

simuPOP  
tutorial

Bo Peng,  
Ph.D.

What is  
simuPOP

An example

simuPOP  
components

# Forward-time simulations using simuPOP, a tutorial

Bo Peng, Ph.D.

Department of Epidemiology  
U.T. M.D. Anderson Cancer Center  
Houston, TX

June. 6, 2007  
Programmers' Cross Training  
U.T. M.D. Anderson Cancer Center

# outline

## simuPOP tutorial

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What is  
simuPOP

An example

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components

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

# simuPOP is ...

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## A forward-time population genetics simulation environment

# simuPOP is ...

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

- A population genetics simulation program

# simuPOP is ...

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

- A population genetics simulation program
- Not coalescent-based

# simuPOP 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  
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## 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, ...

# What simuPOP does

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## 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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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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## What is simuPOP

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## simuPOP components

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

# This is fun, but is it useful?

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## What is simuPOP

## An example

## simuPOP components

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
- study the evolution of (complex) genetic diseases

# This is fun, but is it useful?

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## What is simuPOP

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

# This is fun, but is it useful?

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## What is simuPOP

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## simuPOP components

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

# This is fun, but is it useful?

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## What is simuPOP

## An example simuPOP components

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
- study the evolution of (complex) genetic diseases
- simulate samples to validate gene-mapping methods
- study ascertainment methods in simulated populations
- ...

# I heard about coalescent...

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## Backward-time

- 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

# I heard about coalescent...

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## Backward-time

- 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

## Forward-time

- 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



# 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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## What is simuPOP

## An example simuPOP components

### 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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## What is simuPOP

## An example simuPOP components

### 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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## What is simuPOP

## An example simuPOP components

### 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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## An example

## simuPOP components

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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```
>>> from simuPOP import *  
>>> simu = simulator(  
...     population(size=1000, ploidy=2, loci=[2]),  
...     randomMating(),  
...     rep = 3)
```

Import the default simuPOP module

# population

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## An example

## simuPOP components

```
>>> from simuPOP import *  
>>> simu = simulator(  
...     population(size=1000, ploidy=2, loci=[2]),  
...     randomMating(),  
...     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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## What is simuPOP

## An example

## simuPOP components

```
>>> from simuPOP import *
>>> simu = simulator(
...     population(size=1000, ploidy=2, loci=[2]),
...     randomMating(),
...     rep = 3)
```

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

# Operators!

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## What is simuPOP

## An example

## simuPOP components

```
>>> from simuPOP import *
>>> simu = simulator(
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...         pyEval(r"'\\n'", rep=REP_LAST, step=10)
...     ],
...     end=100
... )
```

`initByValue` is applied before evolution



# Operators!

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## What is simuPOP

## An example

## simuPOP components

```
>>> from simuPOP import *
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...         pyEval(r"'%f    ' % LD[0][1]", step=10),
...         pyEval(r"'\\n'", rep=REP_LAST, step=10)
...     ],
...     end=100
... )
```

**recombinator** is applied at every generation when an offspring is produced

# Operators!

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## What is simuPOP

## An example

## simuPOP components

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

**stat** is applied to the offspring generation at every generation

# Operators!

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## What is simuPOP

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## simuPOP components

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

**pyEval** is applied every 10 generations

# Use R to plot

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## What is simuPOP

## 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!

## simuPOP tutorial

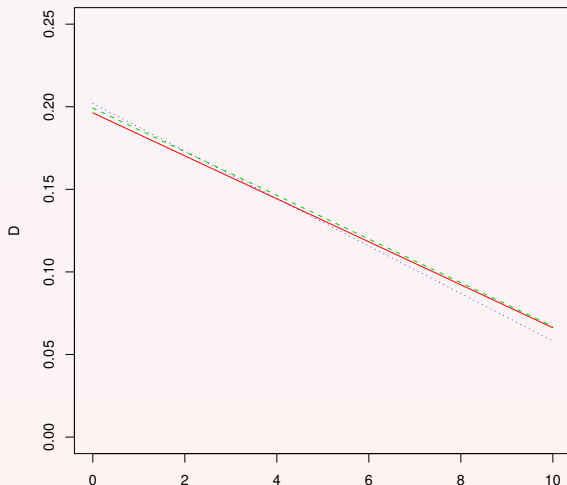
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What is  
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components

LD Decay



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

# Evolve!

## simuPOP tutorial

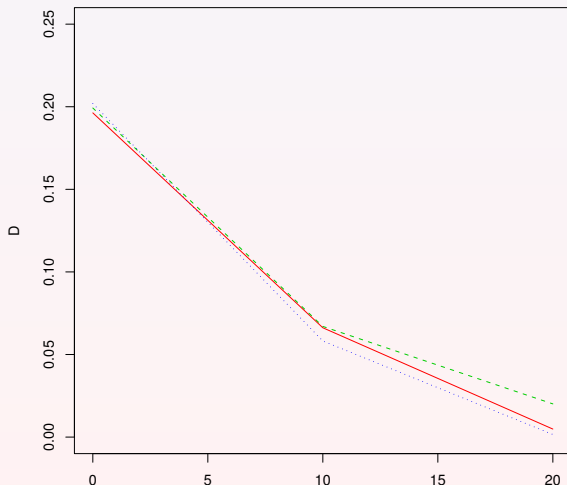
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LD Decay



- Update at every 10 generations
- $LD=0.25$  before generation 0
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# Evolve!

## simuPOP tutorial

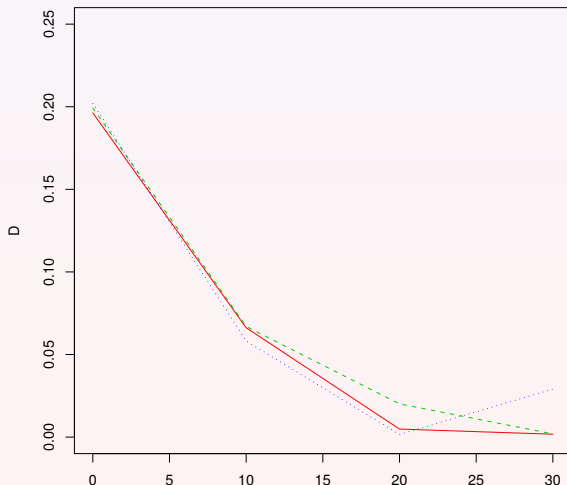
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LD Decay



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- $LD=0.25$  before generation 0
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# Evolve!

## simuPOP tutorial

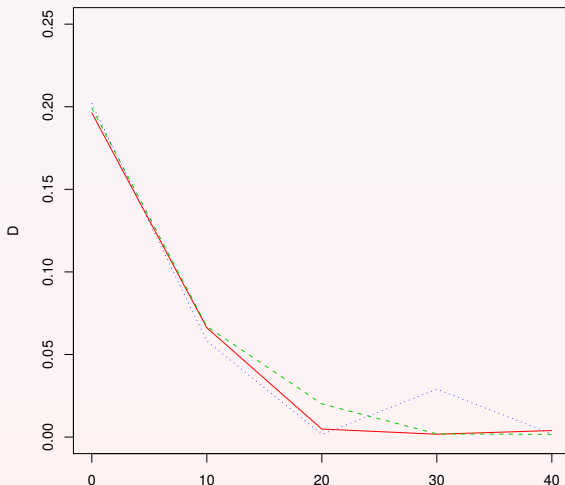
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LD Decay



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# Evolve!

## simuPOP tutorial

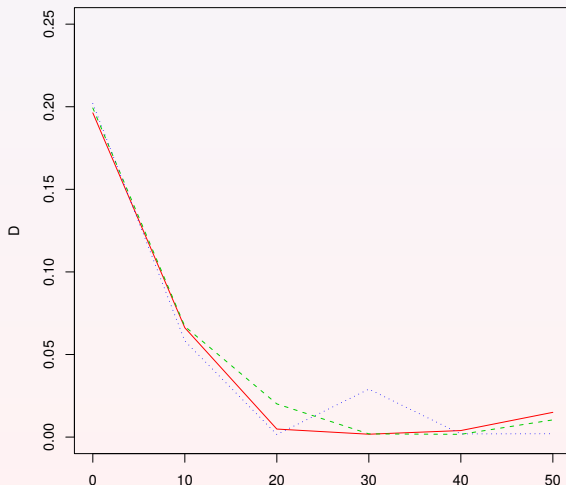
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LD Decay



- Update at every 10 generations
- $LD=0.25$  before generation 0
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# Evolve!

## simuPOP tutorial

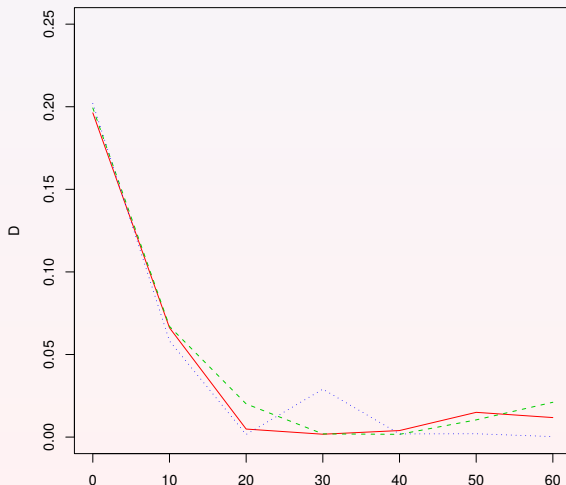
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LD Decay



- Update at every 10 generations
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# Evolve!

## simuPOP tutorial

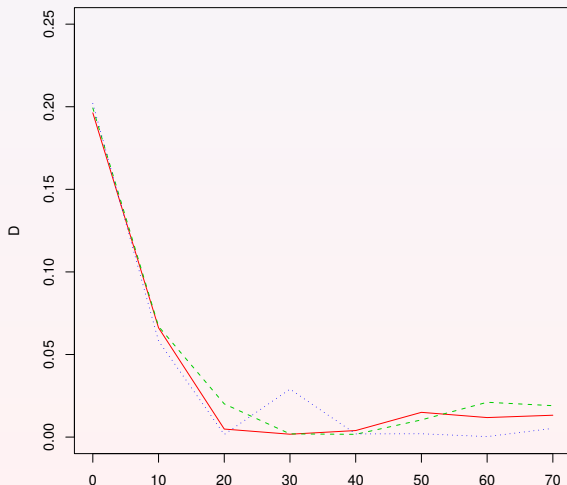
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LD Decay



- Update at every 10 generations
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# Evolve!

## simuPOP tutorial

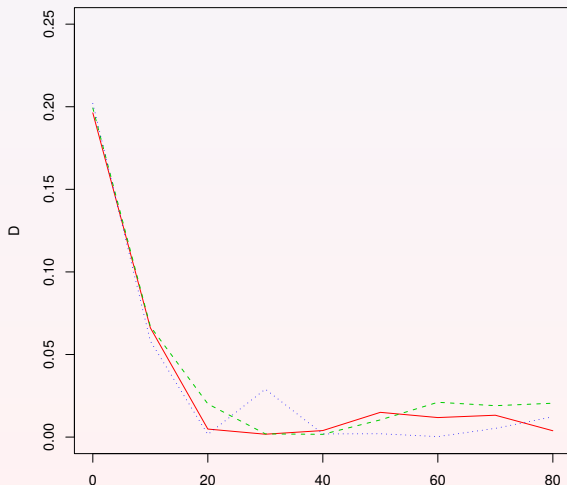
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LD Decay



- Update at every 10 generations
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# Evolve!

## simuPOP tutorial

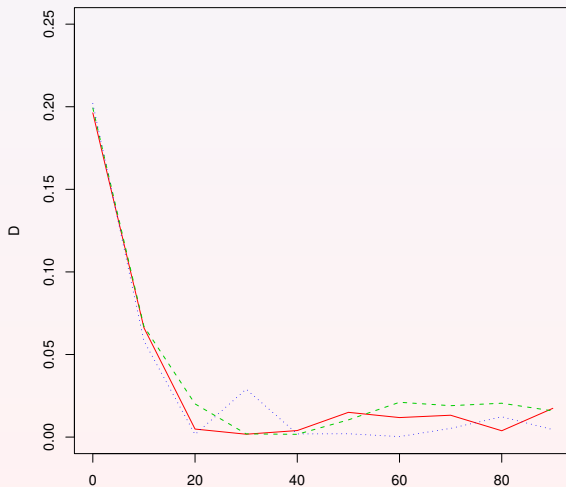
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LD Decay



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

# Evolve!

## simuPOP tutorial

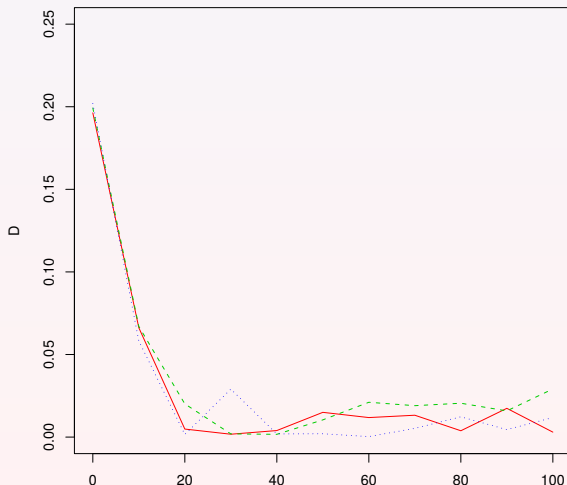
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LD Decay



- 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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## What is simuPOP

## An example

## simuPOP components

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

```
pop.ploidyName( )
```

- run `tutorial_example1.py`

# Outline

## simuPOP tutorial

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What is  
simuPOP

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simuPOP  
components

Population

Individual

Operator

Mating scheme

Simulator

## 3 simuPOP components

- Population
- Individual
- Operator
- Mating scheme
- Simulator



# Structure of a population

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Population

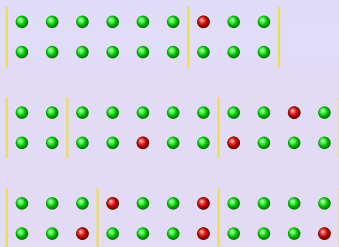
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

# Structure of a population

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Population

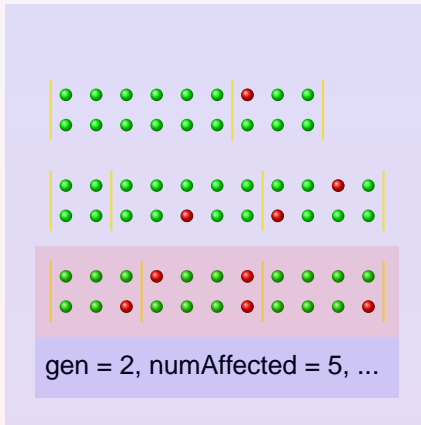
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

# Structure of a population

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Population

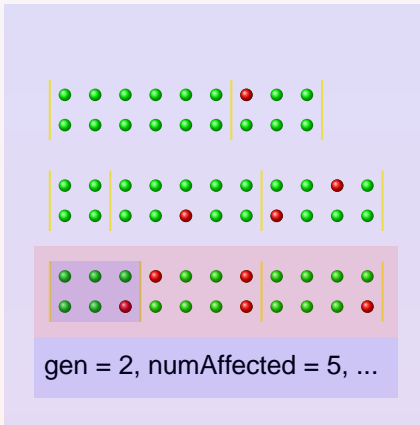
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



# Structure of a population

## simuPOP tutorial

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## What is simuPOP

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## simuPOP components

Population

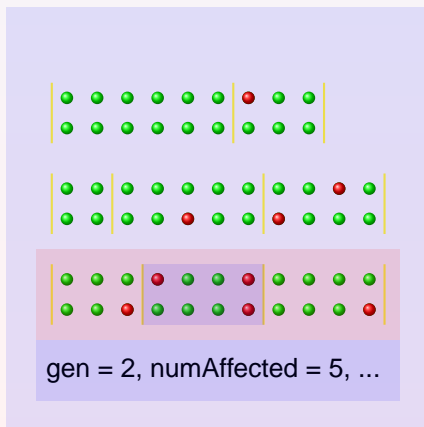
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

# Structure of a population

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Population

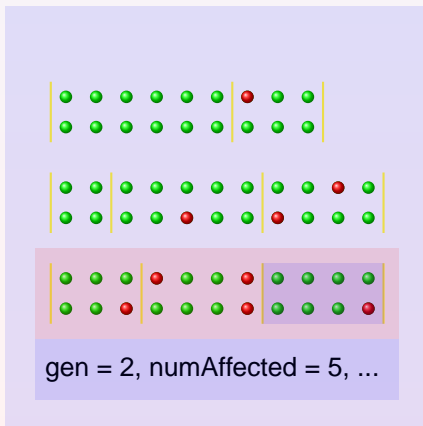
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Current generation

# Structure of a population

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Population

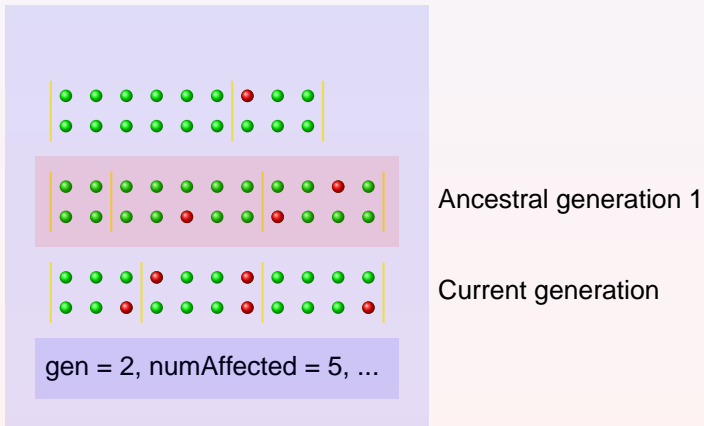
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



# Structure of a population

## simuPOP tutorial

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## What is simuPOP

## An example

## simuPOP components

Population

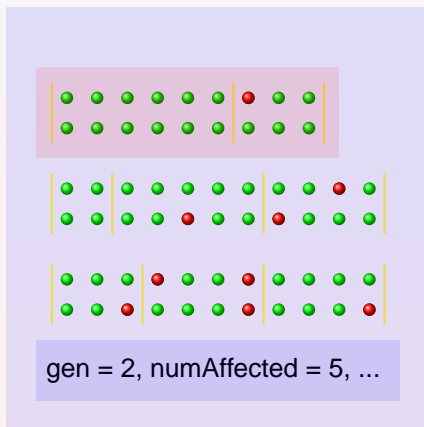
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



Ancestral generation 2

Ancestral generation 1

Current generation

# Structure of a population

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Population

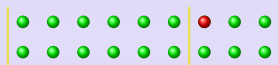
Individual

Operator

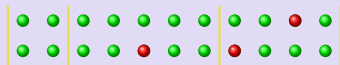
Mating scheme

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
>>>
```

## Simulator

# 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
```

# Outline

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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 | ...

# 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

● 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

Chromosome 1

Male

Sex

● 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

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
>>>
>>>
```



# Outline

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# Life cycle of a generation

**simuPOP**  
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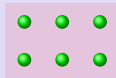
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Parental  
generation

# Life cycle of a generation

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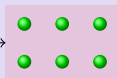
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operators



Parental  
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# Life cycle of a generation

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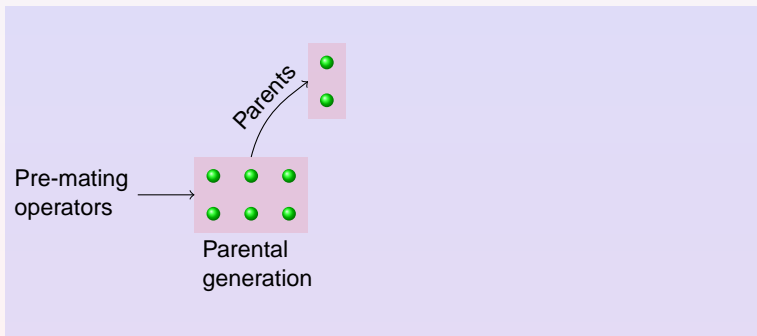
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# Life cycle of a generation

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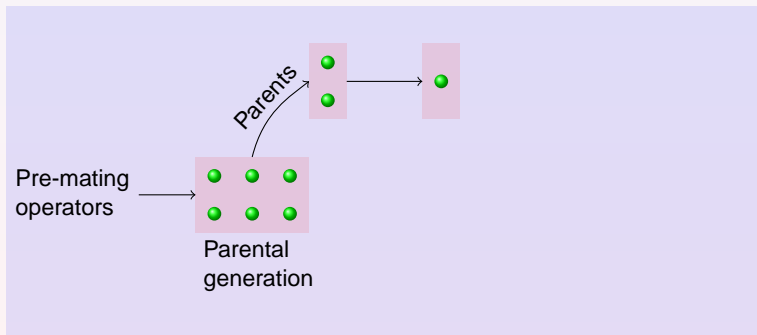
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# Life cycle of a generation

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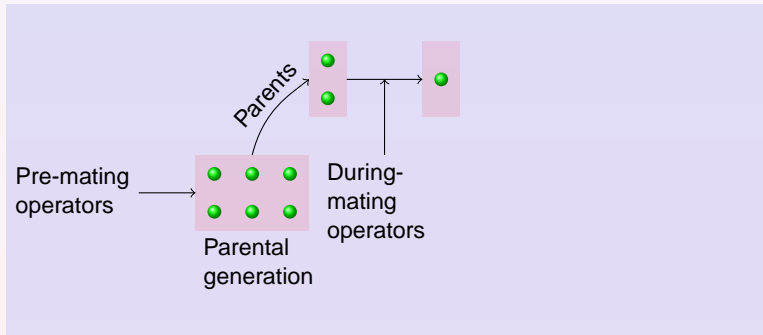
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# Life cycle of a generation

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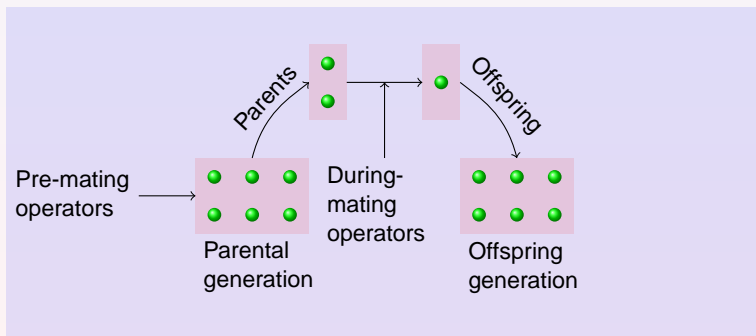
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# Life cycle of a generation

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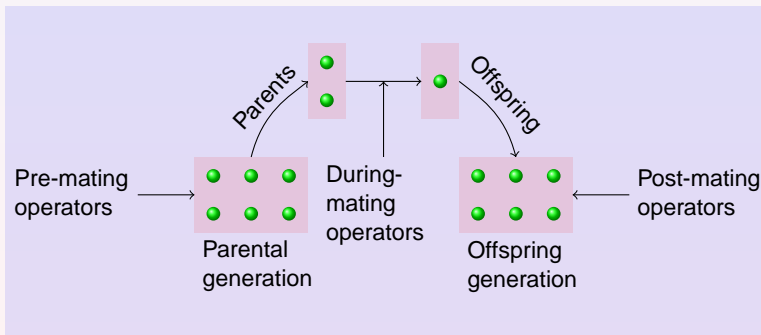
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# Stages

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# Stages, an example

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# Output

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# Table-like output

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# Mating schemes

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# Simulator

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