum() (in module), 63
valueLE() (in module), 62
valueLT() (in module), 62
valueNot() (in module), 62
valueNotEqual() (in module), 63
valueOneOf() (in module), 62
valueOr() (in module), 62
valueTrueFalse() (in module), 62
valueValidDir() (in module), 63
valueValidFile() (in module), 63
varPlotter (class in), 71
vars () (population method), 9
vars () (simulator method), 11
```