

Forward-time simulations using simuPOP, a tutorial

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Programmers' Cross Training
U.T. M.D. Anderson Cancer Center

outline

simuPOP tutorial

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What is
simuPOP

An example

simuPOP
components

- 1 What is simuPOP
- 2 An example
- 3 simuPOP components

simuPOP is ...

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What is
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An example

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components

A forward-time population genetics simulation environment

simuPOP is ...

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What is
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A forward-time population genetics **simulation** environment

- A population genetics simulation program

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What is
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An example

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A **forward-time** population genetics simulation environment

- A population genetics simulation program
- Not coalescent-based

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What is
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A forward-time population genetics simulation **environment**

- A population genetics simulation program
- Not coalescent-based
- Based on an object-oriented scripting language (Python)

What simuPOP does

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What is
simuPOP

An example
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components

simuPOP provides

- a large number of functions to manipulate populations, copy, split, merge, modify genotype, modify individuals, determine affection status, save to and load from various formats, generate sample, ...

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What is
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components

simuPOP provides

- a large number of functions to manipulate populations, copy, split, merge, modify genotype, modify individuals, determine affection status, save to and load from various formats, generate sample, ...
- and a mechanism to evolve populations forward in time, subject to arbitrary demographic and genetic forces such as population size changes, mutation, migration, recombination, selection ...

This is fun, but is it useful?

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What is
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An example

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simuPOP can simulate the change of the genetic composition of a population in a complicated evolutionary process. It can be used to

- demonstrate population genetics phenomena

This is fun, but is it useful?

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simuPOP can simulate the change of the genetic composition of a population in a complicated evolutionary process. It can be used to

- demonstrate population genetics phenomena
- study the impact of genetic and demographic forces on the evolution of a population

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- study the evolution of (complex) genetic diseases

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- study the evolution of (complex) genetic diseases
- simulate samples to validate gene-mapping methods

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- simulate samples to validate gene-mapping methods
- study ascertainment methods in simulated populations

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- ...

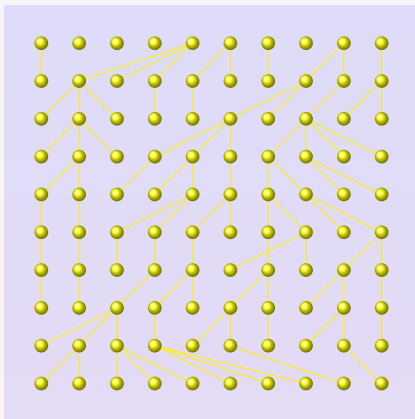
Forward-time simulation

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Forward-time simulation

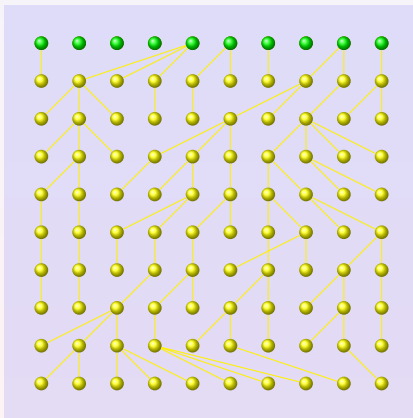
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- Start from an initial population



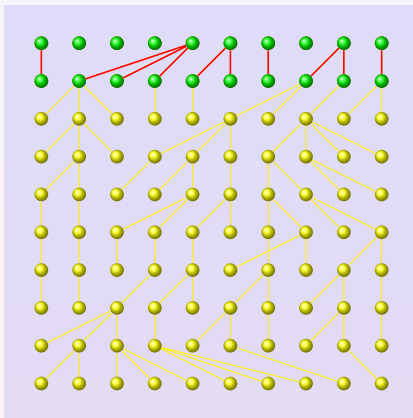
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- Start from an initial population
- Evolve forward in time, generation by generation, subject to certain number of genetic and/or demographic effects

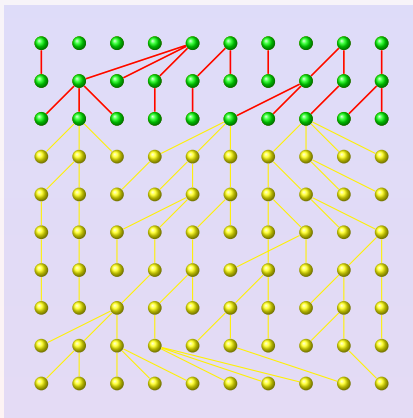
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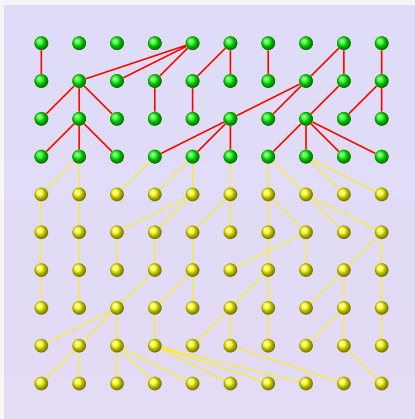
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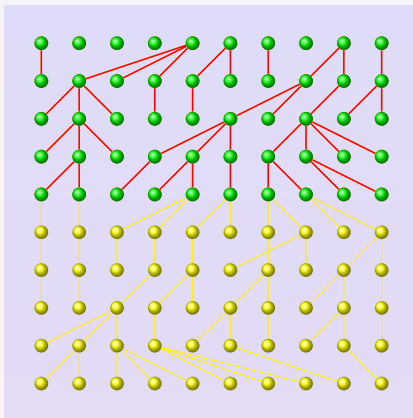
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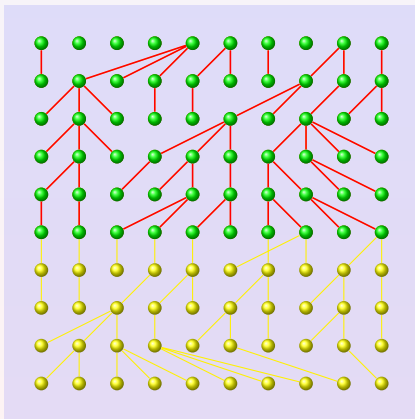
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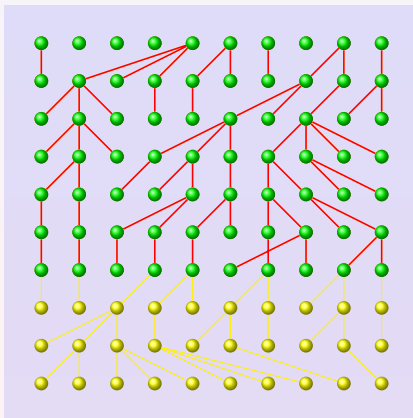
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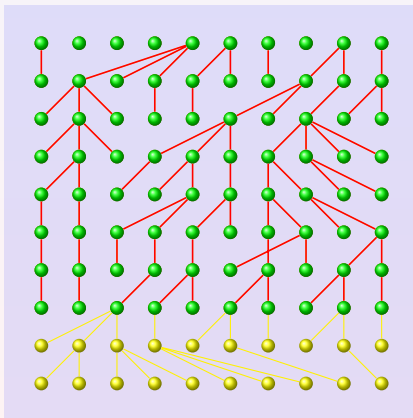
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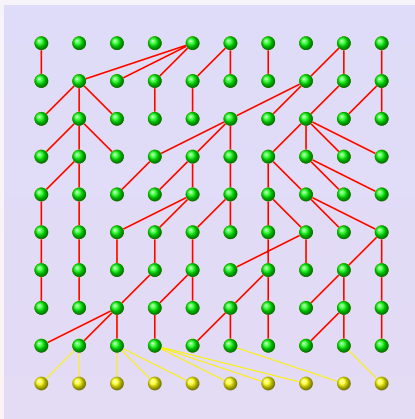
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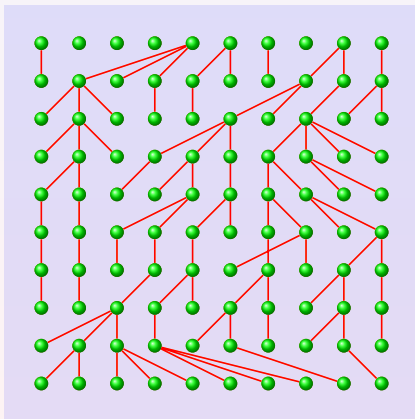
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- Start from an initial population
- Evolve forward in time, generation by generation, subject to certain number of genetic and/or demographic effects
- Samples are collected from the last several generations

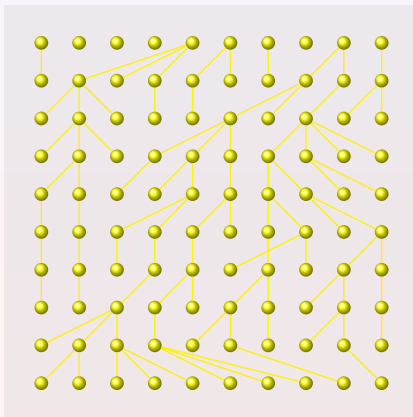
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- Start from a sample with unknown genotype
- Coalesce individuals until the most recent common ancestor of all individuals is found
- Starting from the MRCA, proceed forward in time and fill the genotype of each individual

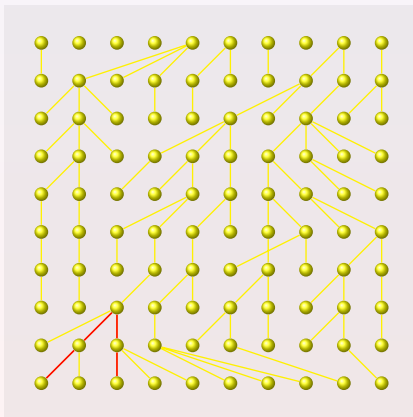
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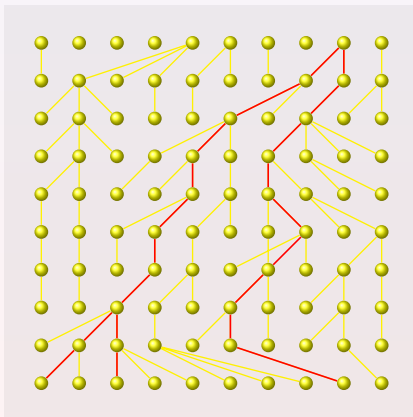
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Forward vs. backward-time simulations

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Backward-time

- Sample based, efficient.

Forward-time

- Population based, inefficient.

Forward vs. backward-time simulations

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Backward-time

- Sample based, efficient.
- Limited selection, recombination models and mating schemes

Forward-time

- Population based, inefficient.
- Can simulate almost arbitrary evolutionary scenarios

Forward vs. backward-time simulations

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Backward-time

- Sample based, efficient.
- Limited selection, recombination models and mating schemes
- Can not study population properties, or properties of ancestral generations

Forward-time

- Population based, inefficient.
- Can simulate almost arbitrary evolutionary scenarios
- Can study population properties and ancestral generations

Forward vs. backward-time simulations

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Backward-time

- Sample based, efficient.
- Limited selection, recombination models and mating schemes
- Can not study population properties, or properties of ancestral generations
- Used mostly for sample generation

Forward-time

- Population based, inefficient.
- Can simulate almost arbitrary evolutionary scenarios
- Can study population properties and ancestral generations
- Wider application area

On the simulations of complex human diseases

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Backward-time

- Haploid simulation only

Forward-time

- No limit on ploidy

On the simulations of complex human diseases

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Backward-time

- Haploid simulation only
- Additive selection and penetrance models

Forward-time

- No limit on ploidy
- Arbitrary selection and penetrance models

On the simulations of complex human diseases

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Backward-time

- Haploid simulation only
- Additive selection and penetrance models
- One disease susceptibility locus

Forward-time

- No limit on ploidy
- Arbitrary selection and penetrance models
- Multiple DSL with interaction

On the simulations of complex human diseases

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Backward-time

- Haploid simulation only
- Additive selection and penetrance models
- One disease susceptibility locus
- Generate independent samples

Forward-time

- No limit on ploidy
- Arbitrary selection and penetrance models
- Multiple DSL with interaction
- Simulate populations, which allows more flexible sampling

I like it, but, oohm, Python??

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What is simuPOP

An example simuPOP components

- For efficiency, the core of simuPOP is written in C++
- Python is used to
 - wrap simuPOP core (the glue language)
 - write simuPOP extensions (GUI etc)
 - pass parameters and more

Availability

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An example

simuPOP components

- **simuPOP website:**
`http://simupop.sourceforge.net`
- **Mailing list:**
`simupop-list@lists.sourceforge.net`
- **License:** GPL 2.0
- **Platforms:** all OS on which Python is available
- **Monthly release,** currently at 0.7.10
- **Documentation:** *simuPOP User's Guide* and *simuPOP Reference Manual*

A simple example

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What is simuPOP

An example

simuPOP components

```
>>> from simuPOP import *
>>> simu = simulator(
...     population(size=1000, ploidy=2, loci=[2]),
...     randomMating(),
...     rep = 3)
>>> simu.evolve(
...     preOps = [initByValue([1,2,2,1])],
...     ops = [
...         recombinator(rate=0.1),
...         stat(LD=[0,1]),
...         pyEval(r"'%3d    ' % gen", rep=0, step=10),
...         pyEval(r"'%f        ' % LD[0][1]", step=10),
...         pyEval(r"'\\n'", rep=REP_LAST, step=10)
...     ],
...     end=100
... )
```

Output of the example

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0	0.198036	0.200709	0.197748
10	0.064744	0.063100	0.078473
20	0.013233	0.019795	0.041057
30	0.002985	0.004931	0.000649
40	0.023492	0.002948	0.004462
50	0.006016	0.014262	0.013900
60	0.011310	0.008717	0.013715
70	0.016652	0.014545	0.014426
80	0.007250	0.002506	0.014372
90	0.016994	0.014455	0.004147
100	0.000425	0.016570	0.008704

simuPOP modules

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An example

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components

```
>>> from simuPOP import *  
>>> simu = simulator(  
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```

Import the default simuPOP module

population

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An example

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```
>>> from simuPOP import *
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...     rep = 3)
```

Create a **population** of 1000 **diploid** individuals, each having two **loci** on the first chromosome

simulator and mating scheme

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An example

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```
>>> from simuPOP import *
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```

Create a **simulator** that has one replicate of this population, and a random mating scheme

Operators!

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```

`initByValue` is applied before evolution

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...     ],
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... )
```

recombinator is applied at every generation when an offspring is produced

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...     ],
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... )
```

stat is applied to the offspring generation at every generation

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```

pyEval is applied every 10 generations

Use R to plot

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An example

simuPOP components

```
>>> from simuPOP import *
>>> from simuRPy import *
>>> simu = simulator(
...     population(size=1000, ploidy=2, loci=[2]),
...     randomMating(),
...     rep = 3)
>>> simu.evolve(
...     preOps = [initByValue([1,2,2,1])],
...     ops = [
...         recombinator(rate=0.1),
...         stat(LD=[0,1]),
...         varPlotter('LD[0][1]', numRep=3, step=10, saveAs='ld',
...             ylim=[0,.25], lty=range(1, 4), col=range(2, 5),
...             xlab='generation', ylab='D', title='LD Decay')),
...     ],
...     end=100
... )
True
>>>
```


Evolve!

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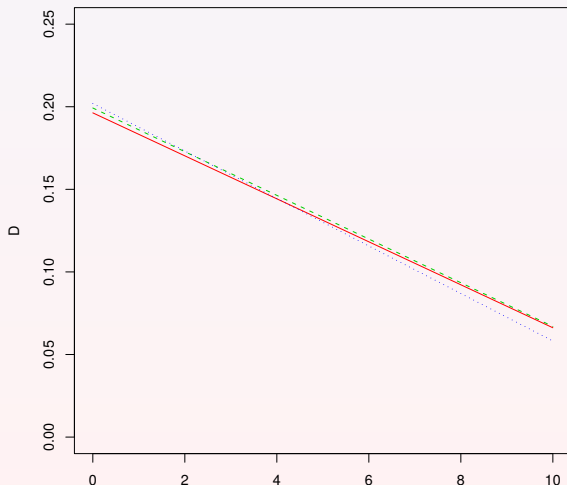
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LD Decay



- Update at every 10 generations
- $LD=0.25$ before generation 0
- LD calculated at the end of each generation

Evolve!

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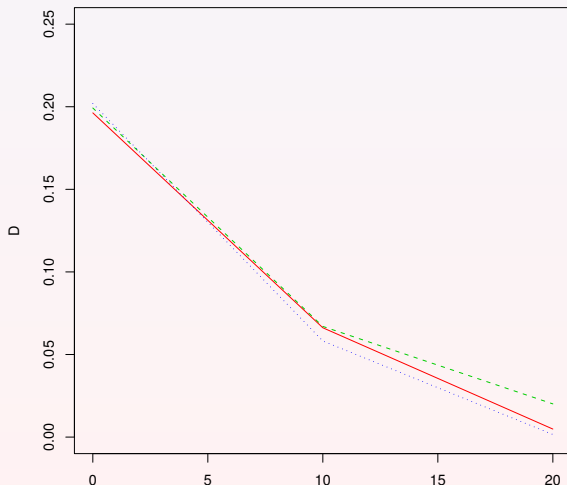
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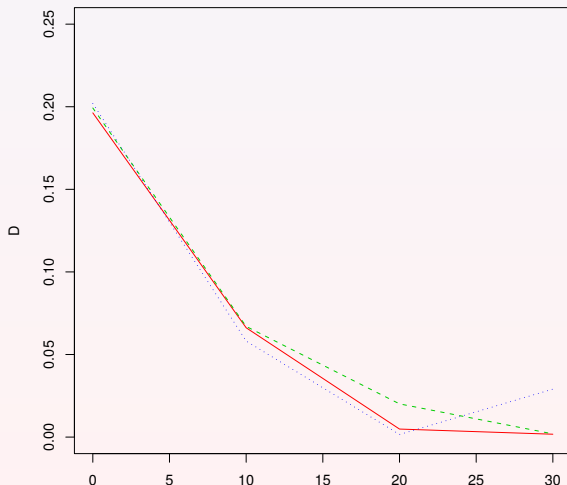
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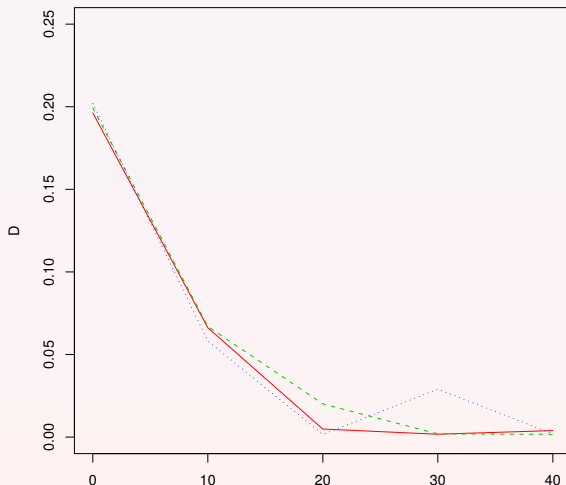
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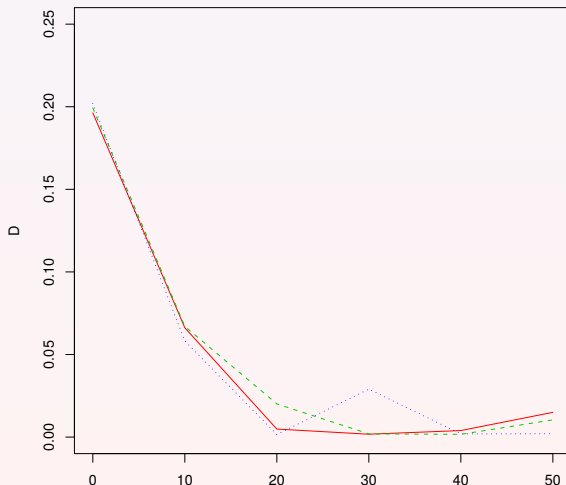
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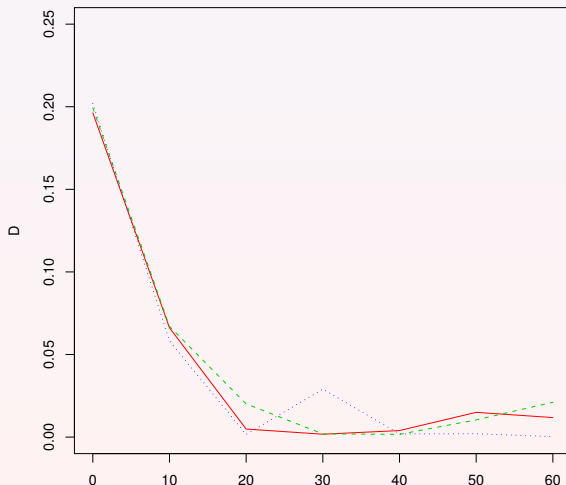
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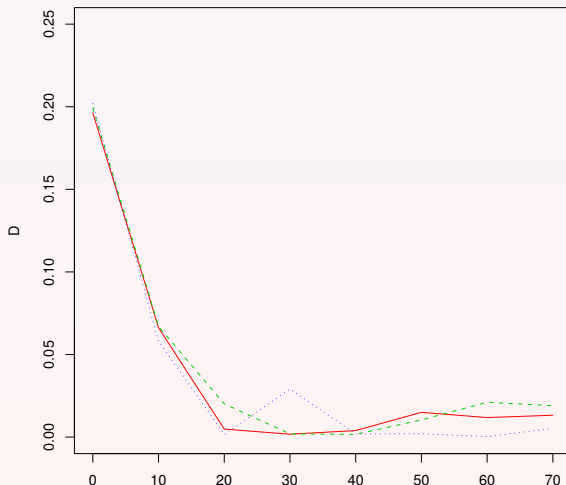
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Evolve!

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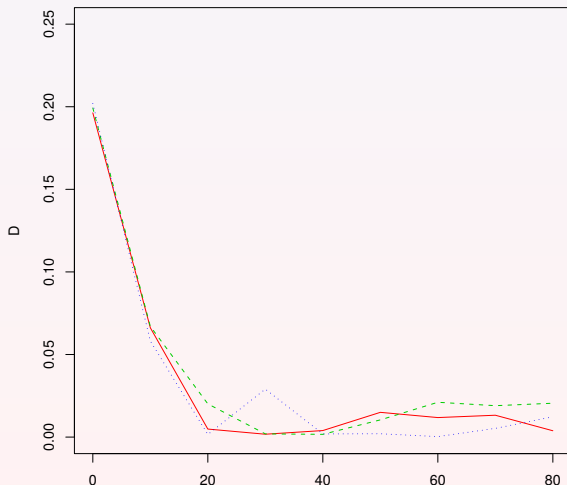
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What is
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An example

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LD Decay



- Update at every 10 generations
- LD=0.25 before generation 0
- LD calculated at the end of each generation

Evolve!

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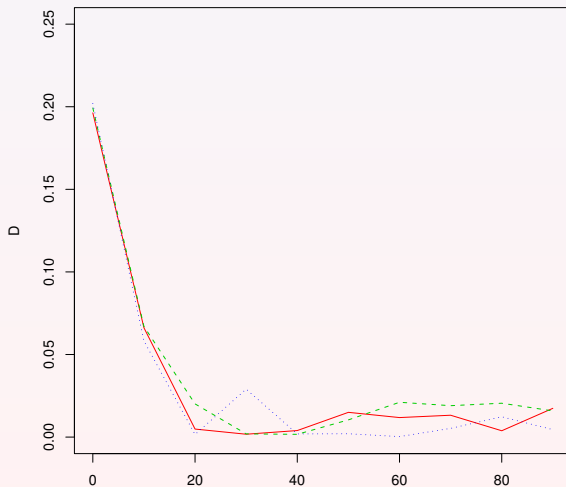
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LD Decay



- Update at every 10 generations
- LD=0.25 before generation 0
- LD calculated at the end of each generation

Evolve!

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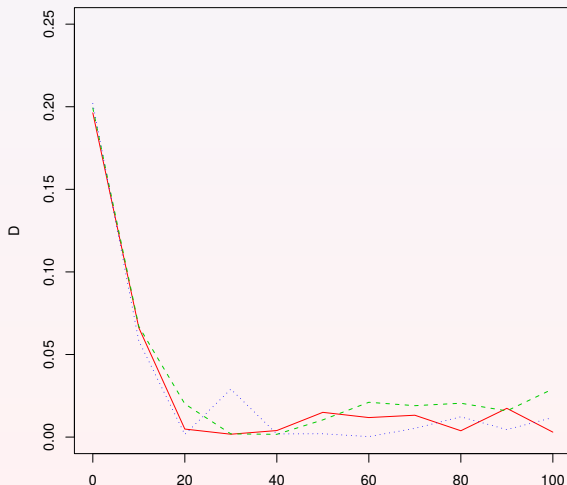
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LD Decay



- Update at every 10 generations
- $LD=0.25$ before generation 0
- LD calculated at the end of each generation

Exercise time

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- Start python
- Load simuPOP
- Create a population and run

```
pop.ploidyName( )
```

- run `tutorial_example1.py`

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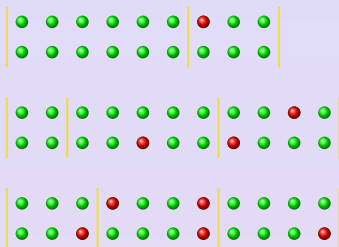
Individual

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- Unaffected
- Affected



gen = 2, numAffected = 5, ...

Structure of a population

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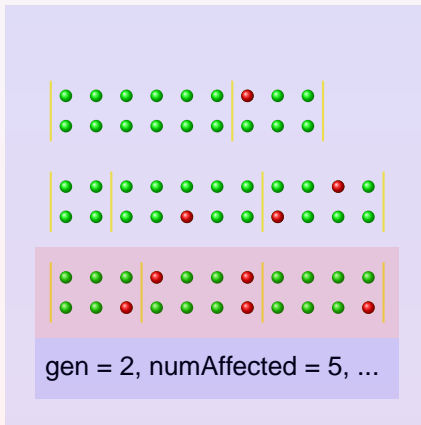
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

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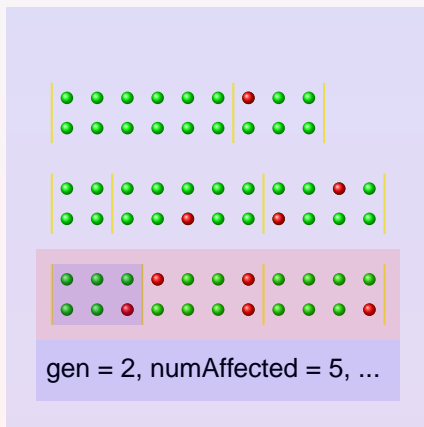
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

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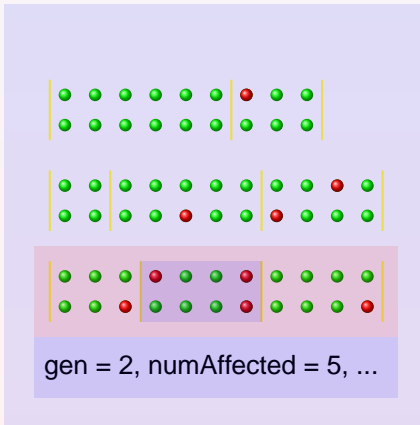
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

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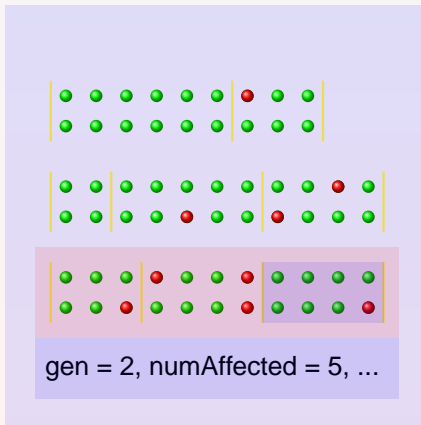
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- Unaffected
- Affected



Current generation

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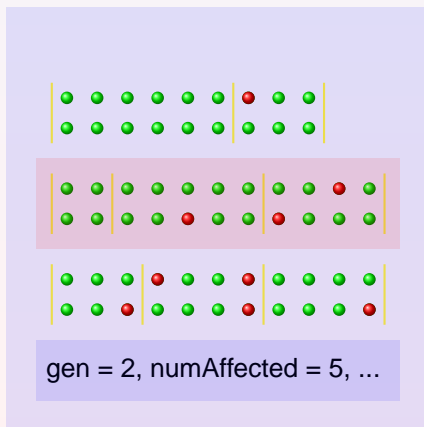
Individual

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Ancestral generation 1

Current generation

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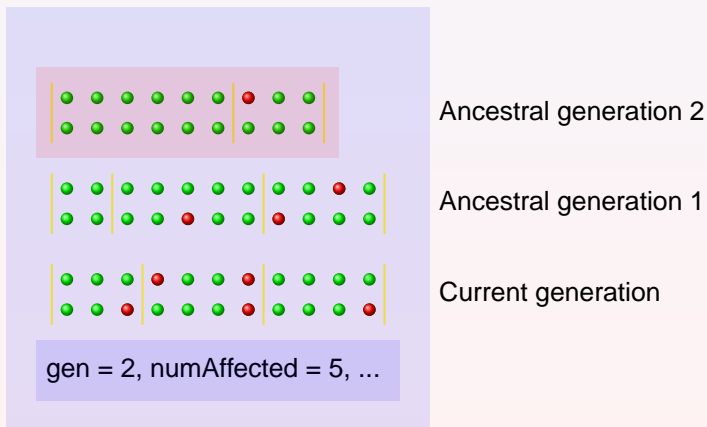
Individual

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- Unaffected
- Affected



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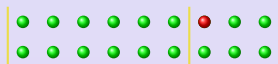
Individual

Operator

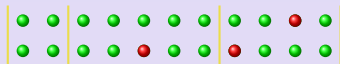
Mating scheme

Simulator

- Unaffected
- Affected



Ancestral generation 2



Ancestral generation 1



Current generation

gen = 2, numAffected = 5, ...

Population variables

Create and manipulate populations

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```
>>> pop = population(size=10, loci=[2, 3])
>>> Dump(pop)
Ploidy:                2
Number of chrom:        2
Number of loci:          2 3
Maximum allele state:    255
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

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```
>>> 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

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```
>>> # 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
[[0.8066666666666666, 0.1933333333333333], [0.7960000000000000, 0.2040000000000000]]
>>> # 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.)

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```
>>> # 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.)

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

>>>
```

Population variables

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```
>>> pop = population(subPop=[5, 10], loci=[5])
>>> InitByFreq(pop, [.6, .3, .1])
>>> Stat(pop, alleleFreq=[1], genoFreq=[2])
>>> print pop.dvars().alleleFreq[1][0]
0.7
>>> from simuUtil import ListVars
>>> ListVars(pop.dvars(), useWxPython=False)
grp : -1
rep : -1
alleleNum :
  [1]
    [0]      21
    [1]       7
    [2]       2
genoFreq :
  [2]
    [0]
      0 :      0.2
      1 :      0.6666666666667
      2 :      0.0666666666667
    [1]
      1 :      0.0666666666667
genoNum :
  [2]
    [0]
      0 :      3.0
      1 :     10.0
      2 :      1.0
    [1]
      1 :      1.0
alleleFreq :
```

Population variables (cont.)

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```
subPop
[0]
  alleleNum :
    [1]
      [0] 8
      [1] 1
      [2] 1
  genoNum :
    [2]
      [0]
        0 : 2.0
        1 : 2.0
      [1]
        1 : 1.0
  genoFreq :
    [2]
      [0]
        0 : 0.4
        1 : 0.4
      [1]
        1 : 0.2
  alleleFreq :
    [1]
      [0] 0.8
      [1] 0.1
      [2] 0.1
```

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Structure of Individuals

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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

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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

Male

● Affected

fitness	father_id	...
---------	-----------	-----

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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

● Affected

fitness	father_id	...
---------	-----------	-----

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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	...
---------	-----------	-----

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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

Affection status

fitness	father_id	...
---------	-----------	-----

Structure of Individuals

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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

Affection status

fitness | father_id | ...

Information
fields

Individuals

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

Information fields

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```
>>> pop = population(100, 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')
56.0 46.0
>>> print ind1.info('father_idx'), ind1.info('mother_idx')
56.0 46.0
>>>
>>>
```

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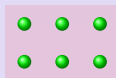
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Parental
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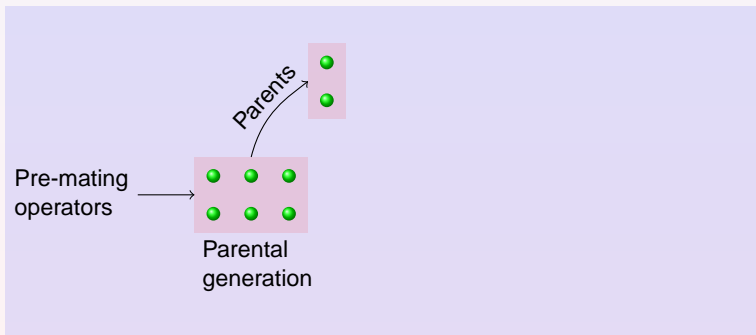
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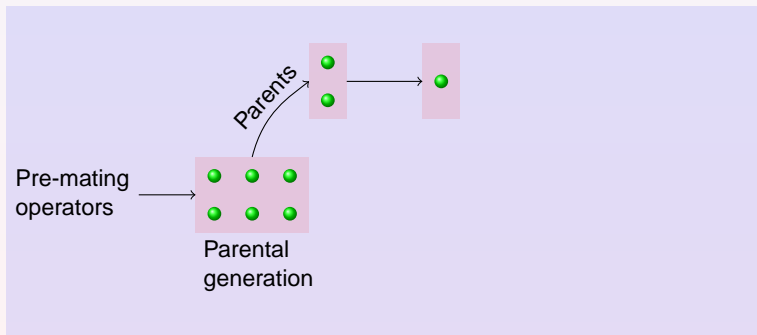
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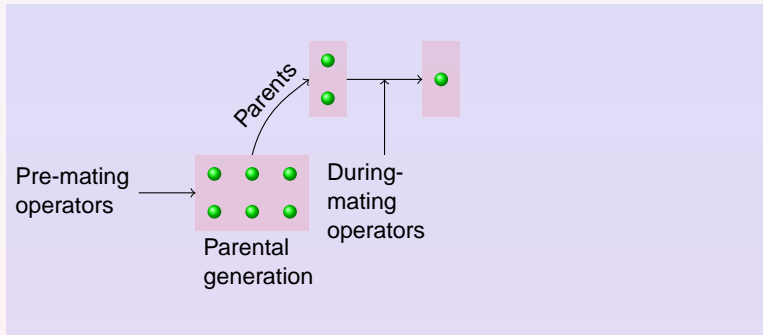
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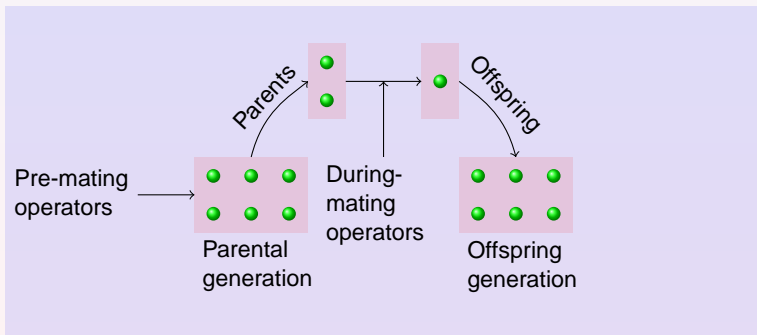
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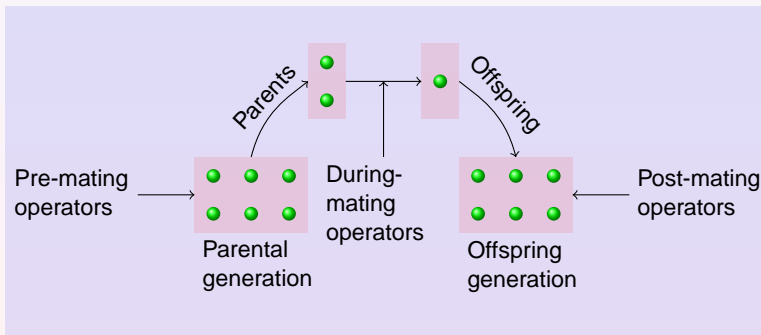
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Table-like output

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