

In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

Mating scheme

Simulator

Forward-time simulations using simuPOP, an in-depth course

Bo Peng, Ph.D.

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June 15th, 2007 simuPOP workshop School of Public Health, Department of Biostatistics University of Alabama Birmingham



outline

In-depth course

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- Loading simuPOP
- **Population**
- Individual
- Operator
- Mating scheme
- Simulator

- Loading simuPOP
- 2 Population
- Individual
- Operator
- **5** Mating scheme
- **6** Simulator



Outline

In-depth course

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Loading simuPOP

Random Number Generator Debug information

Getting help

Population Individual

marriada

Operator

Mating scheme

Simulator

Loading simuPOP

- simuPOP modules
- Random Number Generator
- Debug information
- Getting help



simuPOP modules

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Loading simuPOP

simuPOP modules

Generator
Debug information

Getting help

Population

Individual

Operator

Mating scheme

Simulator

simuPOP provides six types of modules

Possible allele states:

short
$$0 \sim 2^8 - 1$$
 long $0 \sim 2^{16} - 1$ binary 0 and 1

2 Debug information and runtime validation

standard with debug information and runtime validation

optimized without debug information and runtime validation

Note: A Message Passing Interface (parallel) version of simuPOP is under development.



Loading appropriate module

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Loading simuPOP

simuPOP modules
Random Number
Generator
Debug information
Getting help

Population

Individual

Operator

Mating scheme

Simulator

Use simuOpt.setOptions

```
>>> from simuOpt import setOptions
>>> setOptions(alleleType='long', optimized=False, quiet=False)
>>> from simuPOP import *
simuPOP : Copyright (c) 2004-2006 Bo Peng
Developmental Version (Jun 12 2007) for Python 2.3.4
[GCC 3.4.6 20060404 (Red Hat 3.4.6-8)]
Random Number Generator is set to mt19937 with random seed 0x3c5edc074c65ce(0
This is the standard long allele version with 65536 maximum allelic states.
For more information, please visit http://simupop.sourceforge.net,
or email simupop-list@lists.sourceforge.net (subscription required).
>>>
```

- 2 Set environment variables (system dependent)
 - SIMUALLELETYPE = short/long/binary
 - SIMUOPTIMIZED for optimized version
- Command line argument of scripts using the simuOpt module (--optimized)



Standard modules

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Loading simuPOP

simuPOP modules Random Number Generator

Generator

Debug information

Getting help

Population

Individual

Operator

Mating scheme

Simulator

Perform strict runtime check. Produce proper debug information if anything goes wrong.

```
>>> pop = population(10, loci=[2])
>>> pop.locusPos(10)
Traceback (most recent call last):
   File "course.py", line 1, in ?
        #!/usr/bin/env python
IndexError: src/genoStru.h:428 absolute locus index (10) out of range of 0 - 1
>>> pop.individual(20).setAllele(1, 0)
Traceback (most recent call last):
   File "course.py", line 1, in ?
        #!/usr/bin/env python
IndexError: src/population.h:452 individual index (20) is out of range of 0 ~ 9
>>>
```



Optimized modules

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Loading simuPOP

simuPOP modules
Random Number
Generator
Debug information
Getting help

Population

Individual

Operator

Mating scheme

Simulator

No runtime check. Improper usages may crash simuPOP.

```
% seteny SIMUOPTIMIZED
% python
Python 2.3.4 (#1, Jan 9 2007, 16:40:09)
[GCC 3.4.6 20060404 (Red Hat 3.4.6-3)] on linux2
Type "help", "copyright", "credits" or "license" for more information.
>>> from simuPOP import *
simuPOP: Copyright (c) 2004-2006 Bo Peng
Developmental Version (May 21 2007) for Python 2.3.4
[GCC 3.4.6 20060404 (Red Hat 3.4.6-3)]
Random Number Generator is set to mt19937 with random seed 0x2f04b9dc5ca0fc00
This is the optimied short allele version with 256 maximum allelic states.
For more information, please visit http://simupop.sourceforge.net.
or email simupop-list@lists.sourceforge.net (subscription required).
>>> pop = population(10, loci=[2])
>>> pop.locusPos(10)
1.2731974748756028e-313
>>> pop.individual(20).setAllele(1. 0)
Segmentation fault
```



Random Number Generator

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Loading simuPOP

simuPOP modules
Random Number

Debug information

Population

Individual

Operator

Mating scheme

Simulator

simuPOP uses RNG from the GNU Scientific Library

```
>>> rng().name()
'mt19937'
>>> rnq().seed()
4350156213991099904
>>> r = ListAllRNG()
>>> print r[:5]
('qfsr4', 'mt19937', 'mt19937_1999', 'mt19937_1998', 'r250')
>>> SetRNG('taus2', 1234)
>>> rnq().name()
'taus2'
>>> rnq().seed()
1234
>>> rng().randUniform01()
0.82989443955011666
>>>
```

Note: simuPOP uses system clock to set random seeds under windows.



Debug information

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Loading simuPOP modules

Random Number Generator Debug information Getting help

Population

Individual

Operator

Mating scheme

Simulator

Several ways to turn on/off debug information

- Set environment variable SIMUDEBUG
- Use function TurnOnDebug, TurnOffDebug
- Use operator turnOnDebug, turnOffDebug to turn on/off debug at specific generations



Debug information (cont.)

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Loading simuPOP simuPOP modules

Random Number Generator

Debug information Getting help

Population

Individual

Operator

Mating scheme

```
>>> TurnOnDebug(DBG POPULATION)
>>> ind = population(10, loci=[5]).individual(1)
Constructor of population is called
Destructor of population is called
>>> # This line may crash simuPOP
>>> print ind.allele(2)
0
>>> # Show all debug code
>>> ListDebugCode()
Debug code
                            On/Off
DBG ALL
DBG GENERAL
DBG UTILITY
DBG OPERATOR
DBG SIMULATOR
DBG INDIVIDUAL
DBG OUTPUTER
DBG MUTATOR
DBG RECOMBINATOR
DBG INITIALIZER
DBG POPULATION
```



Getting help

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Loading simuPOP simuPOP modules

Random Number Generator Debug information

Debug informati Getting help

Population Individual

Operator

Mating

scheme Simulator

>>> help(population.addInfoFields)
Help on method population_addInfoFields:

 $\label{eq:population_addInfoFields(...)} unbound \ \mbox{simuPOP_la.population method} \\ \mbox{Description:}$

add one or more information fields to a population

Usage:

x.addInfoFields(fields, init=0)

Arguments:

init:

fields: new information fields. If one **or** more of the

fields alreay exist, they will simply be re-

initialized.

initial value for the new fields.

>>>



Outline

In-depth course

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Loading simuPOP

Population

Structure of population Genotypic structure Population

structure Population variables

variables Manipulate population

Individual Operator

Mating scheme

Simulator

Population

- Structure of population
- Genotypic structure
- Population structure
- Population variables
- Manipulate population



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Loading simuPOP

Population

Structure of population

Genotypic

structure Population

structure Population

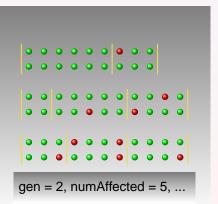
variables
Manipulate

Individual

Operator

Mating scheme

- Unaffected
- Affected





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Loading simuPOP

Population

Structure of population

Genotypic structure

Population structure

Population variables
Manipulate population

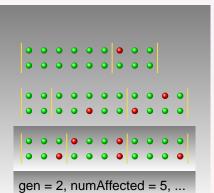
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected





In-depth course

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Loading simuPOP

Population

Structure of population

Genotypic structure

Population

structure Population

variables Manipulate population

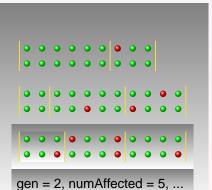
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected





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Loading simuPOP

Population

Structure of population

Genotypic structure

Population structure

Population variables

variables Manipulate population

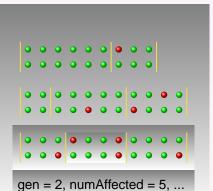
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected





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Loading simuPOP

Population

Structure of population

Genotypic structure

Population structure

Population variables

Manipulate population

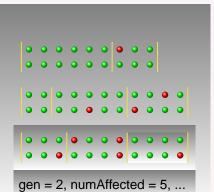
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected





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Loading simuPOP

Population

Structure of population

Genotypic structure Population

Population structure Population variables Manipulate population

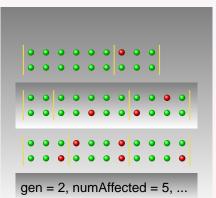
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Ancestral generation 1



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Loading simuPOP

Population

Structure of population

Genotypic structure Population

Population variables Manipulate population

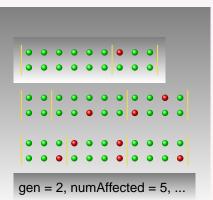
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Ancestral generation 2

Ancestral generation 1



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Population

Structure of population

Genotypic

Population Population

structure Population

variables
Manipulate
population

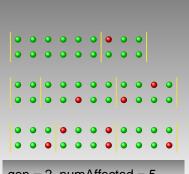
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

Ancestral generation 2

Ancestral generation 1

Current generation

Population variables



Genotypic Structure

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Population
Structure of population

Genotypic structure

Population structure Population

Population variables Manipulate population

Individual Operator

Mating scheme

Simulator

All individuals have the same genotypic structure, which refers to

- Ploidy (diploid, haploid, triploid, ...)
- Number of chromosomes
- Number of loci on each chromosome
- Names and positions of loci
- Names of information fields
- Allele names
- Existence of sex chromosome

```
THE UNIVERSITY OF TEXAS

MD ANDERSON

CANCER CENTER

Making Cancer History*
```

Create a population

0 0

MU MU

```
In-depth
               >>> pop = population(size=10, loci=[2, 3])
  course
               >>> Dump(pop)
  Bo Peng,
               Ploidy:
                                              2
   Ph.D.
               Number of chrom:
                                              2 3
               Number of loci:
Loading
simuPOP
               Maximum allele state:
                                              65535
               Loci positions:
Population
Structure of
population
Genotypic
               Loci names:
Population
structure
                                   1001-1 1001-2
Population
                                   loc2-1 loc2-2 loc2-3
variables
Manipulate
               population size:
                                              10
population
               Number of subPop:
Individual
               Subpop sizes:
                                              10
Operator
               Number of ancestral populations:
               individual info:
Mating
               sub population 0:
scheme
                   0:
                      MIT
                                          0
                                              0
Simulator
                      MIJ
                                              Λ
                                                                   Λ
```



Genotypic structure

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Population Structure of

population Genotypic

structure

structure

Population variables Manipulate

Manipulate population

Operator

Mating scheme

```
>>> pop = population(subPop=[200, 300], loci=[3, 2],
        maxAllele=3, ploidy=4,
        lociPos=[[1, 3, 5], [2.5, 4]],
. . .
        alleleNames=['A', 'C', 'T', 'G'])
>>> pop.numLoci(0)
3
>>> pop.totNumLoci()
5
>>> pop.locusPos(4)
4.0
>>> pop.subPopSize(1)
300
>>> pop.popSize()
500
>>> pop.ploidyName()
'tetraploid'
>>> pop.individual(1).allele(1, 2)
0
>>>
```



Create a population with subpopulations

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Population

Structure of population
Genotypic structure

structure Population

Population variables

Manipulate population

Individual

Operator

Mating scheme

```
>>> pop = population(subPop=[2, 5, 6], loci=[2])
>>> print pop.popSize()
13
>>> print pop.subPopSizes()
(2, 5, 6)
>>> print pop.subPopSize(1)
5
>>> Dump(pop, infoOnly=True)
Ploidy:
                         2
Number of chrom:
Number of loci:
Maximum allele state:
                         65535
Loci positions:
                 1 2
Loci names:
                 1001-1 1001-2
population size:
                         13
Number of subPop:
                         3
Subpop sizes:
                           5
Number of ancestral populations:
>>>
```



Mating happens within subpopulation

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Population Structure of

population Genotypic structure

Population

Population variables Manipulate

population Individual

Operator

Mating scheme

```
>>> pop = population(subPop=[5, 6], loci=[2])
>>> simu = simulator(pop, randomMating())
>>> simu.evolve(
        preOps = [
            initByFreg(alleleFreg=[0.2, 0.8], subPop=[0]),
. . .
            initByFreq([0, 0, 0, 0.5, 0.5], subPop=[1])
. . .
        ops = [
. . .
            dumper(alleleOnly=True, indRange=[[0, 3], [5, 7]]),
            recombinator(rate=0.1)],
        end = 1
```



Mating happens within subpopulation (cont.)

```
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```

Loading

simuPOP Population

Structure of population Genotypic structure

structure Population

structure

variables Manipulate

population

Operator

Mating scheme

Simulator

sub population 1:
5: MU 4 4 | 4 3
6: FU 4 4 | 4 3

End of individual info.

MU



Population variables

```
In-depth
course
```

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Loading simuPOP

Population Structure of

population
Genotypic
structure

Population structure Population

variables Manipulate

population

Operator

Mating

Mating scheme

```
>>> pop = population(subPop=[5, 10], loci=[5])
>>> InitByFreg(pop, [.6, .3, .1])
>>> Stat(pop, alleleFreg=[1], genoFreg=[2])
>>> print pop.dvars().alleleFreg[1][0]
0.7
>>> from simuUtil import ListVars
>>> ListVars(pop.dvars(), useWxPvthon=False)
grp: -1
 rep : -1
 alleleNum :
   [1]
     [0]
                21
     [1]
                8
     [2]
 genoFreg :
   [2]
     f 0 1
                0.26666666667
       0
                0.4
       2:
                0 266666666667
     [1]
       1:
                0.066666666667
 genoNum :
   [2]
     [01
                4.0
                6.0
       2
                4.0
     [1]
                1 0
                                                    4 D > 4 P > 4 B > 4 B >
                                                                                  90 Q
 alleleFreg :
```



Population variables (cont.)

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Loading simuPOP

Population

Structure of population

Genotypic structure

Population structure

Population variables

Manipulate population

Individual Operator

Mating scheme

```
subPop
  [0]
    alleleNum :
       [1]
         [0]
                 6
         [1]
                 3
         [2]
                 1
    genoNum :
       [2]
         [0]
                 3.0
                 2.0
    genoFreg :
       [2]
         [0]
           1:
                 0.6
                 0.4
    alleleFreq :
       [1]
         [0]
                 0.6
         [1]
                 0.3
         [2]
                 0 1
  [1]
    alleleNum :
       [1]
         f 0 1
                 15
```



Population manipulation

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Loading simuPOP

Population
Structure of population
Genotypic structure
Population

Structure
Population
variables
Manipulate
population

Individual Operator

Mating scheme

```
>>> # make a copy of pop
>>> pop = population(1000, loci=[2,3])
>>> pop1 = pop.clone()
>>> # remove loci 2, 3, 4
>>> pop.removeLoci(keep=[0, 1])
>>> # pop2 will have 3 chromosomes, with loci 2, 3, 2
>>> pop2 = MergePopulationsByLoci(pops=[pop, pop1])
>>> # randomly assign alleles using given allele frequencies
>>> InitByFreq(pop2, [0.8, .2])
>>> # assign affection status using a penetrance model
>>> MapPenetrance(pop2, locus=1,
        penetrance=\{'0-0': 0.05, '0-1': 0.2, '1-1': 0.8\})
>>> # draw case control sample
>>> (sample,) = CaseControlSample(pop2, cases=5, controls=5)
>>> # save sample in Merlin OTDT format
>>> from simuUtil import SaveOTDT
>>> SaveQTDT(sample, output='sample', affectionCode=['U', 'A'],
        fields=['affection'])
```



Population manipulation (cont.)

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Population Structure of

population
Genotypic
structure

Population structure Population

variables Manipulate

Individual Operator

Mating scheme

```
>>> # have a look at the sample in Merlin-OTDT Format
>>> print open('sample.map').read()
CHROMOSOME MARKER POSITION
        loc1-1
                1,000000
        1001-2 2.000000
        loc1-1 1
                        1,000000
        loc1-2 1
                         2.000000
3
        1002-1 1.000000
3
        loc2-2 2.000000
3
        1002-3 3.000000
>>> print open('sample.dat').read()
        affection
Α
М
        loc1-1
        1001-2
M
        loc1-1 1
M
М
        loc1-2 1
        loc2-1
M
        loc2-2
М
        loc2-3
```



Population manipulation (cont.)

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Loading simuPOP

Population

Structure of population
Genotypic structure

structure Population

Structure Population variables

Manipulate population

Individual Operator

Operator

>>>

Mating scheme



Outline

In-depth course

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Loading simuPOP
Population

ropulation

Individual

Structure of individual Individual object

Individual object Information fields Iterate through a population

Operator

Mating scheme

Simulator

Individual

- Structure of individual
- Individual object
- Information fields
- Iterate through a population



In-depth course

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Loading simuPOP

Population

Individual

Structure of

individual
Individual object

Information fields
Iterate through a population

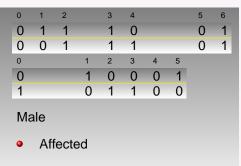
Operator

Mating scheme

Simulator

fitness

Assume ploidy = 2, maxAllele = 1



father idx



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Loading simuPOP

Population

Individual

Structure of

individual
Individual object

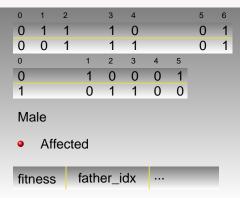
Information fields
Iterate through a population

Operator

Mating scheme

Simulator

Assume ploidy = 2, maxAllele = 1



Chromosome 0



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Loading simuPOP

Population

Individual

Structure of individual

Individual object

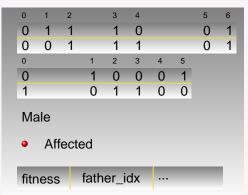
Information fields Iterate through a population

Operator

Mating scheme

Simulator

Assume ploidy = 2, maxAllele = 1



Chromosome 0

Chromosome 1



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Loading simuPOP

Population

Individual

Structure of individual

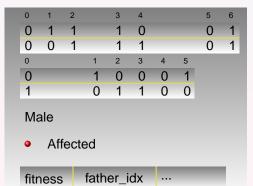
Individual object Information fields Iterate through a population

Operator

Mating scheme

Simulator

Assume ploidy = 2, maxAllele = 1



Chromosome 0

Chromosome 1

Sex



Structure of individual

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Loading simuPOP

Population

Individual

Structure of

Structure of individual

Individual object Information fields Iterate through a population

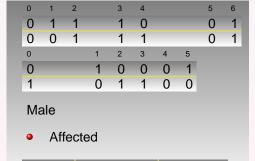
Operator

Mating scheme

Simulator

fitness

Assume ploidy = 2, maxAllele = 1



father idx

Chromosome 0

Chromosome 1

Sex

Affection status



Structure of individual

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Loading simuPOP

Population

Individual

Structure of

Structure of individual

Individual object Information fields Iterate through a population

Operator

Mating scheme

Simulator

fitness

Assume ploidy = 2, maxAllele = 1



father idx

Chromosome 0

Chromosome 1

Sex

Affection status

Information fields



Individual

In-depth course

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Loading simuPOP

Population

Individual Structure of

individual
Individual object

Information fields
Iterate through a population

Operator

Mating scheme

```
>>> pop = population(subPop=[100, 200], loci=[2, 3])
>>> # the first individual
>>> ind1 = pop.individual(0)
>>> # the second individual in the second subpop
>>> ind2 = pop.individual(1, 1)
>>> # genotypic strcuture
>>> print ind1.numLoci(1)
3
>>> print ind1.numChrom()
2
>>> # an editable allele list
>>> alleles = ind1.arrGenotype(0)
>>> alleles[:] = range(ind1.totNumLoci())
>>> print indl.arrGenotype(0)
[0, 1, 2, 3, 4]
>>> # ploidy 1, index 4
>>> ind1.setAllele(3, 4, 1)
>>> print indl.allele(4, 1)
3
>>>
```



Information fields

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Loading simuPOP

Population

Individual
Structure of individual
Individual object
Information fields

Iterate through a population

Operator

Mating scheme

Simulator

Pieces of information that can be attached to each individual, e.g.

- fitness: fitness of each individual, calculated by selectors
- father_idx, mother_idx: index of parents in the parental generation
- old_index: index of an individual in the population where it is sampled

Or, self-defined

- birthday
- geographic location
- ...



Information fields

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Loading simuPOP

Population

Individual

Structure of individual

Individual object

Information fields

population

Operator

Mating scheme



Iterate through a population

In-depth course

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Loading simuPOP

Population

Individual Structure of

Structure of individual Individual object

Information fields

Iterate through a population

Operator

Mating scheme

```
>>> pop = population(subPop=[5, 8], loci=[5],
        infoFields=['penetrance'])
>>> InitByFreq(pop, [.6, .3, .1])
>>> MaPenetrance(pop, locus=2, penetrance=[0.05, 0.2, 0.5],
        wildtype=[0], infoFields=['penetrance'])
>>> # iterate through all inviduals in subPop 1
>>> for ind in pop.individuals(1):
        print 'Aff: %d Fit: %.3f Geno: %d %d' % \
. . .
            (ind.affected(), ind.info('penetrance'), \
. . .
            ind.allele(2, 0), ind.allele(2, 1))
. . .
Aff:
    1 Fit: 0.200 Geno: 0 1
Aff:
       Fit:
            0.200 Geno: 0.2
Aff:
     0 Fit: 0.200 Geno: 1 0
Aff:
           0.200 Geno: 1.0
    0 Fit:
Aff:
     0 Fit: 0.200 Geno: 2.0
Aff: 0 Fit: 0.050 Geno: 0 0
Aff: 0 Fit: 0.050 Geno: 0.0
Aff: 0 Fit: 0.500 Geno: 1 1
>>>
```



Outline

In-depth course

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Loading simuPOP

Population

Individual

Operator

Stage of an

operator Applicable

generations
Replicates and replicate groups
Output and output expression
Python Operators

Mating scheme

Simulator

Operator

- Stage of an operator
- Applicable generations
- Replicates and replicate groups
- Output and output expression
- Python Operators



In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

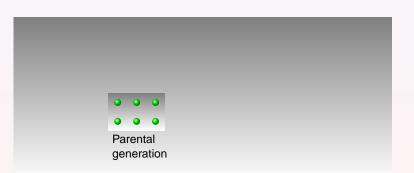
Stage of an

operator

Applicable generations

Replicates and replicate groups Output and output expression Python Operators

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

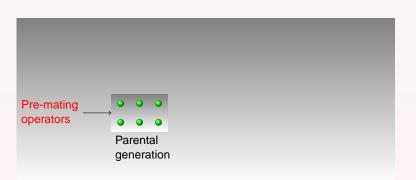
Stage of an operator

Applicable

generations

Replicates and replicate groups **Output and output** expression **Python Operators**

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

Operat

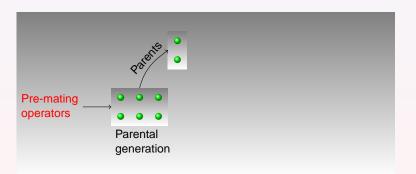
Stage of an

operator

Applicable generations

Replicates and replicate groups Output and output expression Python Operators

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

Operat

Stage of an operator

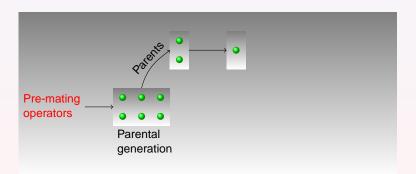
Applicable

generations
Replicates and
replicate groups

Output and output expression

Python Operators

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

. .

Operator

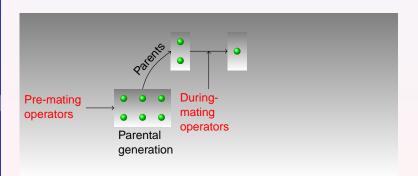
Stage of an

operator

Applicable generations

Replicates and replicate groups Output and output expression Python Operators

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

Operator

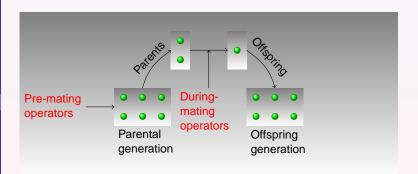
Stage of an

operator Applicable

generations
Replicates and
replicate groups
Output and output
expression

Python Operators

Mating scheme





In-depth course

Bo Peng, Ph.D.

Loading simuPOP

Population

Individual

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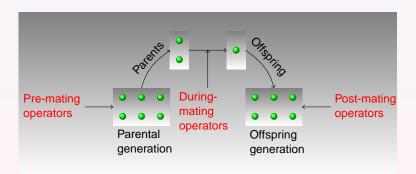
Operator

Stage of an

operator Applicable

generations
Replicates and
replicate groups
Output and output
expression
Python Operators

Mating scheme





Pre-, During-, and PostMating operators

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Population Individual

Operator

Stage of an operator

Applicable generations
Replicates and replicate groups
Output and output expression

Python Operators

Mating

scheme

```
>>> simu = simulator(
        population(subPop=[20, 80], loci=[3]),
        randomMating())
>>> simu.evolve(
        preOps = [initBvFreq([0.2, 0.8])],
        l = ago
            kamMutator(maxAllele=10. rate=0.00005. atLoci=[0.2]).
            recombinator(rate=0.001).
            dumper(stage=PrePostMating),
            stat(alleleFreg=[1]),
        drvrun=True
Dryrun mode: display calling seguence
Apply pre-evolution operators
  Replicate 0
      - <simuPOP::initByFreg> end at 1
Start evolution
  Replicate 0
    Pre-mating operators
      - <simuPOP::dumper> at all generations
    Start mating
      - <simuPOP::recombination> at all generations
    Apply post-mating operators
      - <simuPOP::k-allele model mutator K=10> at all generations
      - <simuPOP::dumper> at all generations
      - <simuPOP::statistics> at all generations
True
>>>
```



Applicable generations

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Population

Individual

Operator

Stage of an operator

Applicable generations

Replicates and replicate groups Output and output expression Python Operators

Mating

scheme

```
>>> simu = simulator(
        population(10000, loci=[3]),
        randomMating())
>>> eval1 = r"'Gen: %3d Freg: %f\n' % (gen, alleleFreg[1][0])"
   eval2 = r"'Last Gen: %3d Freg: %s\n' % (gen, alleleFreg[1])"
   simu.evolve(
        preOps = [initByFreq([0.3, 0.7])],
        l = ago
            recombinator(rate=0.01, begin=10, end=30),
            stat(alleleFreq=[1], step=10),
            pvEval(eval1, step=10),
            pvEval(eval2, at=[-1])
        ],
        end = 50
...)
          Freq: 0.304200
Gen:
Gen:
          Freq: 0.290700
          Freq: 0.285300
Gen:
Gen:
      30
          Freq: 0.288750
          Freq: 0.283750
Gen:
      40
          Freq: 0.284100
Gen:
           50 Freq: [0.2841000000000002, 0.7158999999999998]
Last Gen:
True
>>>
```



Applicable replicates

```
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course
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Ph.D.
```

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Population

Individual

Operator

Stage of an operator

Applicable generations

Replicates and replicate groups

Output and output expression

Python Operators

Mating
scheme

```
>>> simu = simulator(
        population(100, loci=[3]),
        randomMating(),
        rep=5, qrp=[1,1,2,2,2])
. . .
>>> simu.evolve(
        preOps = [initByFreq([0.5, 0.5])],
. . .
        ops = [
. . .
             stat(alleleFreq=[1]),
             recombinator(rate=0.01, grp=1),
. . .
             recombinator(rate=0.01, grp=2),
. . .
             pvEval(r"'%.2f' % alleleFreg[1][0]", grp=1),
             pyEval(r"'\n'", rep=REP LAST),
. . .
         1,
        end=5
. . .
0.470.52
0.49 0.56
0.51 0.60
0.52 0.62
0.56 0.60
0.52 0.62
True
                                         4 D > 4 A > 4 B > 4 B > B 90 C
>>>
```



Output

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Population

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Individual

Operator

Stage of an operator

Applicable generations Replicates and replicate groups Output and output

Python Operators

Mating

scheme

```
>>> simu = simulator(
        population(100, loci=[3]),
        randomMating(),
        rep=5, grp=[1,1,2,2,2])
>>> simu.evolve(
        preOps = [initBvFreq([0.5, 0.5])].
        ops = [
            stat(alleleFreg=[1]).
            pvEval(r"'%,2f ' % alleleFreg[1][0]".
                output='>>out'),
            pyEval(r"'\n'", rep=REP LAST, output='>>out'),
            pvEval(r"'%,2f ' % alleleFreg[1][0]".
                outputExpr="'>>out%d' % grp"),
        ],
        end=2
True
>>> print open('out').read()
0.56 0.55 0.46 0.47 0.54
0.56 0.55 0.42 0.55 0.57
0.58 0.56 0.40 0.57 0.56
>>> print open('out1').read()
0.56 0.55 0.56 0.55 0.58 0.56
>>> print open('out2').read()
0.46 0.47 0.54 0.42 0.55 0.57 0.40 0.57 0.56
>>>
```



Python operator

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Population

Individual

Operator

Stage of an operator Applicable generations Replicates and replicate groups Output and output expression

Python Operators

Mating scheme

Simulator

A Python operator is an operator that calls a user-provided Python function when it is applied to a population. A hybrid operator performs its main function at the C++ level, and a pure Python operator depends on this user-provided function for its functionality.



A hybrid operator

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Population

Individual

Operator

Stage of an operator
Applicable generations
Replicates and replicate groups
Output and output expression
Python Operators

Mating scheme

Simulator

A (weird) selector with fitness

	BB	Bb	bb
AA	1.	1.01	1.02
Aa	1.	0.99	0.98
aa	1.	1.01	1.02

Note: This operator can be more efficiently implemented using other non-Python operators.



True

>>>

A hybrid operator (cont.).

```
In-depth
               >>> expr = r'"%.3f %.3f\n" % (alleleFreq[0][0], alleleFreq[1][0]
  course
               >>> simu = simulator(
  Bo Peng,
                         population(10000, loci=[1,1],
   Ph.D.
                              infoFields=['fitness']),
               . . .
                         randomMating(),
Loading
               . . .
simuPOP
Population
               >>> simu.evolve(
                         preOps = [initBvFreq([0.3, 0.7])],
Individual
                         ops = [
               . . .
Operator
                              pySelector(loci=[0, 1], func=mySelector),
Stage of an
                              stat(alleleFreq=[0, 1], step=20),
operator
Applicable
                              pyEval(expr, step=20)
               . . .
generations
Replicates and
replicate groups
                         end = 100
               . . .
Output and output
expression
Python Operators
               0.294 0.298
Mating
               0.252 0.278
scheme
               0.184 0.246
Simulator
               0.134 0.232
               0.078 0.215
               0.047 0.209
```

4 D > 4 A > 4 B > 4 B > B 90 C



A pure Python operator

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Population

Individual Operator

Stage of an operator
Applicable generations
Replicates and replicate groups

Output and output expression

Python Operators

Mating scheme

```
>>> from random import normalvariate
>>> def trait(ind):
        return [ind.info('trait') + normalvariate(0, 1)]
   def avgTrait(pop):
>>>
        t = sum(pop.indInfo('trait', False))/pop.popSize()
        pop.dvars().trait = t
        print 'Average trait at gen %4d : %.4f' % (pop.gen(), t)
        return True
   simu = simulator(
>>>
        population(100, infoFields=['trait']),
        randomMating()
>>> simu evolve(
        0 = 800
            pyIndOperator(func=trait, infoFields=['trait']),
            pvOperator(func=avgTrait, step=100),
        end = 500
Average trait at gen
                        0 : -0.0216
                      100: -0.7387
Average trait at gen
Average trait at gen
                     200 : -0.6641
Average trait at gen
                     300 : 0.0523
Average trait at gen
                     400 : -0.4510
Average trait at gen
                     500 : -0.7781
True
>>>
```



Outline

In-depth course

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Loading simuPOP Population

Individual

Operator

Mating scheme

Demographic model Number of offspring

- Mating scheme
 - Demographic model
 - Number of offspring



Mating schemes

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Population Individual

Operator

Mating scheme

Demographic model Number of offspring

Simulator

Mating schemes

- Populate offspring subpopulation from corresponding parental subpopulation
- Can not change number of subpopulations
- Can change subpopulation size
- Select parents according to their fitness value (information field)
- Can produce more than one offspring



Demographic model

```
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course
```

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Population

Individual

Operator

Mating scheme

Demographic model

Number of offspring

```
>>> def lin inc(gen, oldsize=[]):
        return [10+gen]*5
>>> simu = simulator(
        population(subPop=lin_inc(1), loci=[1]),
        randomMating(newSubPopSizeFunc=lin inc)
. . .
. . .
>>> simu.evolve(
        ops = [
             stat(popSize=True),
             pvEval(r'"%d %d\n"%(gen, subPop[0]["popSize"])').
        end=5
 10
  11
 12
 13
 14
5 15
True
>>>
                                        4 N D D A R D D A R D D D D D D
```



Number of offspring

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Population

Individual

Operator

Operato

Mating scheme Demographic

Number of offspring

```
>>> simu = simulator(
        population(size=10000, loci=[1]),
     randomMating(),
>>> simu.evolve(
        preOps = [initByFreq([0.1, 0.9])],
. . .
   ops = [], end=100
. . .
True
>>> simu.setMatingScheme(randomMating(numOffspring=2))
>>> simu.addInfoFields(['father idx', 'mother idx'])
>>> simu.setAncestralDepth(1)
>>> simu.step(ops=[parentsTagger()])
True
>>> pop = simu.getPopulation(0)
>>> MaPenetrance(pop, locus=0, penetrance=[0.05, 0.1, 0.5])
>>> AffectedSibpairSample(pop, size=100)
[<simuPOP::population of size 200>]
>>>
```



Outline

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Population Individual

Operator

Mating

scheme

Simulator What a simulator

Simulator operations

Populations

- What a simulator does
- Simulator operations
- Populations



Simulator

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Loading simuPOP

Population

Individual

Operator

Mating scheme

Simulator

What a simulator

Simulator operations
Populations

A simulator manages

- Replicates of a population
- A mating scheme
- Many operators

and evolve the populations.



simulator operations

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Population

Individual

Operator

Mating scheme

Simulator What a simulator

does Simulator

operations
Populations

```
>>> simu = simulator(
        population(size=10000, loci=[3]),
        randomMating(),
>>> # genotypic structure can be accessed at the simulator level
>>> print simu.lociPos()
(1.0, 2.0, 3.0)
>>> simu.step(ops = [])
True
>>> print simu.gen()
1
>>> # add information fields to all populations
>>> simu.addInfoFields(['father_idx', 'mother_idx'])
>>> simu.setMatingScheme(randomMating(numOffspring=2))
>>>
```



simulator populations

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Population

Individual

Operator

Mating

scheme

Simulator What a simulator

Simulator operations

Populations

```
>>> # get a reference to the first replicate
>>> pop = simu.population(0)
>>> pop.individual(0).setAllele(1, 0)
>>> print simu.population(0).individual(0).allele(0)
1
>>> # get a real copy
>>> pop = simu.getPopulation(0)
>>> pop.individual(0).setAllele(1, 1)
>>> print simu.population(0).individual(0).allele(1)
0
>>>
```