Writing forward-time simulations, an in-depth course

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simuPOP workshop
School of Public Health, Department of Biostatistics
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outline

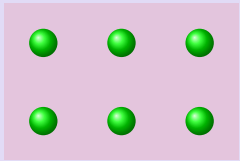
Outline

1 The global view

- Population
- Individual
- Operator
- Mating scheme
- Simulator
- Other utilities

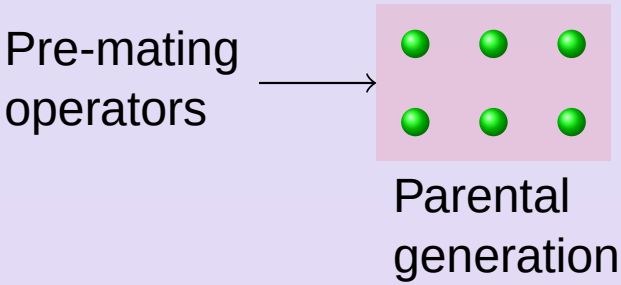
simuPOP modules

Illustration of the evolutionary process



Parental generation

Illustration of the evolutionary process



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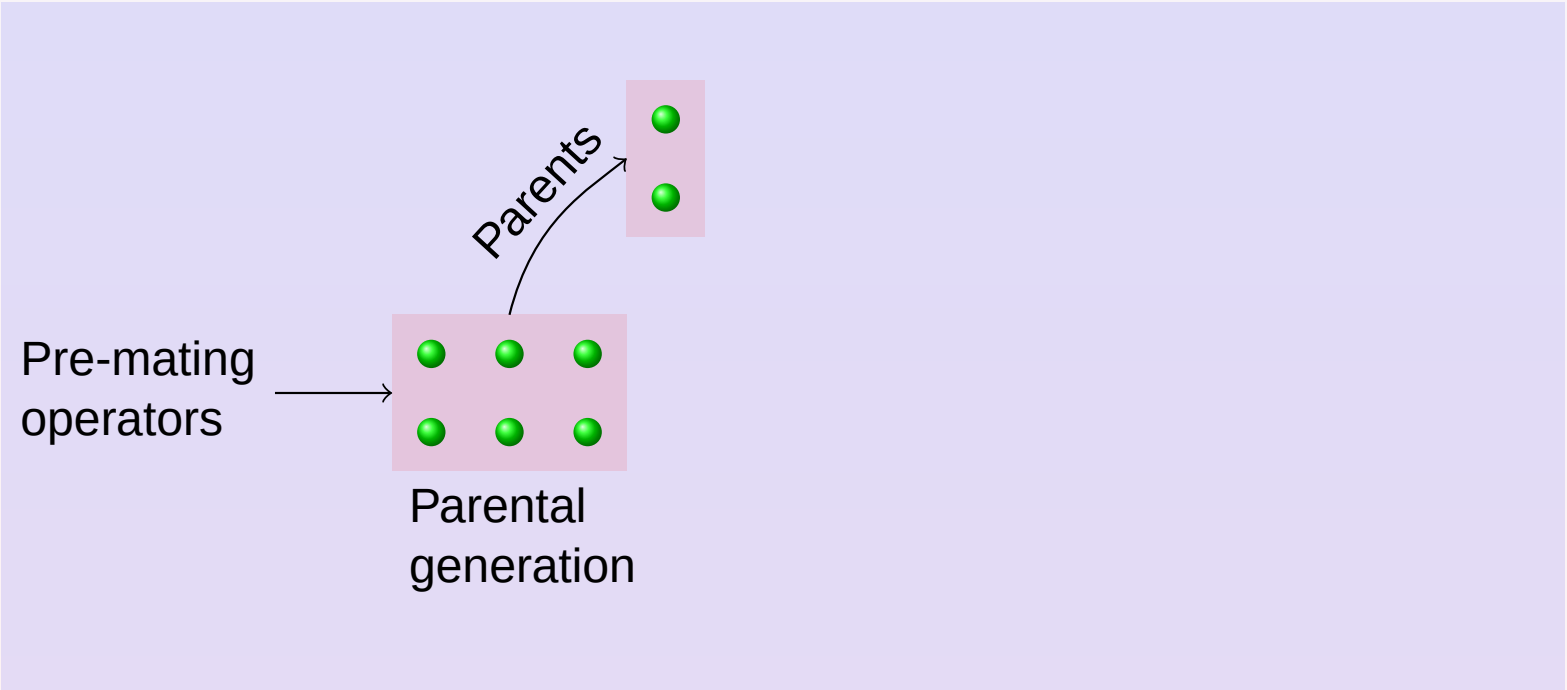

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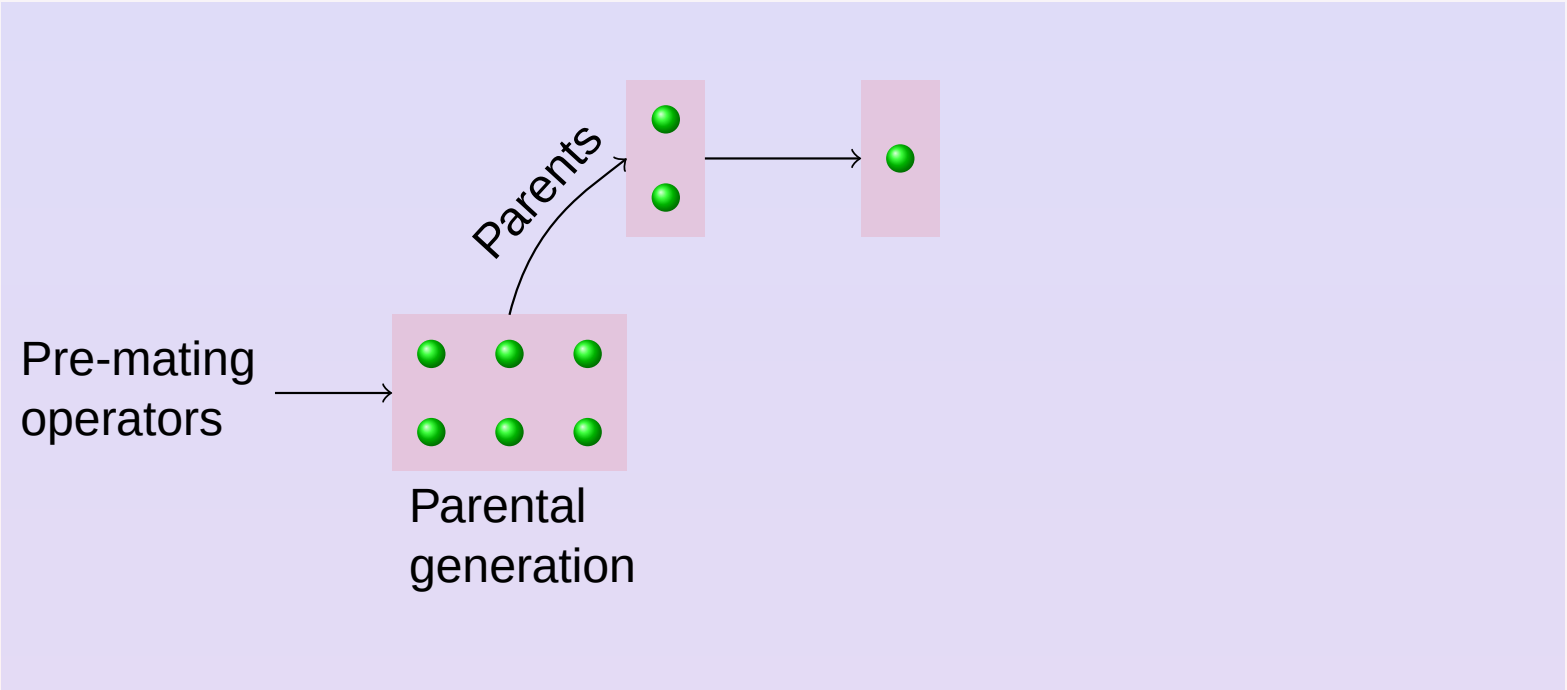

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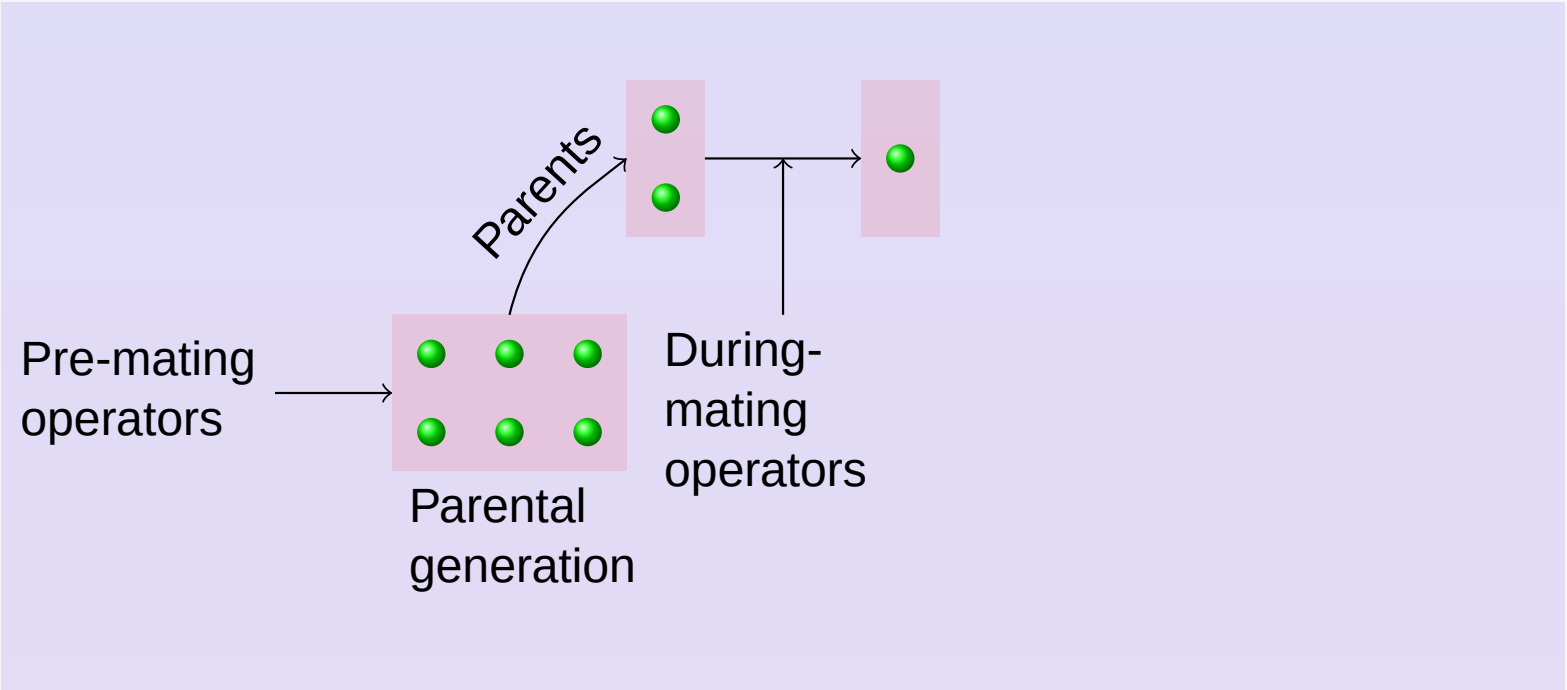

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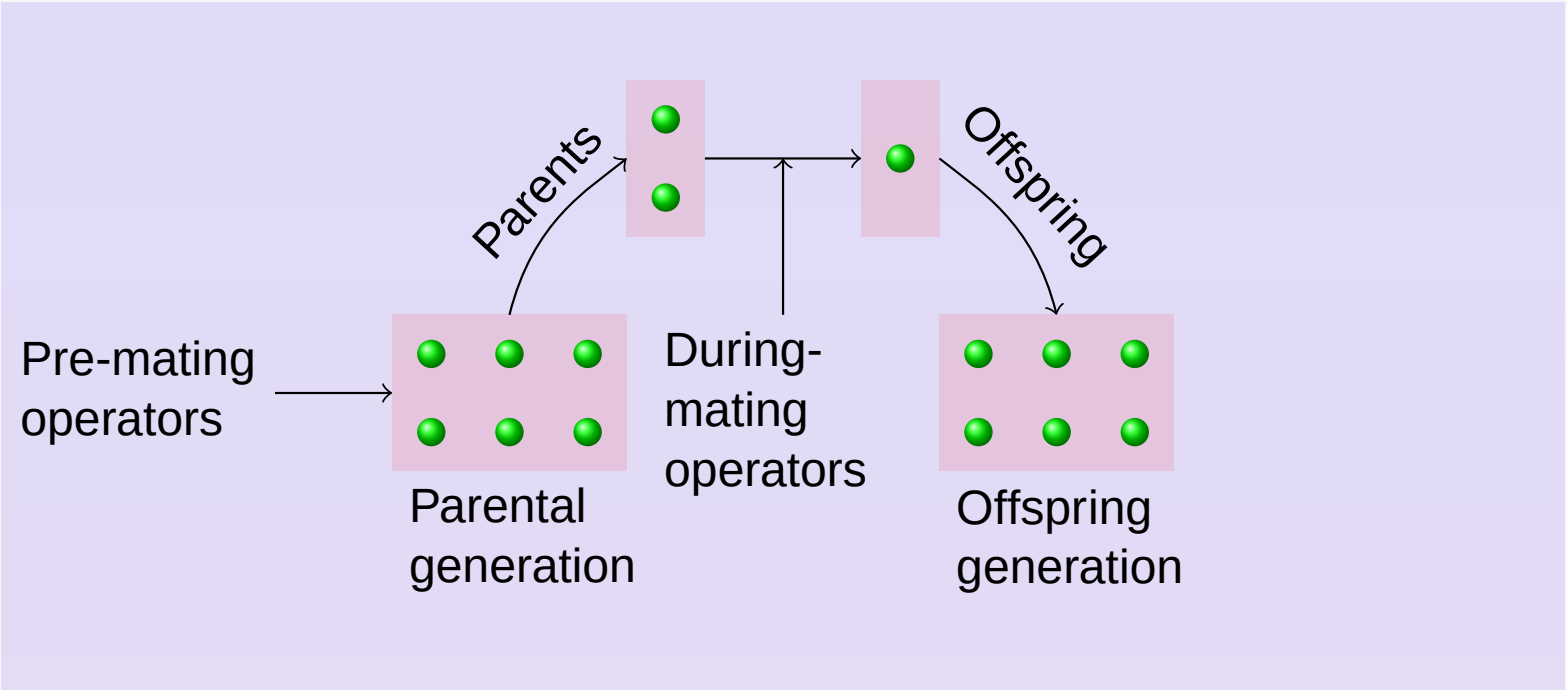

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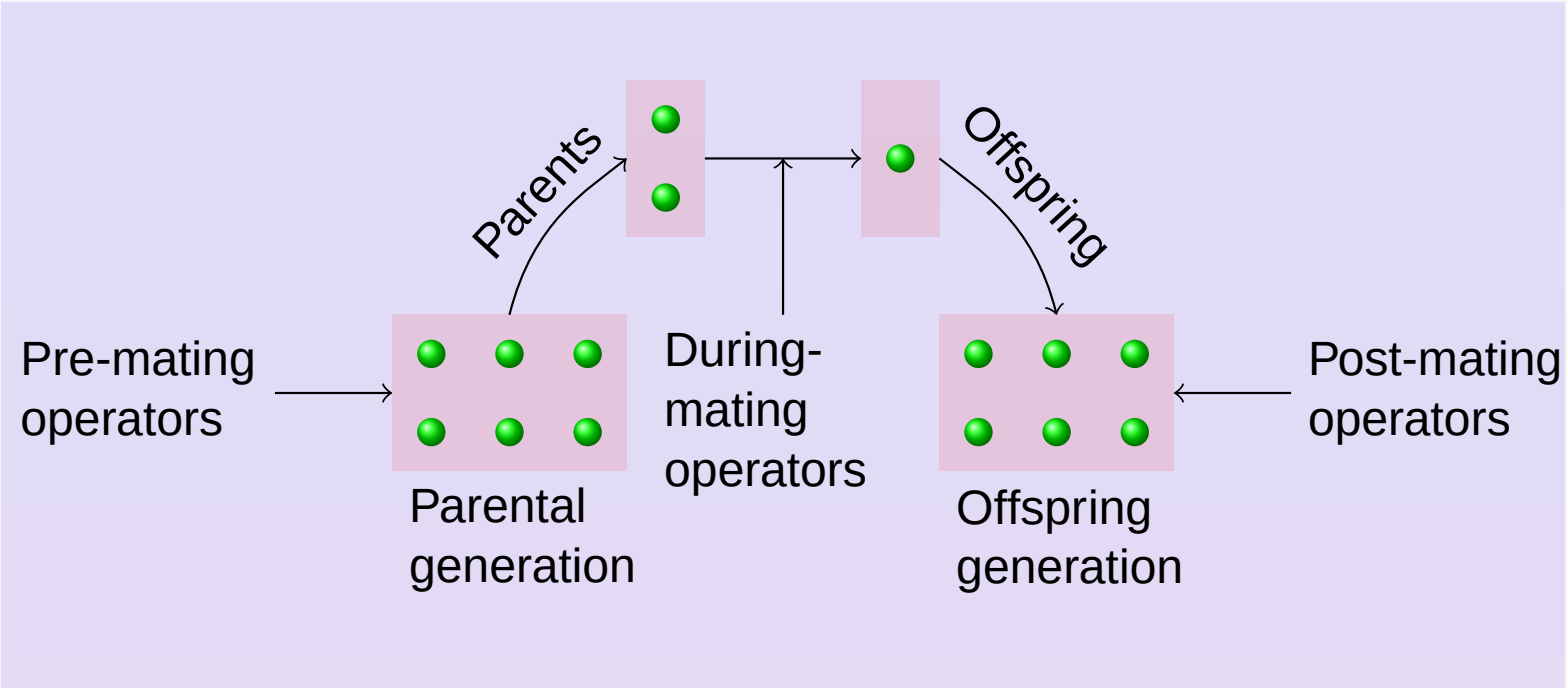


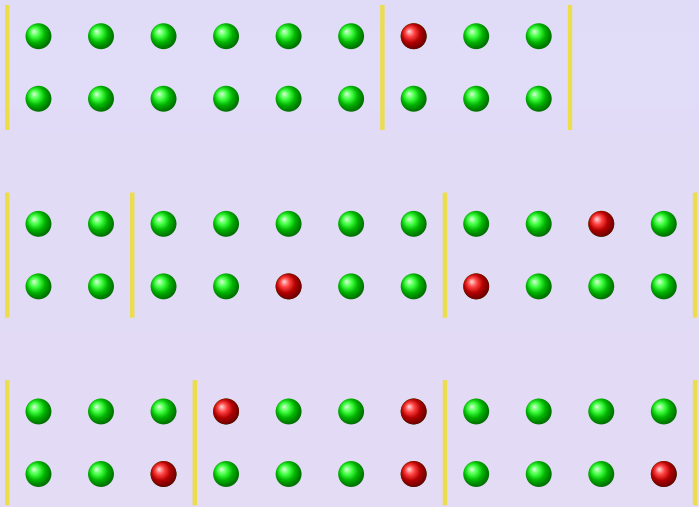
Load simuPOP


```
>>> from simuOpt import setOptions
>>> setOptions(alleleType='long', optimized=False)
>>> from simuPOP import *
simuPOP : Copyright (c) 2004-2006 Bo Peng
Development 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 0x224a5b0a187b5c00
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).
>>>
```

- Allele type: short, long, binary
- Standard and Optimized
- MPI (parallel) version, not ready

Structure of a population

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

Structure of a population

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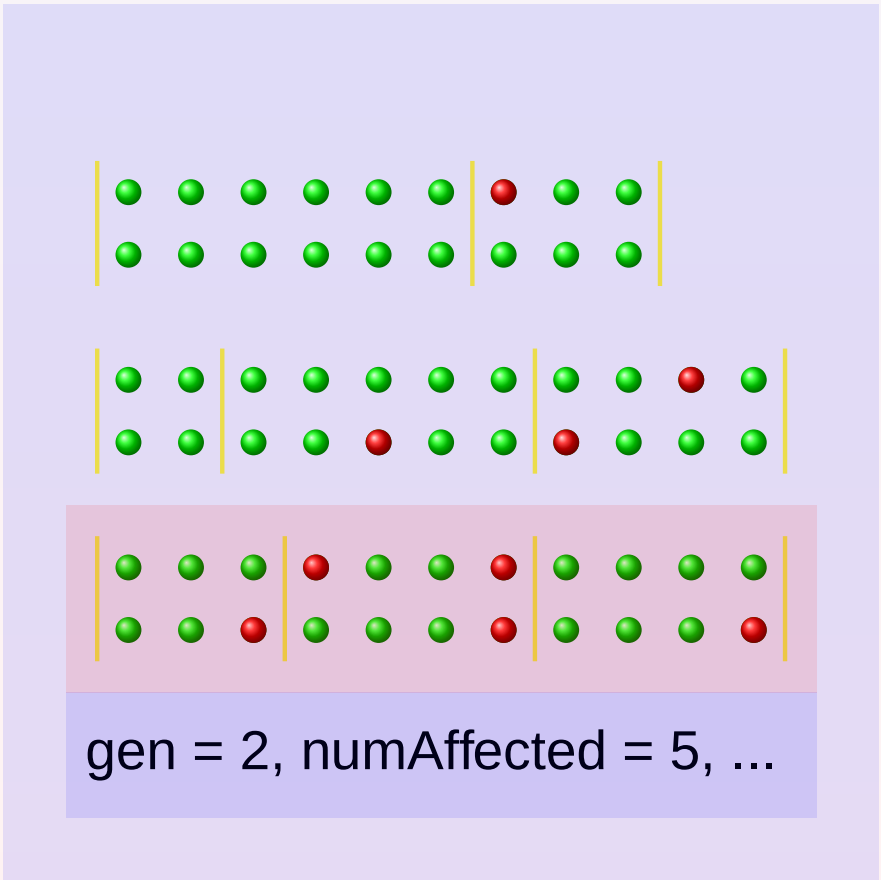
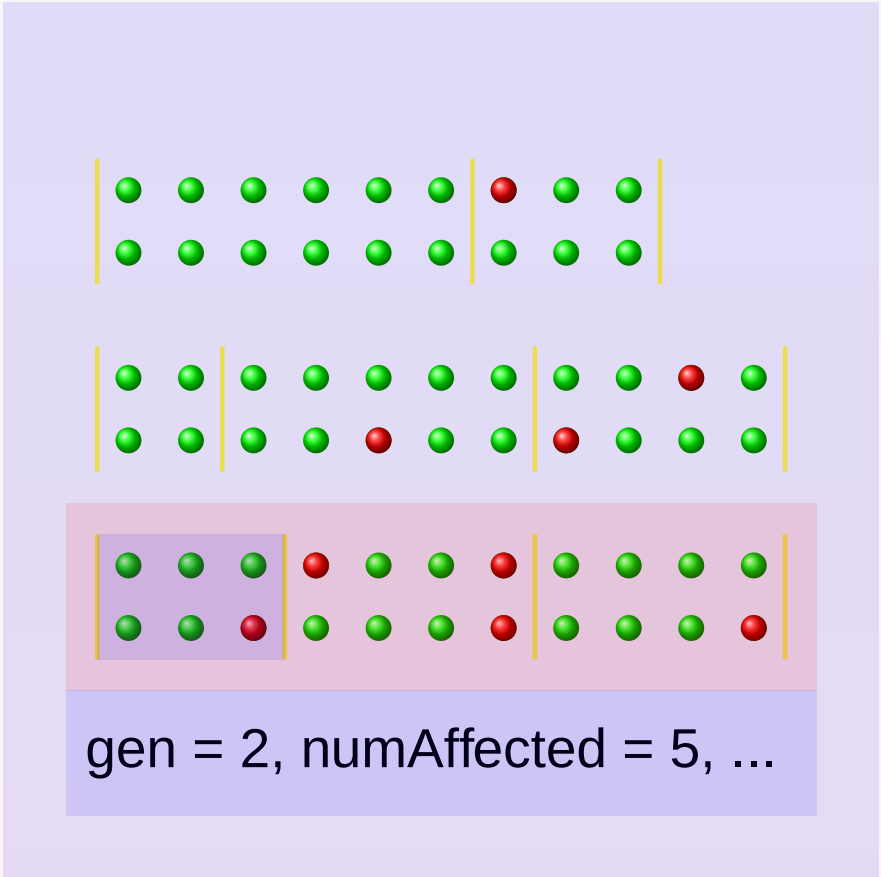
- Affected



Current generation

Structure of a population

- Unaffected
- Affected



Current generation

Structure of a population

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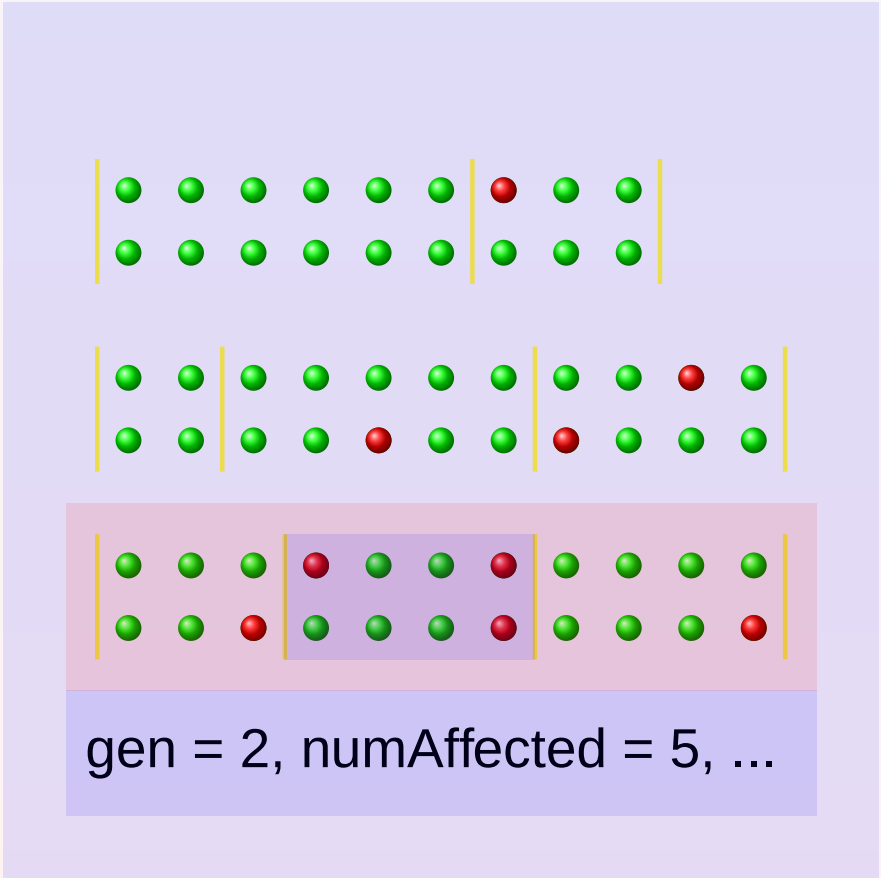

Current generation

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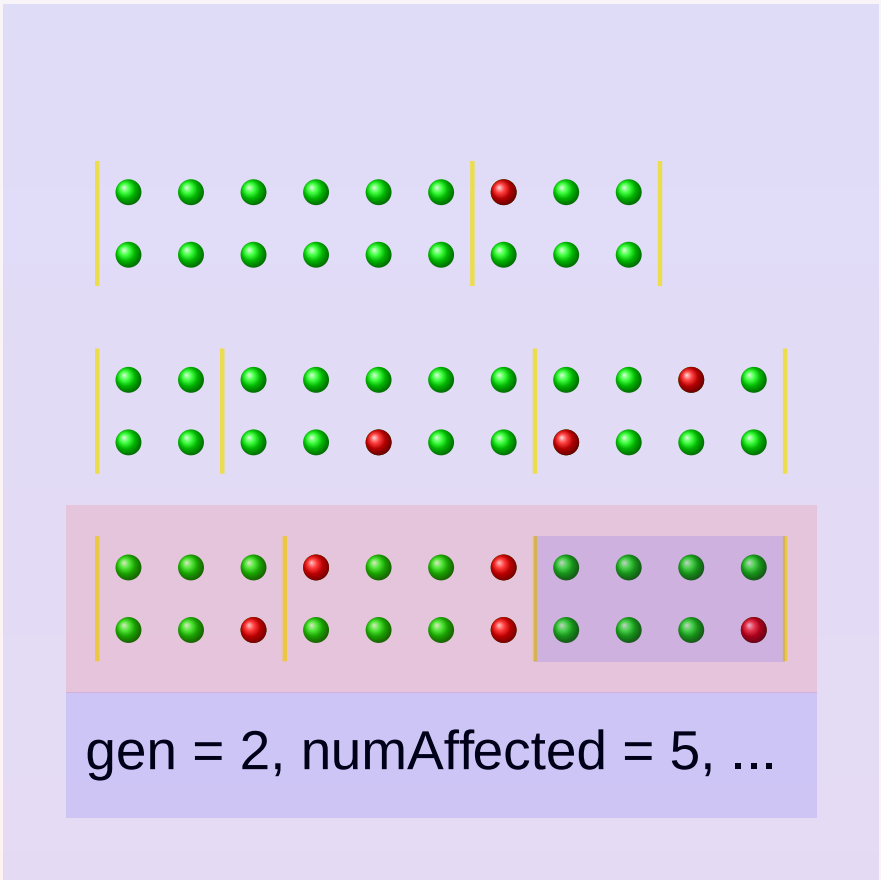

Current generation

Structure of a population

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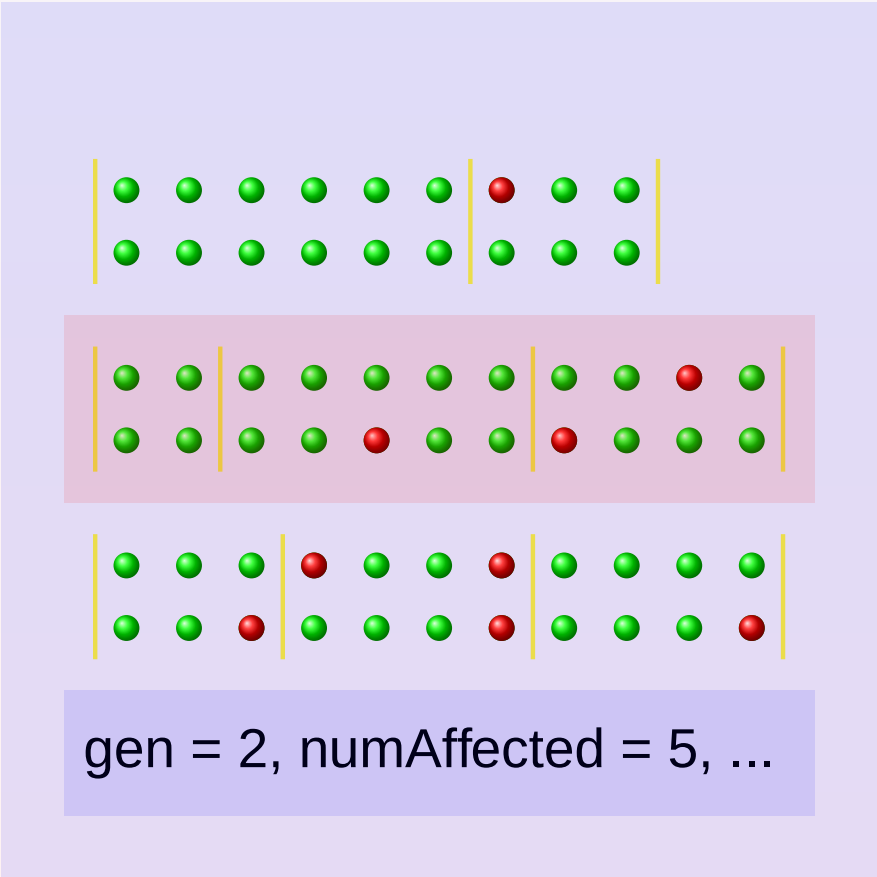

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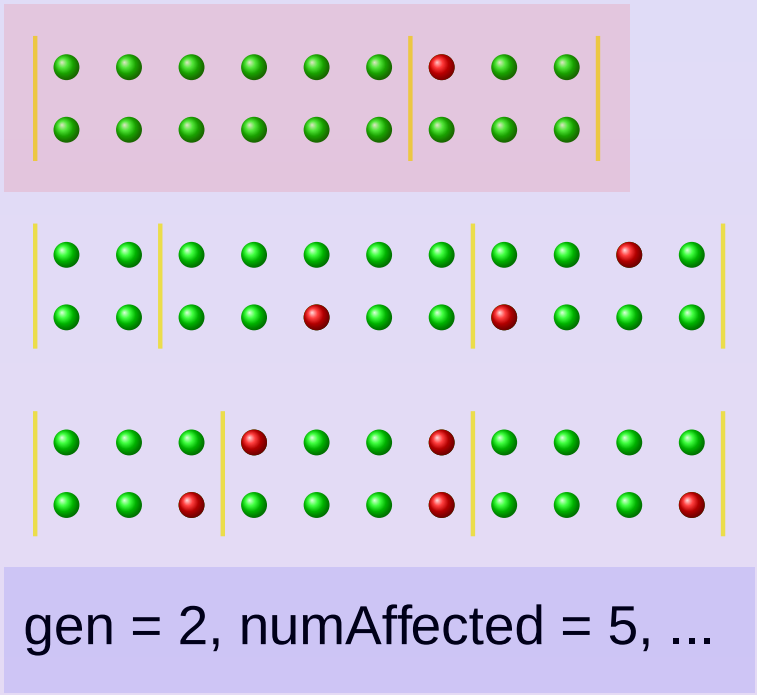


Ancestral generation 2

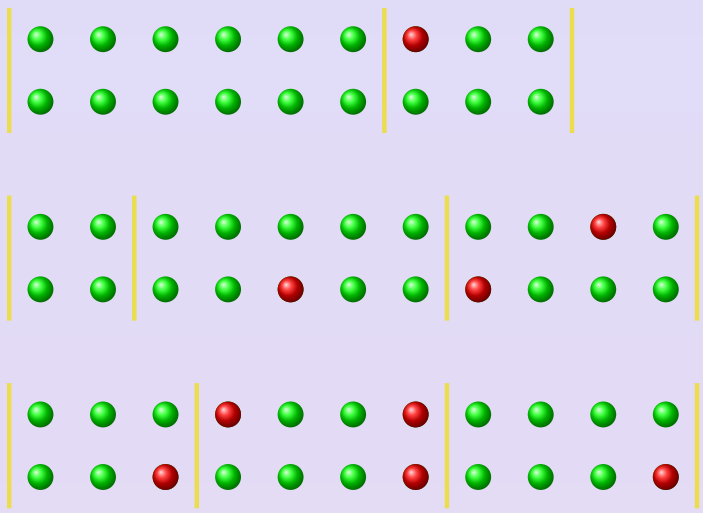
Ancestral generation 1

Current generation

gen = 2, numAffected = 5, ...

Structure of a population

- Unaffected
- Affected



Ancestral generation 2

Ancestral generation 1

Current generation

gen = 2, numAffected = 5, ...

Population variables

Genotypic Structure

Common properties of all individuals

All individuals have the same genotypic structure, which refers to

- Ploidy (diploid, haploid, triploid, ...)
- Number of chromosomes
- Number of loci on each chromosome
- Name and position of loci
- Name of information fields

And less importantly

- Allele names
- Existence of sex chromosome

Chromosome structure


```
>>> pop = population(size=10, loci=[2, 4, 5])
>>> print pop.numLoci()
(2, 4, 5)
>>> # index starts at zero!
>>> print pop.numLoci(1)
4
>>> print pop.ploidy()
2
>>> print pop.ploidyName()
diploid
>>> print pop.chromBegin(1)
2
>>> print pop.locusPos(3)
2.0
>>> print pop.locusName(4)
loc2-3
>>>
```

Loci position and names


```
>>> pop = population(size=10, loci=[2, 4], maxAllele=3,
...     lociPos=[[1.5, 2.5], [1, 2, 5, 10]],
...     lociNames=['loc%x' % x for x in range(6)],
...     alleleNames=['A', 'T', 'C', 'G'])
>>> print pop.locusPos(3)
2.0
>>> print pop.locusName(4)
loc4
>>> print pop.alleleName(1)
T
>>>
```

Create and manipulate populations


```
>>> pop = population(size=10, loci=[2, 3])
>>> Dump(pop)
Ploidy:                    2
Number of chrom:           2
Number of loci:            2 3
Maximum allele state:      65535
Loci positions:
                  1 2
                  1 2 3
Loci names:
                  loc1-1 loc1-2
                  loc2-1 loc2-2 loc2-3
population size:           10
Number of subPop:          1
Subpop sizes:              10
Number of ancestral populations:          0
individual info:
sub population 0:
   0: MU    0  0    0  0  0 |    0  0    0  0  0
   1: MU    0  0    0  0  0 |    0  0    0  0  0
   2: MU    0  0    0  0  0 |    0  0    0  0  0
   3: MU    0  0    0  0  0 |    0  0    0  0  0
```

Genotypic structure


```
>>> pop = population(subPop=[200, 300], loci=[3, 2],
...     maxAllele=3, ploidy=3,
...     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()
'triploid'
>>> pop.individual(1).allele(1, 2)
0
>>>
```

Population manipulation


```
>>> # make a copy of pop
>>> 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])
>>> # calculate population allele frequency
>>> Stat(pop2, alleleFreq=range(pop2.totNumLoci()))
>>> # print allele frequency
>>> print pop2.dvars().alleleFreq
[[0.8006666666666664, 0.1993333333333333], [0.7933333333333333
>>> # 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 QTDT format
>>> from simuUtil import SaveQTDT
>>> SaveQTDT(sample, output='sample', affectionCode=['U', 'A'],
...     fields=['affection'])
```

Population manipulation (cont.)


```
>>> # have a look at the sample in Merlin-QTDT Format
>>> print open('sample.map').read()
CHROMOSOME MARKER POSITION
1        loc1-1  1.000000
1        loc1-2  3.000000
2        loc1-1_1        1.000000
2        loc1-2_1        3.000000
2        loc1-3  5.000000
3        loc2-1  2.500000
3        loc2-2  4.000000

>>> print open('sample.dat').read()
A        affection
M        loc1-1
M        loc1-2
M        loc1-1_1
M        loc1-2_1
M        loc1-3
M        loc2-1
M        loc2-2
```

Population manipulation (cont.)


```
>>> print open('sample.ped').read()
1 1 0 0 2 A 1 2 2 1 1 1 1 1 1 1 2 1 1 2
2 1 0 0 2 A 1 2 2 2 1 1 1 1 2 2 1 1 1 2
3 1 0 0 1 A 1 2 1 2 1 1 1 2 1 1 1 1 2 1
4 1 0 0 2 A 1 1 2 2 1 1 1 1 2 1 1 1 1 1
5 1 0 0 2 A 1 1 1 1 1 2 1 1 2 1 2 1 1 2
6 1 0 0 1 U 1 1 2 1 2 2 1 1 1 1 1 1 1 1
7 1 0 0 1 U 1 1 1 1 2 1 1 1 1 1 1 1 2 1
8 1 0 0 1 U 1 2 1 1 2 1 1 1 1 2 2 2 1 1
9 1 0 0 1 U 1 1 1 1 1 1 1 1 2 1 1 1 1 1
10 1 0 0 1 U 2 1 2 1 1 1 1 1 2 2 1 2 2 2

>>>
```

Population variables


```
>>> pop = population(subPop=[5, 10], loci=[5])
>>> InitByFreq(pop, [.6, .3, .1])
>>> Stat(pop, alleleFreq=[1], genoFreq=[2])
>>> print pop.dvars().alleleFreq[1][0]
0.533333333333
>>> from simuUtil import ListVars
>>> ListVars(pop.dvars(), useWxPython=False)
 grp :  -1
 rep :  -1
 alleleNum :
   [1]
     [0]        16
     [1]        13
     [2]        1
 genoFreq :
   [2]
     [0]
       0 :      0.4
       1 :      0.333333333333
       2 :      0.2
     [1]
       2 :      0.0666666666667
 genoNum :
   [2]
     [0]
       0 :      6.0
       1 :      5.0
       2 :      3.0
     [1]
       2 :      1.0
 alleleFreq :
```

Population variables (cont.)


```
subPop
  [0]
    alleleNum :
      [1]
        [0]    6
        [1]    4
    genoNum :
      [2]
        [0]
          0 :  4.0
          1 :  1.0
    genoFreq :
      [2]
        [0]
          0 :  0.8
          1 :  0.2
    alleleFreq :
      [1]
        [0]    0.6
        [1]    0.4
  [1]
    alleleNum :
      [1]
        [0]    10
        [1]    9
        [2]    1
```

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2		3	4			5	6
0	1	1		1	0			0	1
0	0	1		1	1			0	1

0			1	2	3	4	5
0			1	0	0	0	1
1			0	1	1	0	0

Male

- Affected

fitness	father_id	···

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2		3	4			5	6
0	1	1		1	0			0	1
0	0	1		1	1			0	1

0			1	2	3	4	5
0			1	0	0	0	1
1			0	1	1	0	0

Chromosome 0

Male

- Affected

fitness	father_id	···

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2		3	4			5	6
0	1	1		1	0			0	1
0	0	1		1	1			0	1

0	1	2	3	4	5
0	1	0	0	0	1
1	0	1	1	0	0

Chromosome 0

Chromosome 1

Male

- Affected

fitness	father_id	···

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2	3	4	5	6
0	1	1	1	0	0	1
0	0	1	1	1	0	1

Chromosome 0

0	1	2	3	4	5
0	1	0	0	0	1
1	0	1	1	0	0

Chromosome 1

Male

Sex

- Affected

fitness	father_id	···

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2	3	4	5	6
0	1	1	1	0	0	1
0	0	1	1	1	0	1

0	1	2	3	4	5
0	1	0	0	0	1
1	0	1	1	0	0

Chromosome 0

Chromosome 1

Male

Sex

- Affected

Affection status

fitness	father_id	···

Structure of Individuals

Assume ploidy = 2, maxAllele = 1

0	1	2		3	4			5	6
0	1	1		1	0			0	1
0	0	1		1	1			0	1

0			1	2	3	4	5
0			1	0	0	0	1
1			0	1	1	0	0

Male

- Affected

fitness	father_id	...

Chromosome 0

Chromosome 1

Sex

Affection status

Information fields

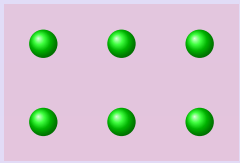
Individuals


```
>>> 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: 0 Fit: 0.500 Geno: 2 1
Aff: 0 Fit: 0.200 Geno: 0 1
Aff: 0 Fit: 0.050 Geno: 0 0
Aff: 0 Fit: 0.050 Geno: 0 0
Aff: 0 Fit: 0.200 Geno: 1 0
Aff: 0 Fit: 0.200 Geno: 2 0
Aff: 0 Fit: 0.200 Geno: 0 1
Aff: 0 Fit: 0.200 Geno: 0 1
>>>
```

Information fields


```
>>> pop = population(100, loci=[5, 8],
...     infoFields=['father_idx', 'mother_idx'])
>>> simu = simulator(pop, randomMating(numOffspring=2))
>>> simu.evolve(ops=[parentsTagger()], end=5)
True
>>> ind = simu.population(0).individual(0)
>>> ind1 = simu.population(0).individual(1)
>>> print ind.info('father_idx'), ind.info('mother_idx')
34.0 76.0
>>> print ind1.info('father_idx'), ind1.info('mother_idx')
34.0 76.0
>>>
>>>
```

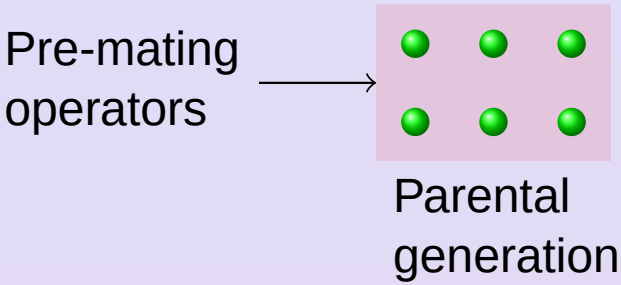
Life cycle of a generation



Parental generation

Every operator has a default stage, and a `stage` parameter to change it.

Life cycle of a generation



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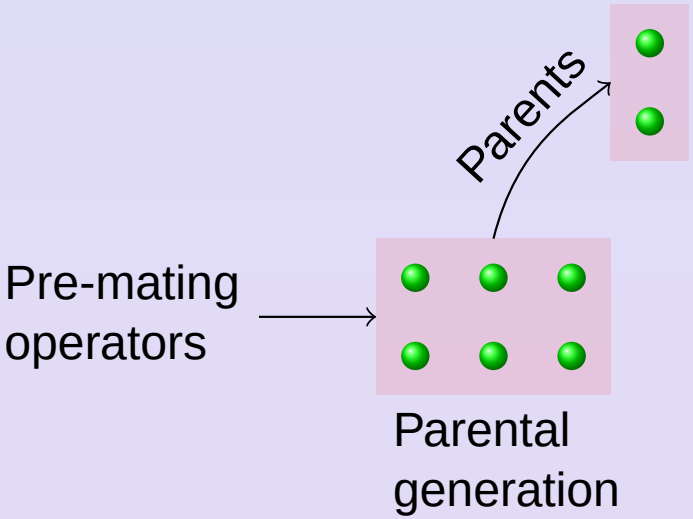

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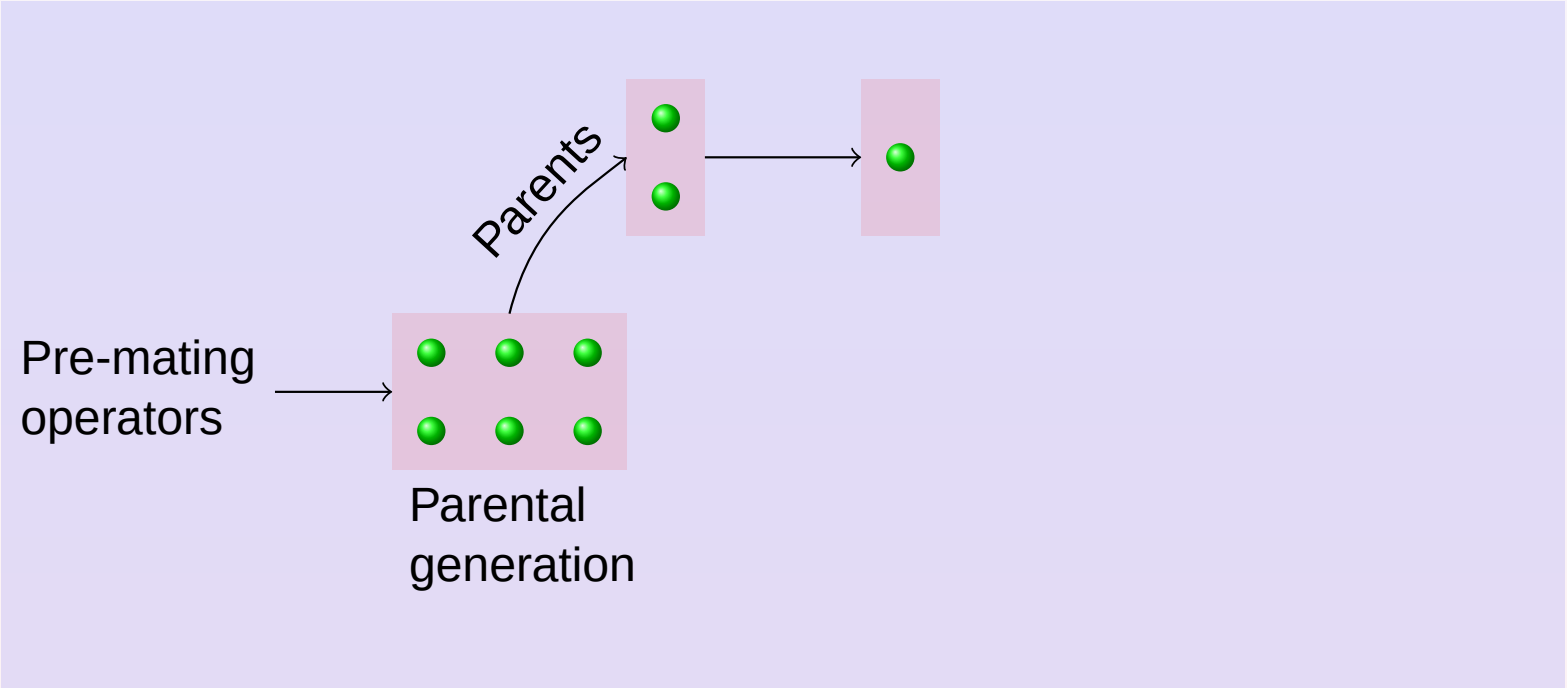
Life cycle of a generation



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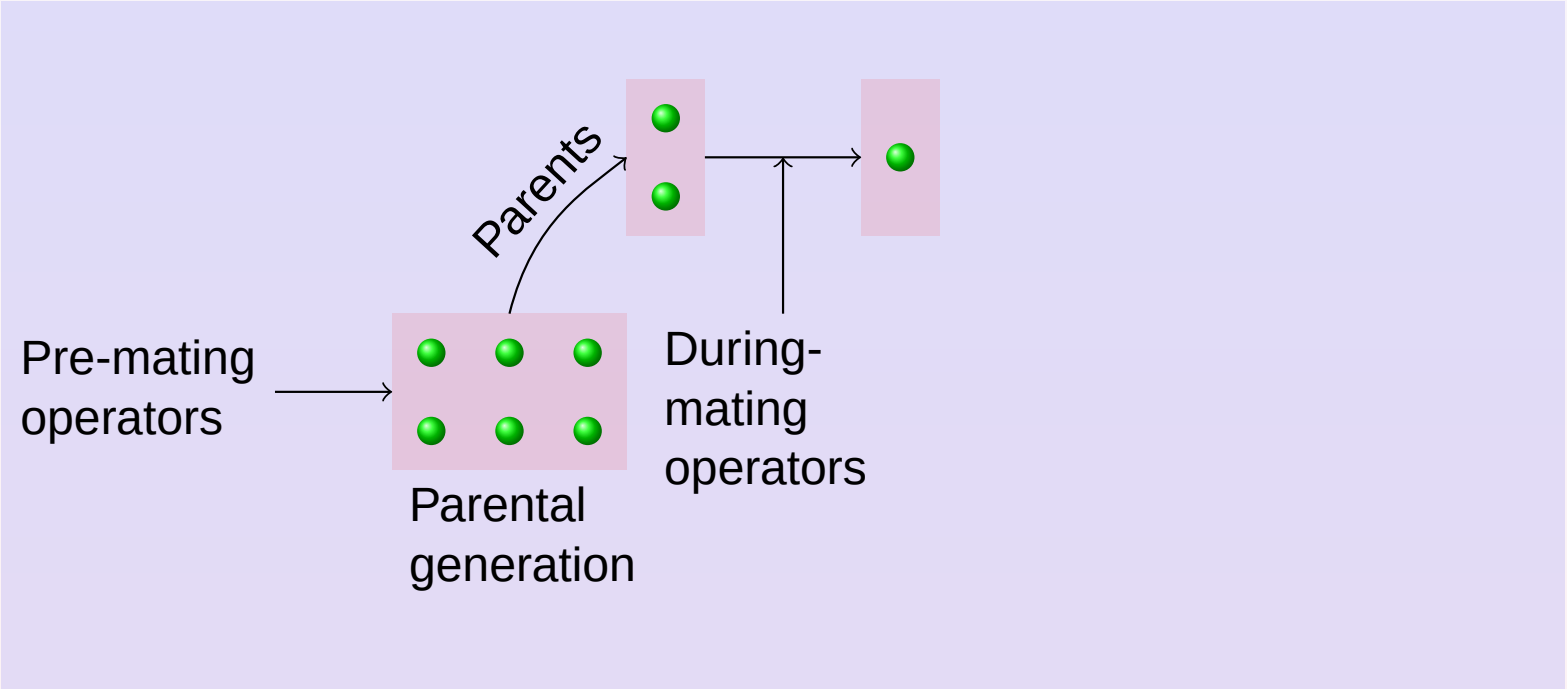
Life cycle of a generation



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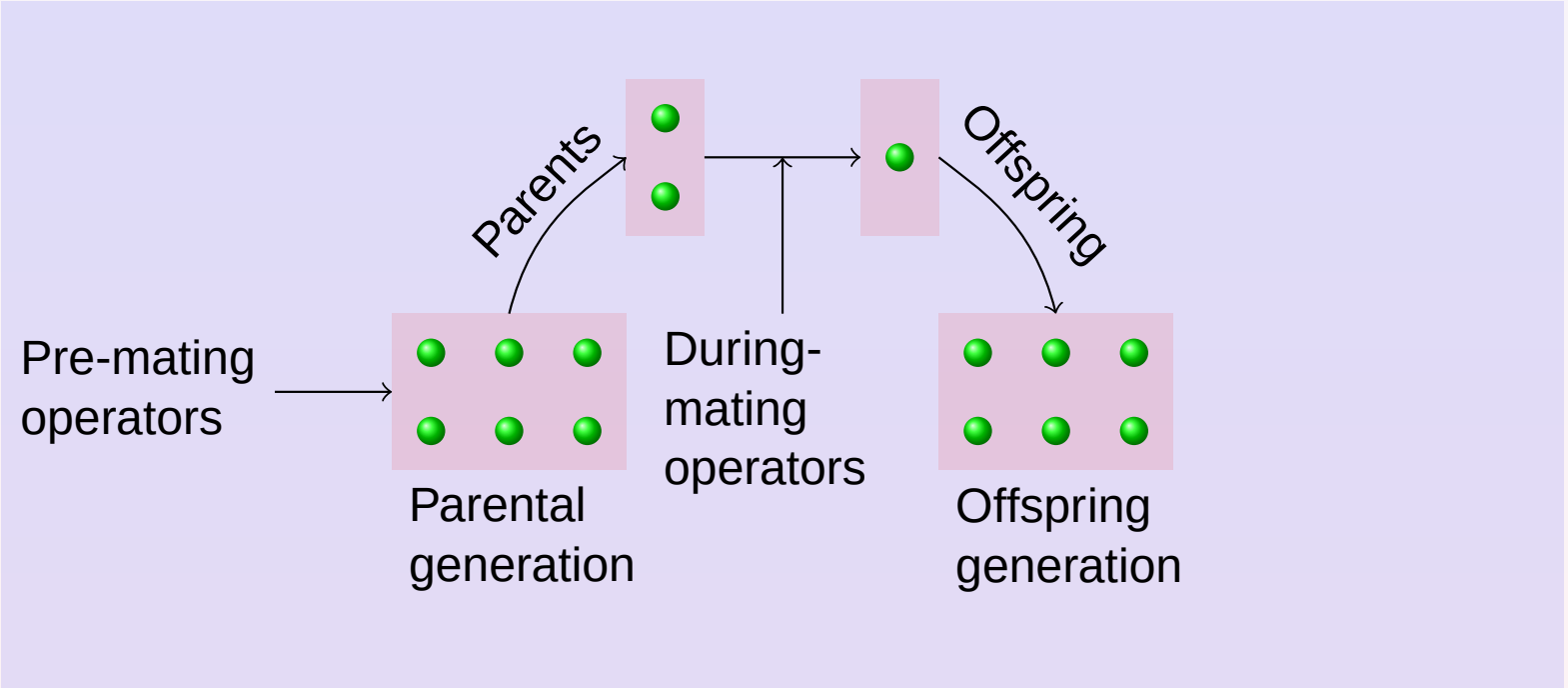
Life cycle of a generation



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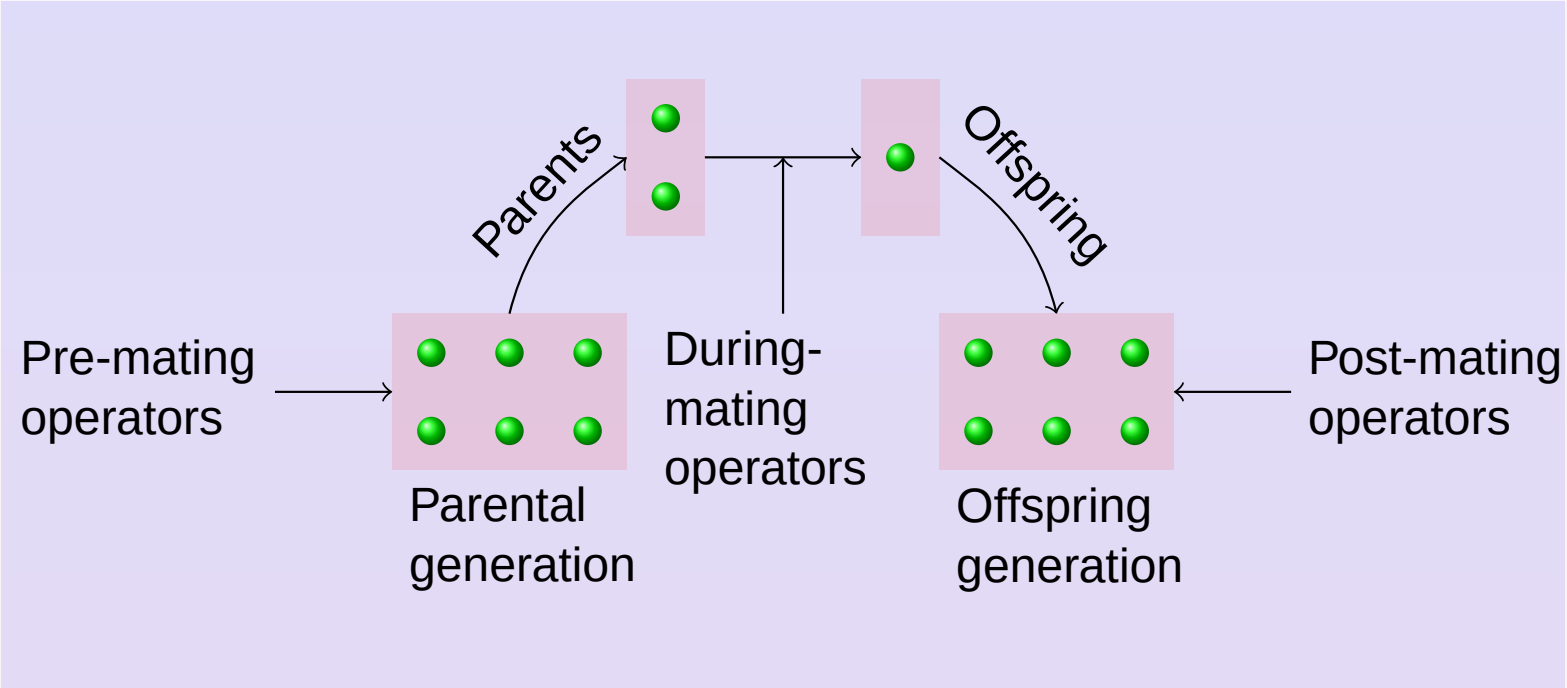
Life cycle of a generation



Every operator has a default stage, and a `stage` parameter to change it.

Pre-, During- and PostMating operators


```
>>> simu = simulator(
...     population(subPop=[20, 80], loci=[3]),
...     randomMating())
>>> simu.evolve(
...     preOps = [initByFreq([0.2, 0.8])],
...     ops = [
...         kamMutator(maxAllele=10, rate=0.00005, atLoci=[0,2]),
...         recombinator(rate=0.001),
...         dumper(stage=PrePostMating),
...         stat(alleleFreq=[1]),
...     ],
...     dryrun=True
... )
Dryrun mode: display calling sequence
Apply pre-evolution operators
  Replicate 0
    Apply pre-mating ops
      - <simuPOP::initByFreq> 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


```
>>> simu = simulator(
...     population(10000, loci=[3]),
...     randomMating())
>>> eval1 = r"'Gen: %3d  Freq: %f\n' % (gen, alleleFreq[1][0])"
>>> eval2 = r"'Last Gen: %3d  Freq: %s\n' % (gen, alleleFreq[1])"
>>> simu.evolve(
...     preOps = [initByFreq([0.3, 0.7])],
...     ops = [
...         recombinator(rate=0.01, begin=10, end=30),
...         stat(alleleFreq=[1], step=10),
...         pyEval(eval1, step=10),
...         pyEval(eval2, at=[-1])
...     ],
...     end = 50
... )
Gen:   0  Freq: 0.300050
Gen:  10  Freq: 0.310100
Gen:  20  Freq: 0.294950
Gen:  30  Freq: 0.297350
Gen:  40  Freq: 0.292450
Gen:  50  Freq: 0.292550
Last Gen:  50  Freq: [0.29254999999999998, 0.70745000000000002]
True
>>>
```

Applicable replicates


```
>>> simu = simulator(
...     population(100, loci=[3]),
...     randomMating(),
...     rep=5, grp=[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),
...         pyEval(r"'%.2f ' % alleleFreq[1][0]", grp=1),
...         pyEval(r"'\n'", rep=REP_LAST),
...     ],
...     end=5
... )
Warning: More than one during mating operators. Make sure they a
0.48 0.47
0.52 0.46
0.45 0.42
0.46 0.47
0.45 0.48
0.50 0.47
True
```

Output


```
>>> simu = simulator(
...     population(100, loci=[3]),
...     randomMating(),
...     rep=5, grp=[1,1,2,2,2])
>>> simu.evolve(
...     preOps = [initByFreq([0.5, 0.5])],
...     ops = [
...         stat(alleleFreq=[1]),
...         pyEval(r"'%.2f ' % alleleFreq[1][0]",
...             output='>>out'),
...         pyEval(r"'\n'", rep=REP_LAST, output='>>out'),
...         pyEval(r"'%.2f ' % alleleFreq[1][0]",
...             outputExpr="'>>out%d' % grp"),
...     ],
...     end=2
... )
True
>>> print open('out').read()
0.55 0.47 0.47 0.51 0.47
0.50 0.42 0.52 0.55 0.44
0.51 0.47 0.56 0.52 0.43

>>> print open('out1').read()
0.55 0.47 0.50 0.42 0.51 0.47
>>> print open('out2').read()
0.47 0.51 0.47 0.52 0.55 0.44 0.56 0.52 0.43
>>>
```

Mating schemes

Mating schemes

- Population offspring subpopulation from corresponding parental subpopulation
- Can change subpopulation size
- Select parents according to their `fitness` value (information field)
- Can produce more than one offspring

Demographic model


```
>>> 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),
...         pyEval(r'"%d %d\n"%(gen, subPop[0]["popSize"])'),
...     ],
...     end=5
... )
0 10
1 11
2 12
3 13
4 14
5 15
True
>>>
```

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>]
>>>
```

Simulator

A simulator manages

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

and evolve the populations.

Utility modules and scripts

simuOpt.py provides an easy way to handle parameters.

simuUtil.py provides functions to save/load in many formats, gene mapping functions, list variables etc

simuCluster.py a control script to send jobs to cluster systems

simuLDDecay.py a simple script to demonstrate the decay of linkage disequilibrium under recombination

simuForward.py implements a traditional forward-time simulation scenario

simuComplexDisease.py implements a new forward-time simulation method (PLoS Genetics, 2007)

simuCDCV.py demonstrate the evolution of allelic spectrum

...

Outline

2 Populations

- Overview
- Population structure
- Information fields

```
>>> Dump(pop)
Ploidy:                    2
Number of chrom:           2
Number of loci:            2 3
Maximum allele state:   65535
Loci positions:
                  1 2
                  1 2 3
Loci names:
                  loc1-1 loc1-2
                  loc2-1 loc2-2 loc2-3
population size:           10
Number of subPop:          1
Subpop sizes:              10
Number of ancestral populations:         0
individual info:
sub population 0:
   0: MU   0  0   0  0  0 |   0  0   0  0  0
   1: MU   0  0   0  0  0 |   0  0   0  0  0
   2: MU   0  0   0  0  0 |   0  0   0  0  0
   3: MU   0  0   0  0  0 |   0  0   0  0  0
   4: MU   0  0   0  0  0 |   0  0   0  0  0
   5: MU   0  0   0  0  0 |   0  0   0  0  0
   6: MU   0  0   0  0  0 |   0  0   0  0  0
   7: MU   0  0   0  0  0 |   0  0   0  0  0
   8: MU   0  0   0  0  0 |   0  0   0  0  0
   9: MU   0  0   0  0  0 |   0  0   0  0  0
End of individual info.
```

```
>>> InitByFreq(pop, alleleFreq=[0.3, 0.7])
>>> Dump(pop)
Ploidy:                    2
Number of chrom:           2
Number of loci:            2 3
Maximum allele state:   65535
Loci positions:
                  1 2
                  1 2 3
Loci names:
                  loc1-1 loc1-2
                  loc2-1 loc2-2 loc2-3
population size:           10
Number of subPop:          1
Subpop sizes:              10
Number of ancestral populations:         0
individual info:
sub population 0:
   0: FU   0  1   0  0  1 |   1  1   1  0  0
   1: MU   1  1   1  0  1 |   1  1   1  1  1
   2: MU   1  1   1  1  1 |   1  0   1  0  1
   3: MU   0  1   1  1  1 |   1  1   1  1  0
   4: MU   0  1   1  0  1 |   1  1   1  0  1
   5: MU   1  1   1  1  0 |   1  1   1  1  1
   6: FU   1  1   1  1  1 |   1  0   1  0  0
   7: MU   1  0   1  1  1 |   0  1   0  1  0
   8: MU   0  0   1  1  1 |   1  1   1  0  1
   9: MU   0  0   1  1  0 |   0  1   1  1  1
```

```
>>> 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:           1
Number of loci:            2
Maximum allele state:   65535
Loci positions:
                  1 2
Loci names:
                  loc1-1 loc1-2
population size:           13
Number of subPop:          3
Subpop sizes:              2 5 6
Number of ancestral populations:         0
>>>
```

Mating is within subpopulation only


```
>>> pop = population(subPop=[5, 6], loci=[2])
>>> simu = simulator(pop, randomMating())
>>> simu.evolve(
...     preOps = [
...         initByFreq(alleleFreq=[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 is within subpopulation only – continue


```
individual info:
sub population 0:
   0: MU   1  1 |   0  1
   1: FU   1  0 |   0  1
   2: FU   1  1 |   1  1
sub population 1:
   5: FU   3  4 |   3  4
   6: FU   3  4 |   3  4
End of individual info.


No ancenstral population recorded.
individual info:
sub population 0:
   0: MU   1  1 |   0  1
   1: MU   0  1 |   1  1
   2: FU   1  1 |   1  1
sub population 1:
   5: MU   3  4 |   4  3
   6: MU   4  3 |   3  4
End of individual info.
```

Subpopulation manipulations

Information fields

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 – an example

Outline

3 Operators

- Python Operators

The most flexible operators that can perform any operation, but are less efficient.

The idea: user provide a function with specified input and output, simuPOP calls this function during evolution.

Python operator


```
func(pop [, param])
```

Python Individual operator

`func(ind [, genotype] [, param]), return True/False or an array`

- `ind`: individual
- `genotype`: if parameter loci is given, genotype at these loci are passed to the function
- `param`: if parameter param is given, param passed from simuPOP
- `return`: if parameter infoFields is given, assign return values to these information fields

An example of `pyIndOperator`

Specialized Python operators: pyPenetrance

pySelector

Outline

4 Simulator

simulator

mating scheme

evolve!

Exercise time!

simuLDDecay.py

Outline

5 simuPOP components

- Population object
- Operators
- Mating scheme, Simulator and forward-time simulation

Create a population

Genotypic structure

Individuals

Population strcuture

Information fields

Variables

Stages

Stages, an example

Output

Table-like output

Mating schemes

Simulator

Evolve?!

Outline

6 A real example

- Handling of HapMap data

Outline

7 A quick Python tutorial

Outline

8 Some more examples

- Example 1
- Example 2

Manipulating of HapMap data

Outline

9 Advanced topics