Forward-time simulations using simuPOP, a tutorial

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

outline

1 What is simuPOP

2 An example

3 simuPOP components

simuPOP is ...

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What is simuPOP

An example

simuPOP components

A forward-time population genetics simulation environment

simuPOP is ...

A forward-time population genetics simulation environment

- A population genetics simulation program

simuPOP is ...

A forward-time population genetics simulation environment

- A population genetics simulation program
- Not coalescent-based

simuPOP is ...

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

simuPOP tutorial

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What is simuPOP

An example

simuPOP 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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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?

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 phenomina

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- ...

I heard about coalescent...

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

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Backward-time

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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

Backward-time

- Sample based, efficient.

Forward-time

- Population based, inefficient.

Forward vs. backward-time simulations

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

Forward-time

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Forward vs. backward-time simulations

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- Can study population properties and ancestral generations

Forward vs. backward-time simulations

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

Backward-time

- Haploid simulation only

Forward-time

- No limit on ploidy

On the simulations of complex human diseases

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

Backward-time

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

Forward-time

- No limit on ploidy
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- Multiple DSL with interaction

On the simulations of complex human diseases

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??

- 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

A simple example

```
>>> 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

```
  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


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

Import the default simuPOP module

population

```
>>> 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


```
>>> 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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...     ],
...     end=100
... )
```

`initByValue` is applied before evolution

Operators!

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...     ],
...     end=100
... )
```

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

Operators!

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```

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

Operators!

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...         pyEval(r"'\n'", rep=REP_LAST, step=10)
...     ],
...     end=100
... )
```
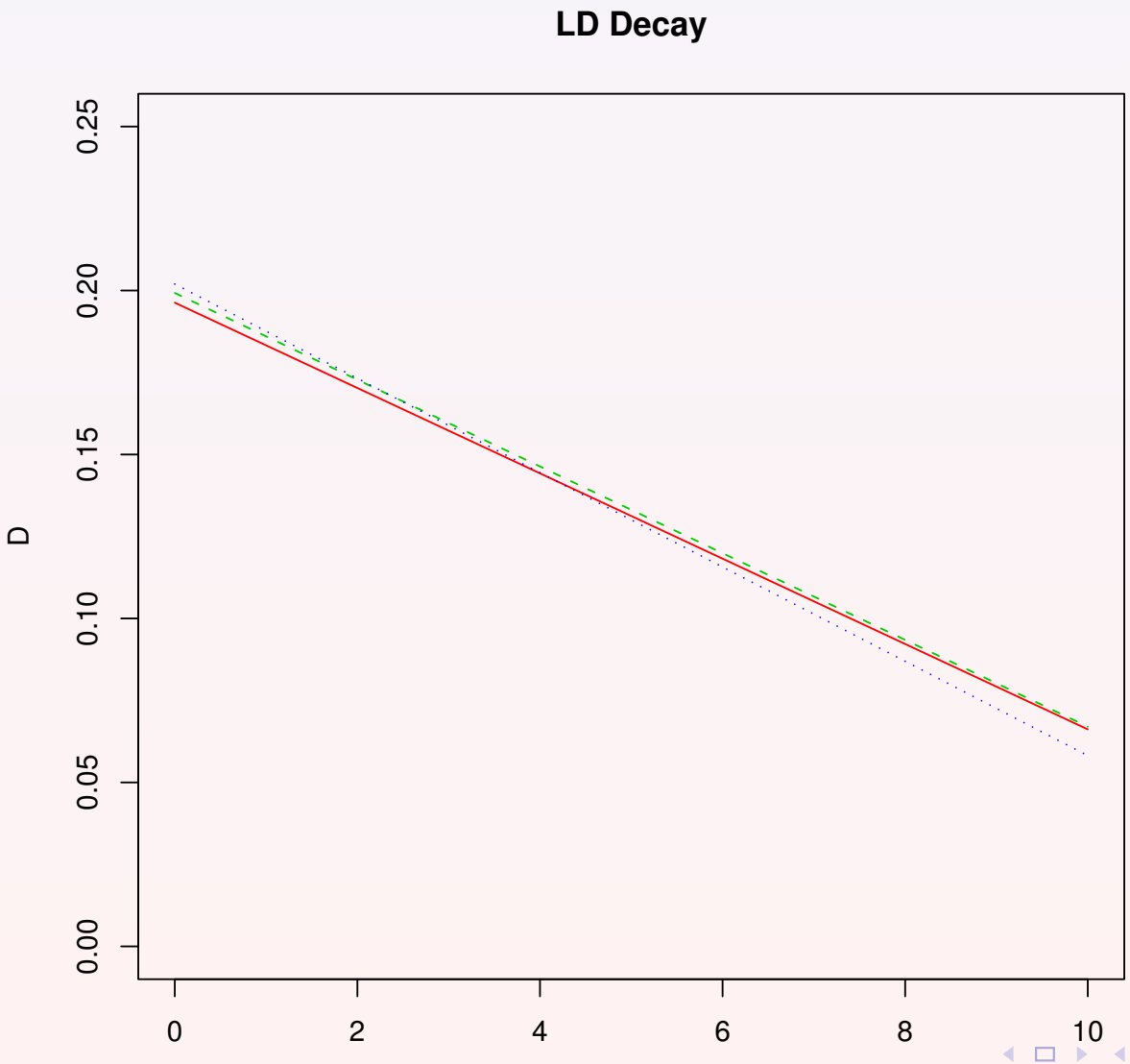

`pyEval` is applied every 10 generations

Use R to plot

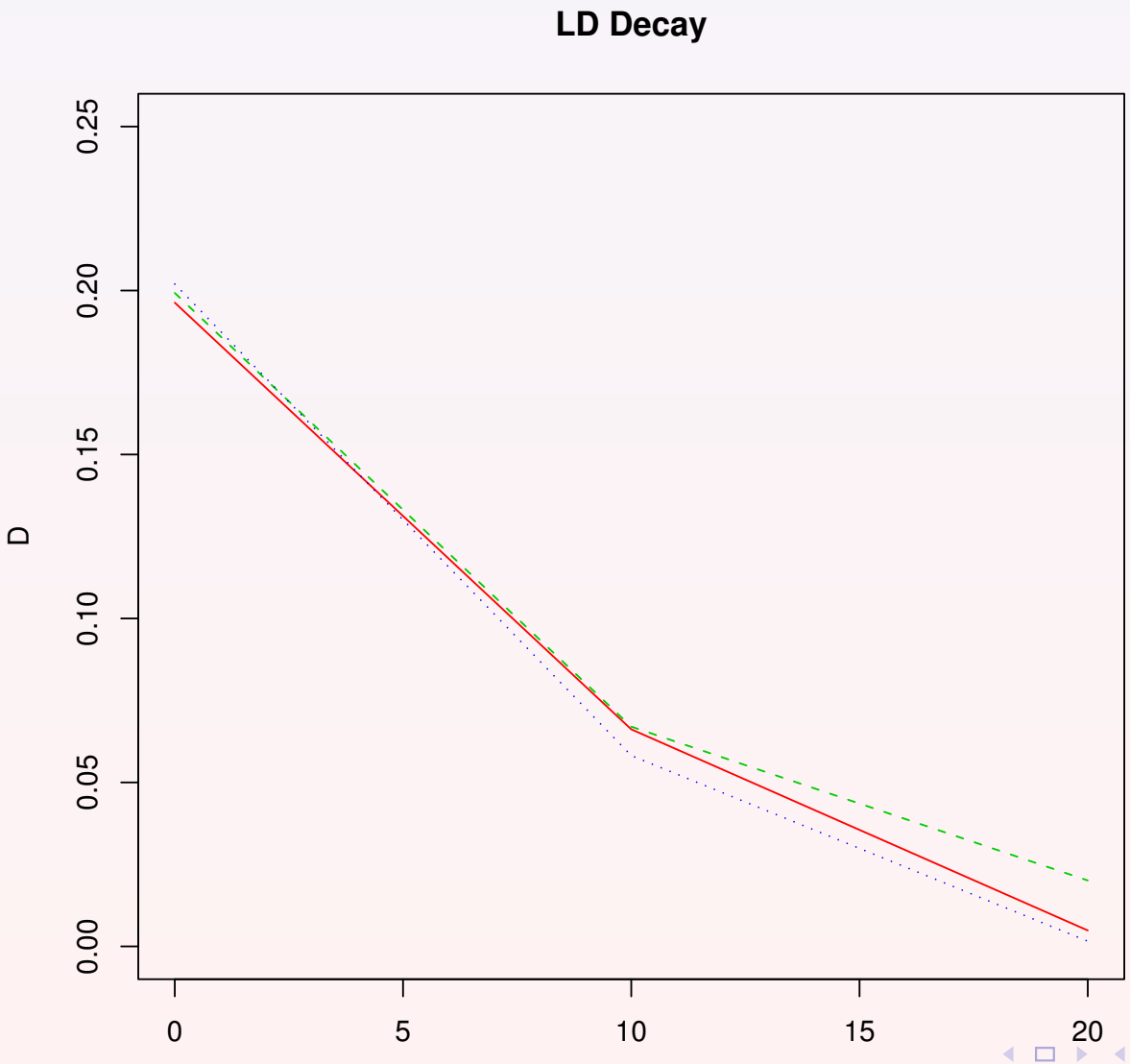
```
>>> from simuPOP import *
>>> from simuRPy import *
>>> simu = simulator(
...     population(size=1000, ploidy=2, loci=[2]),
...     randomMating(),
...     rep = 3)
>>> simu.evolve(
...     preOps = [initByValue([1,2,2,1])],
...     ops = [
...         recombinator(rate=0.1),
...         stat(LD=[0,1]),
...         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!



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

Evolve!



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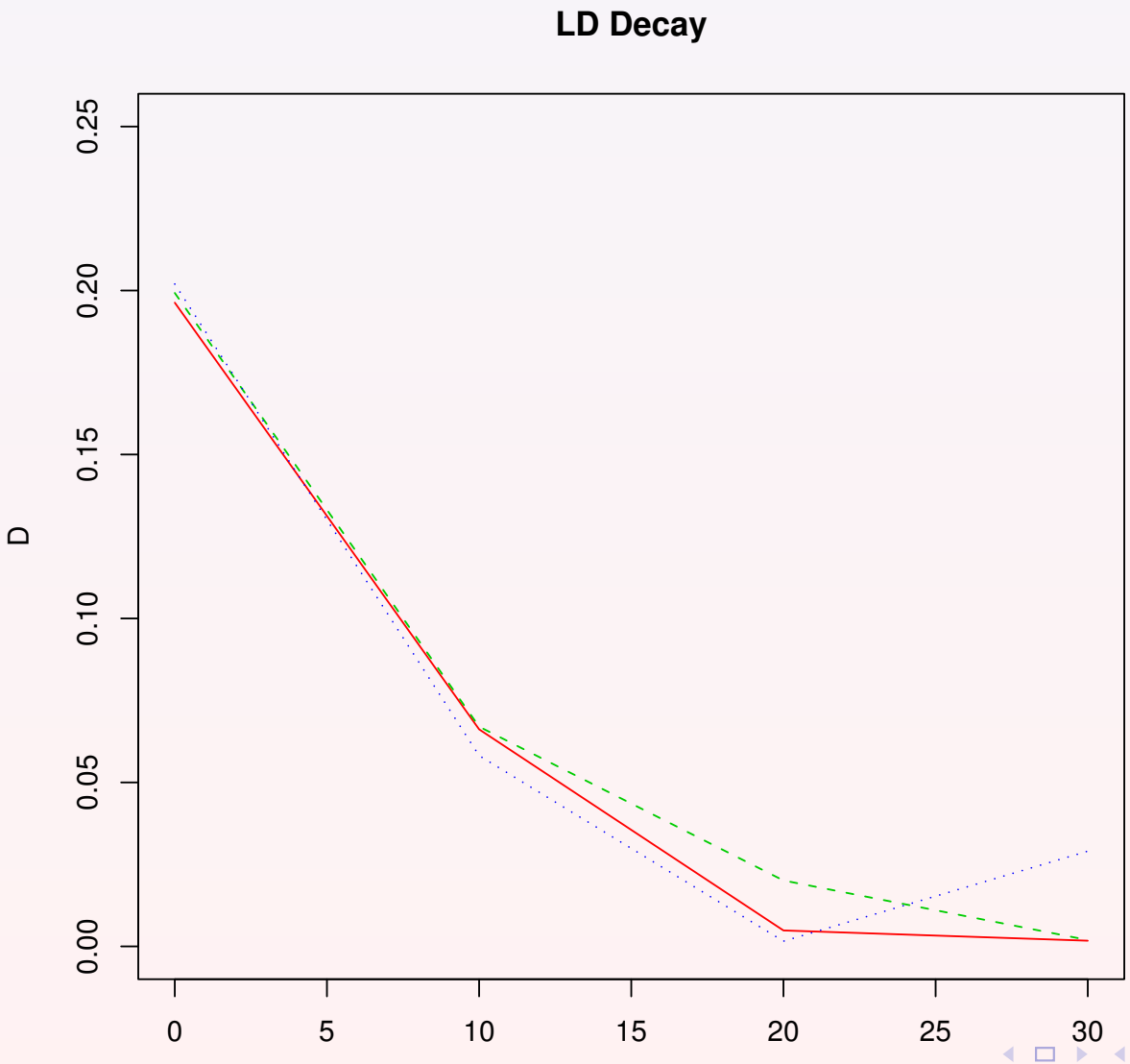

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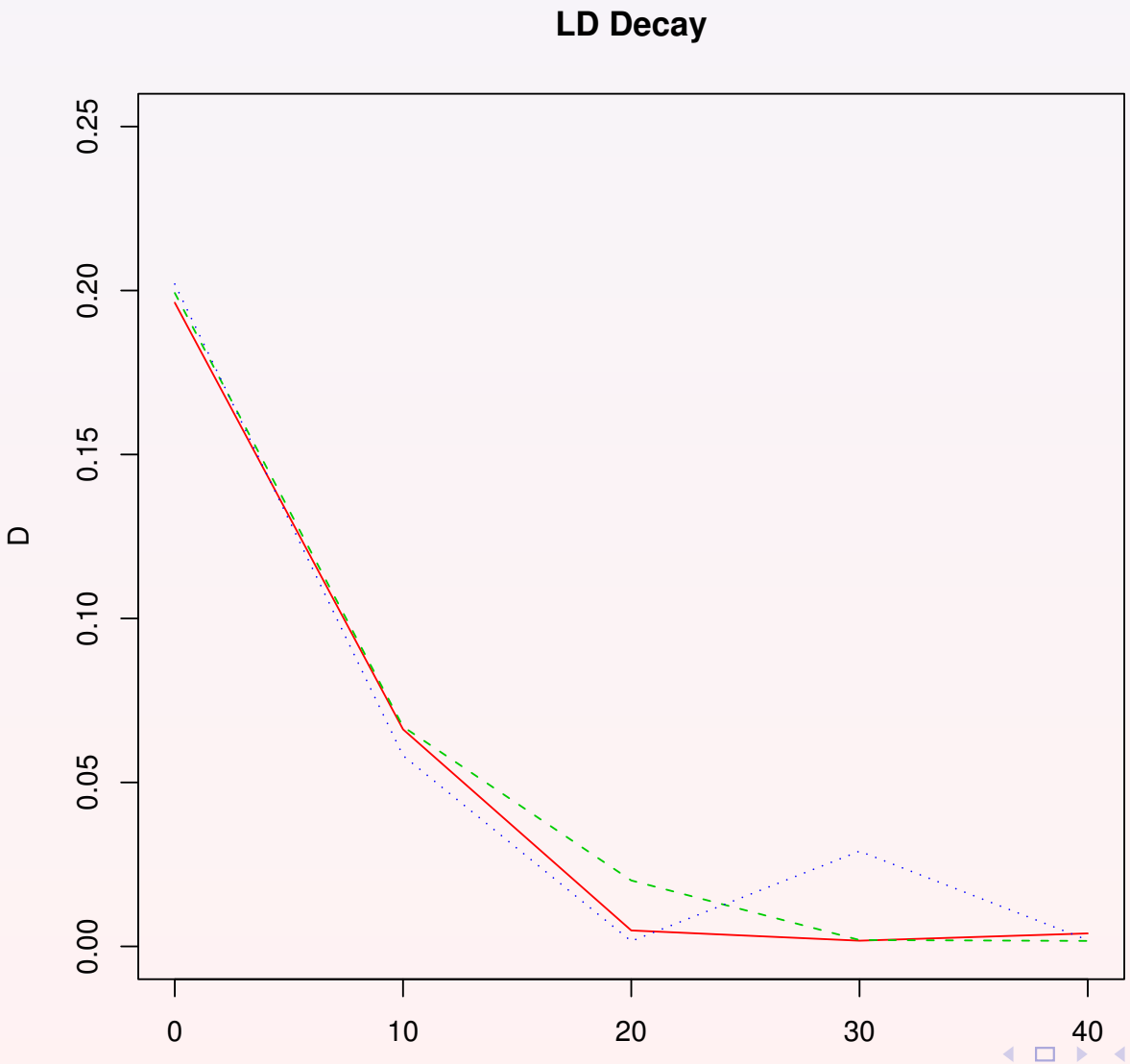

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Evolve!

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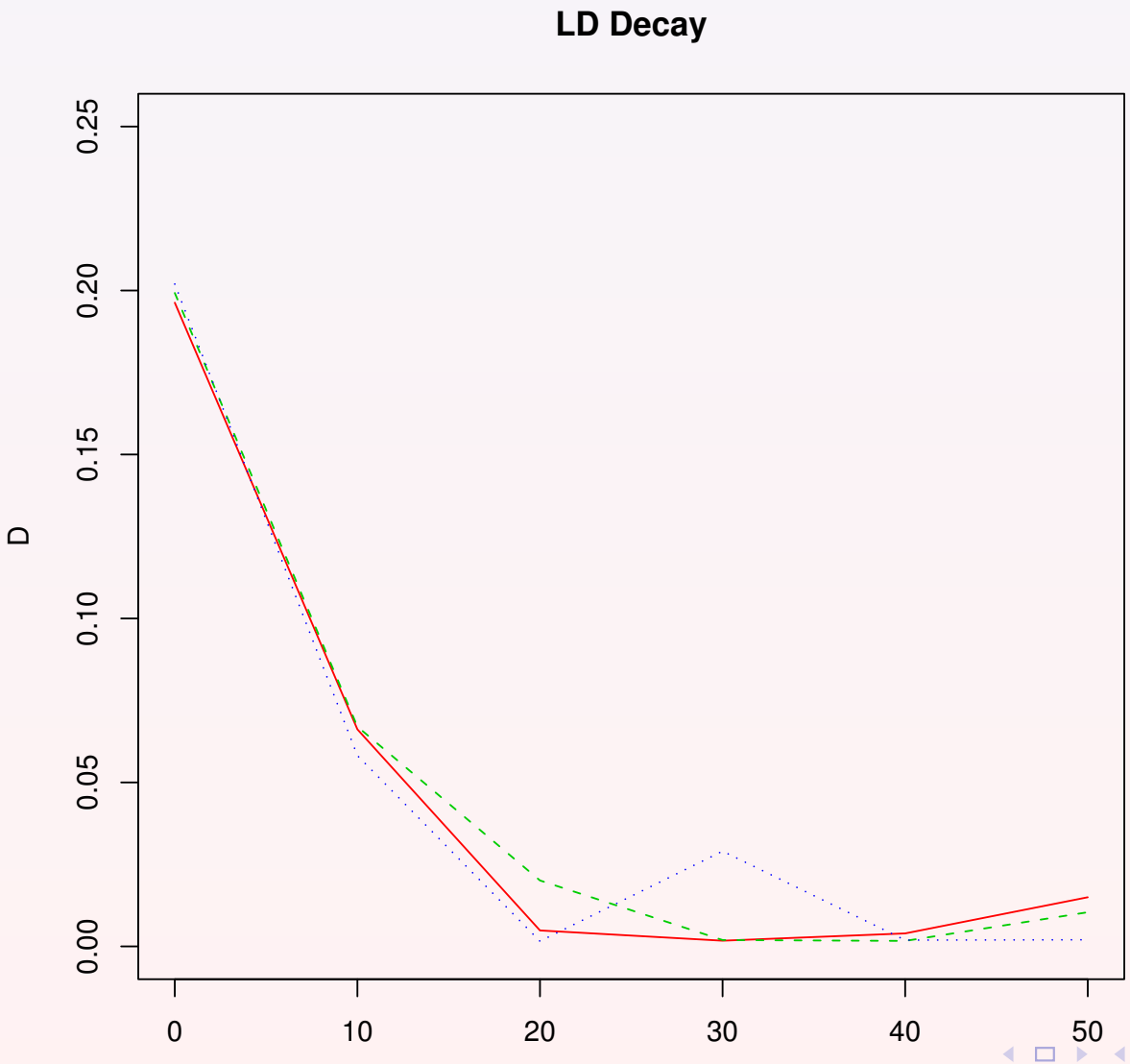
What is simuPOP

An example

simuPOP components



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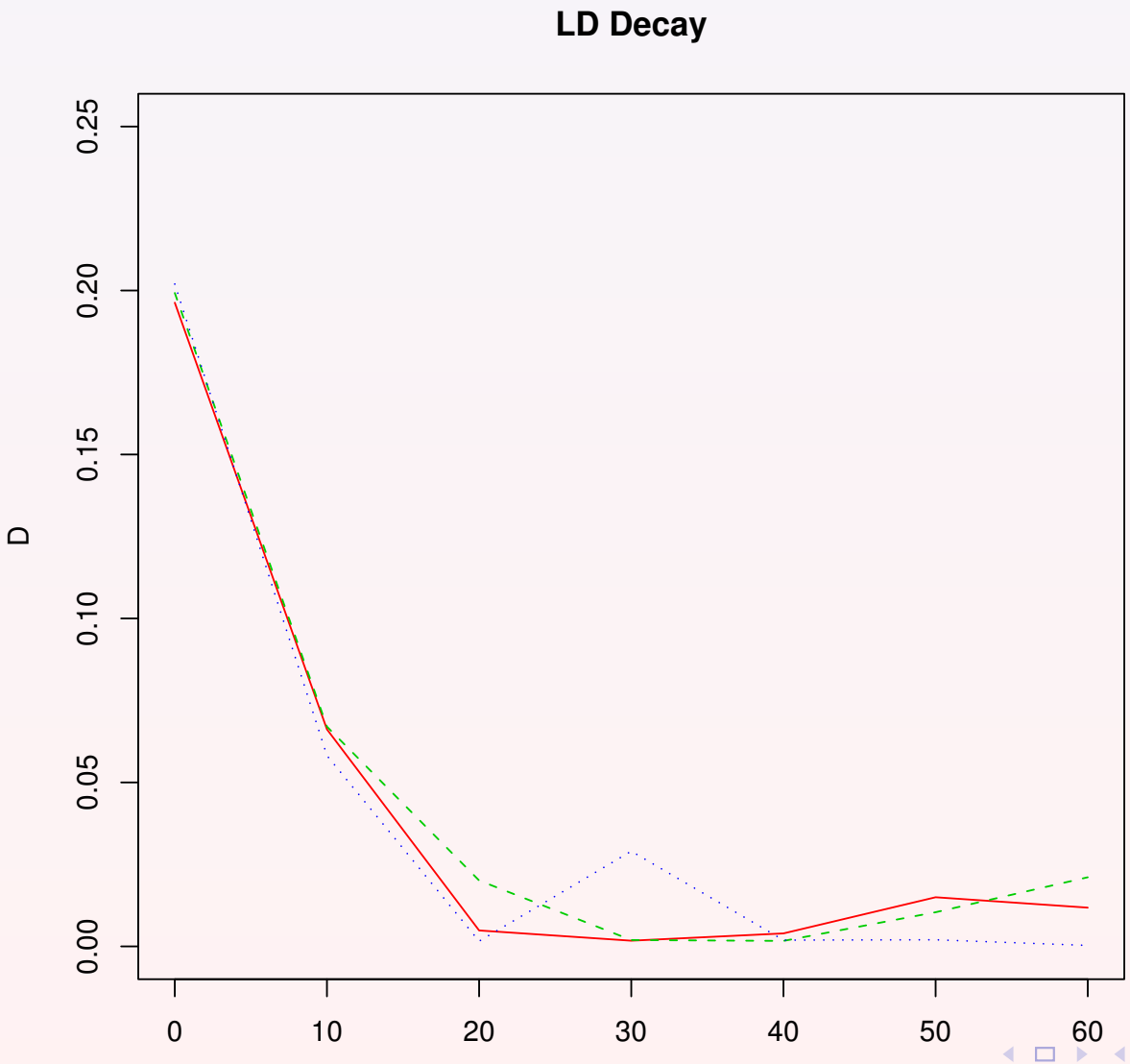

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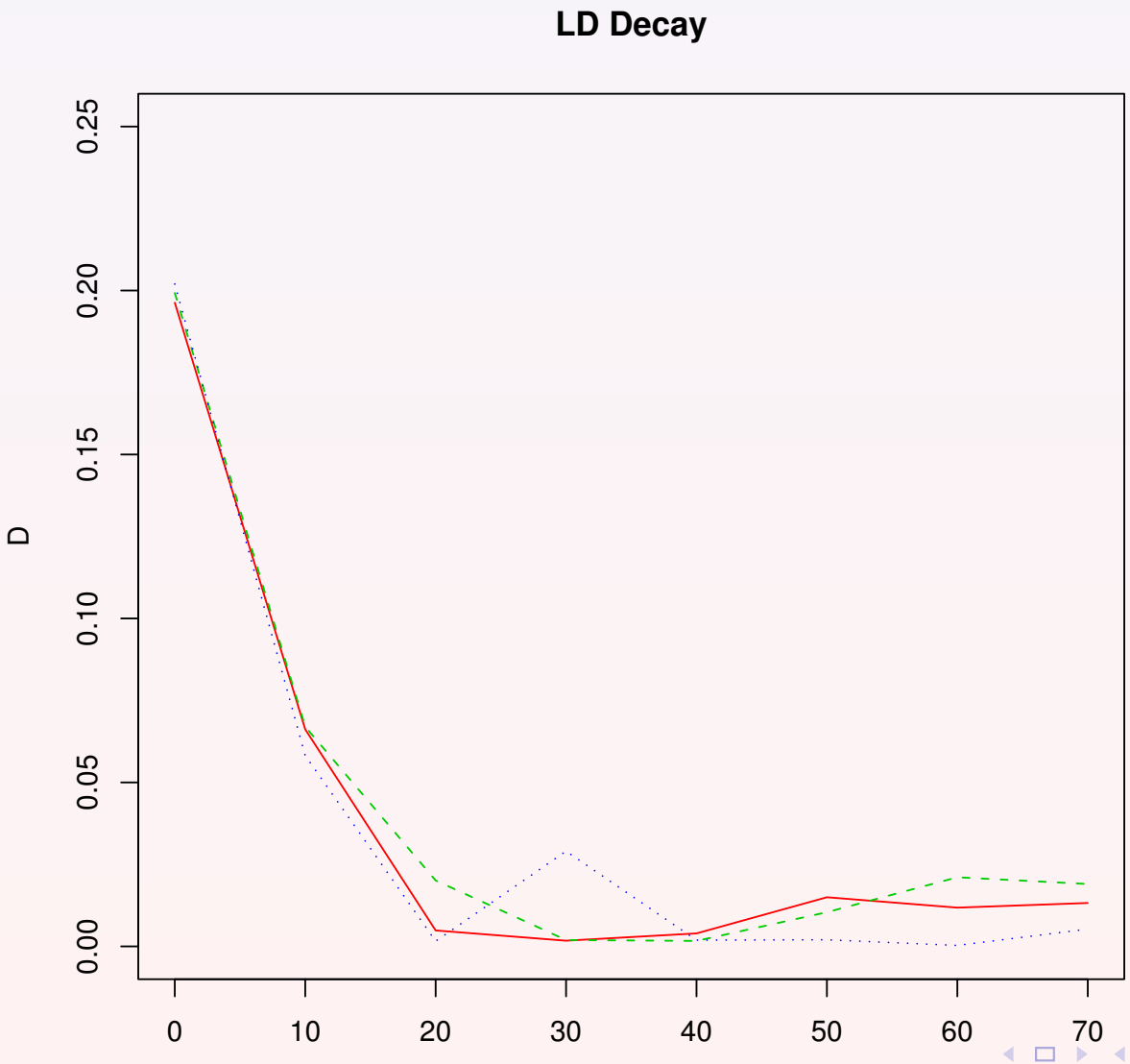

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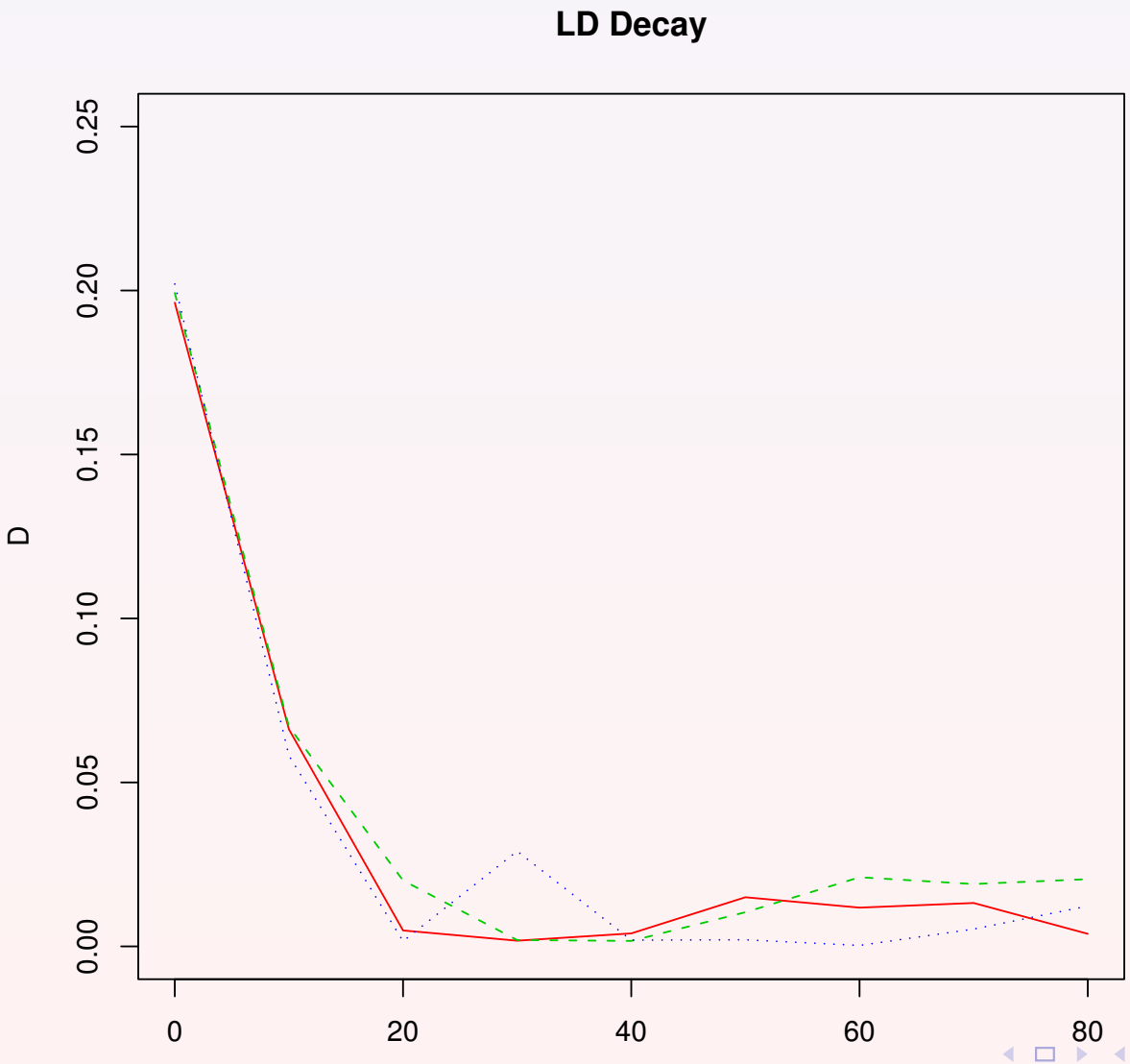

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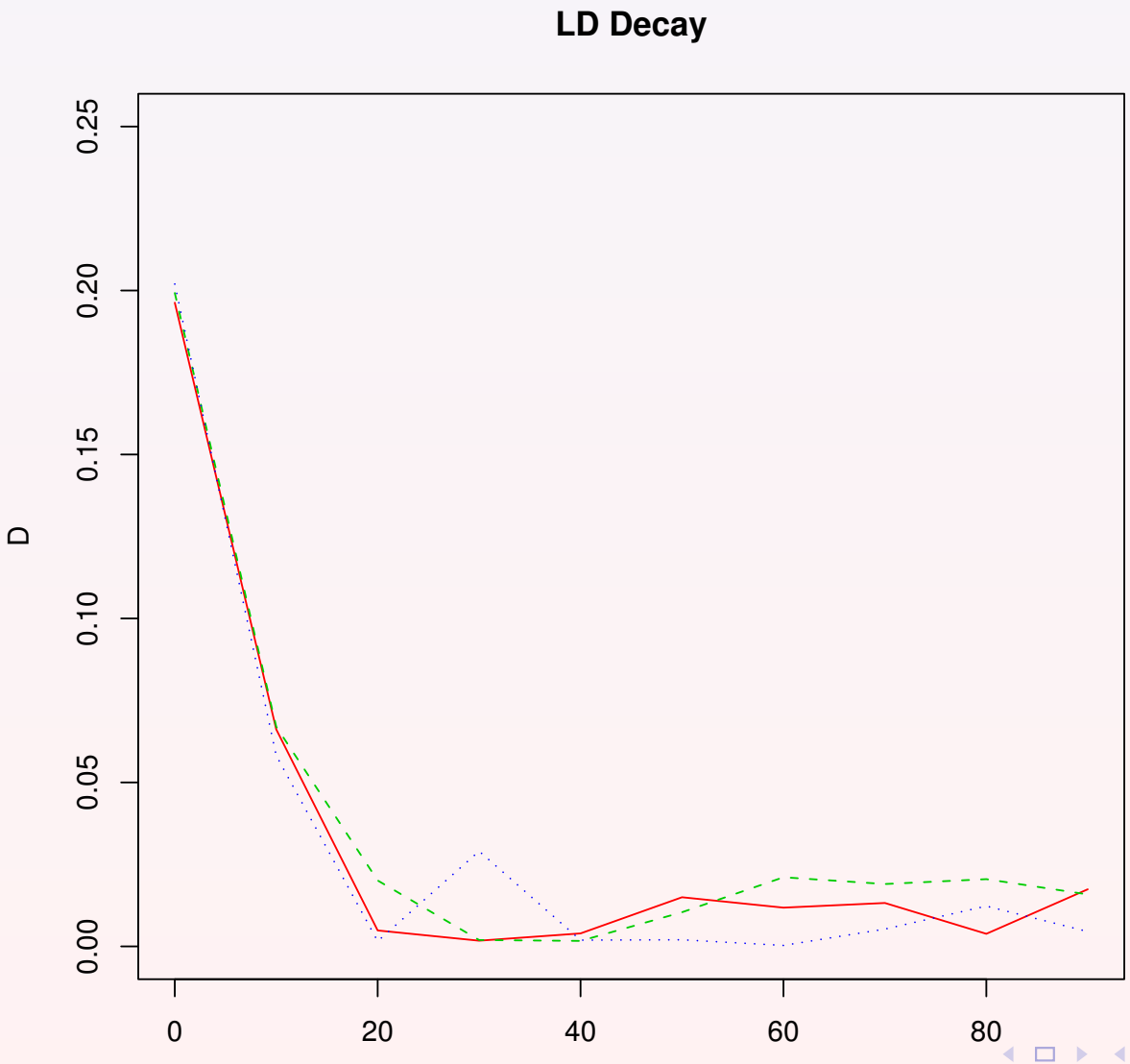

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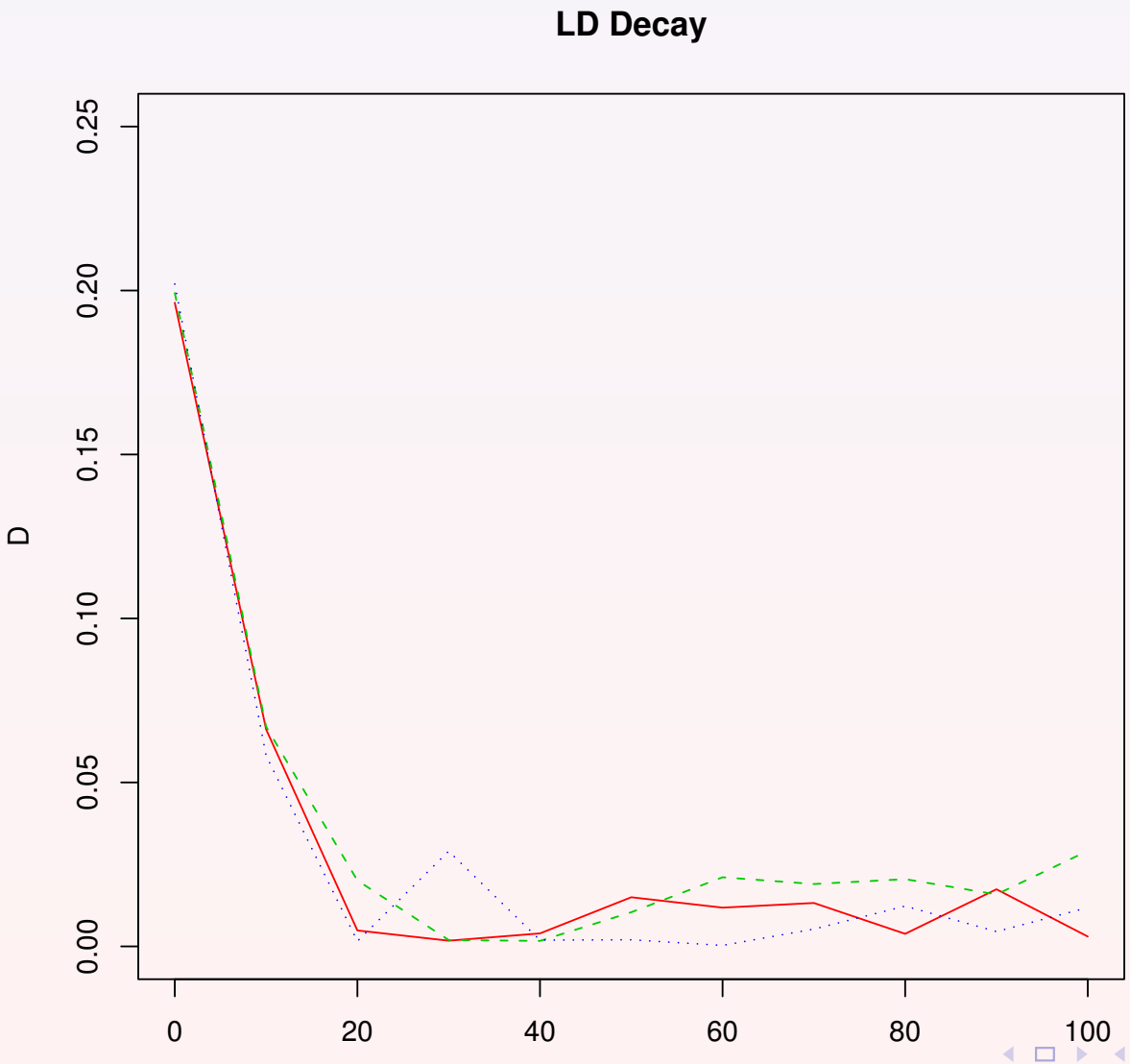

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Exercise time

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

```
pop.ploidyName()
```

- run `tutorial_example1.py`

Outline

3 simuPOP components

- Population
- Individual
- Operator
- Mating scheme
- Simulator

Structure of a population

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What is simuPOP

An example

simuPOP components

Population

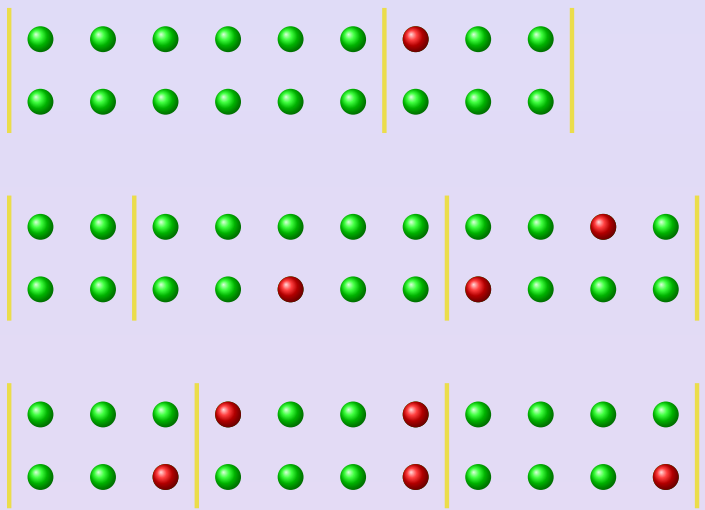
Individual

Operator

Mating scheme

Simulator

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

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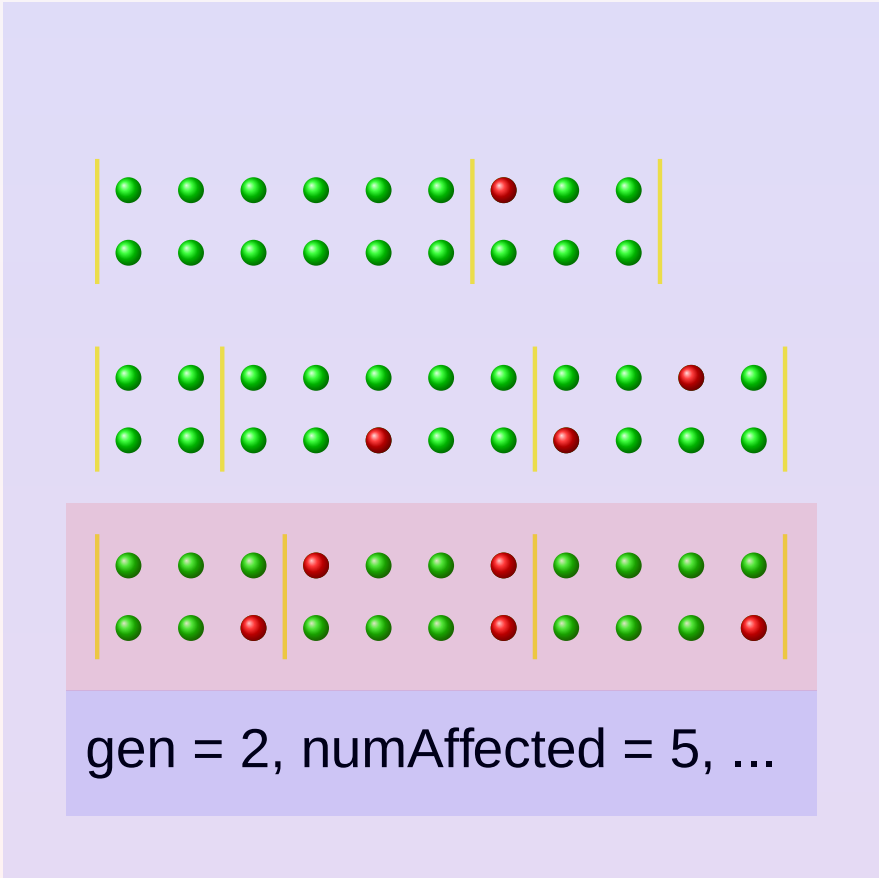

Current generation

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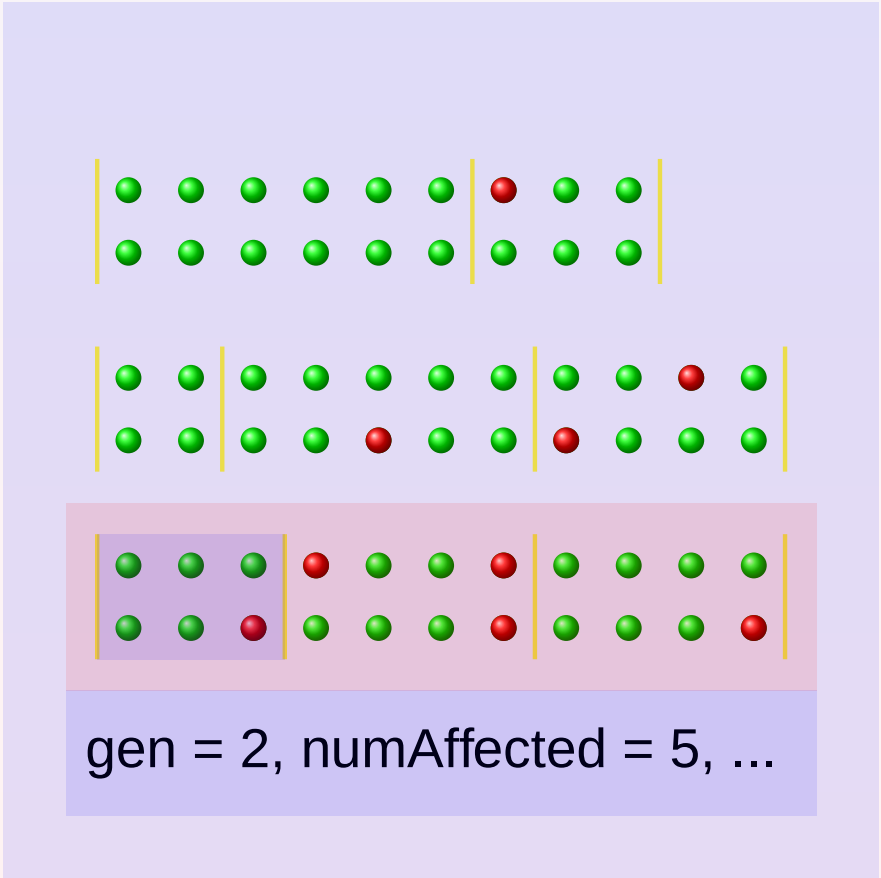

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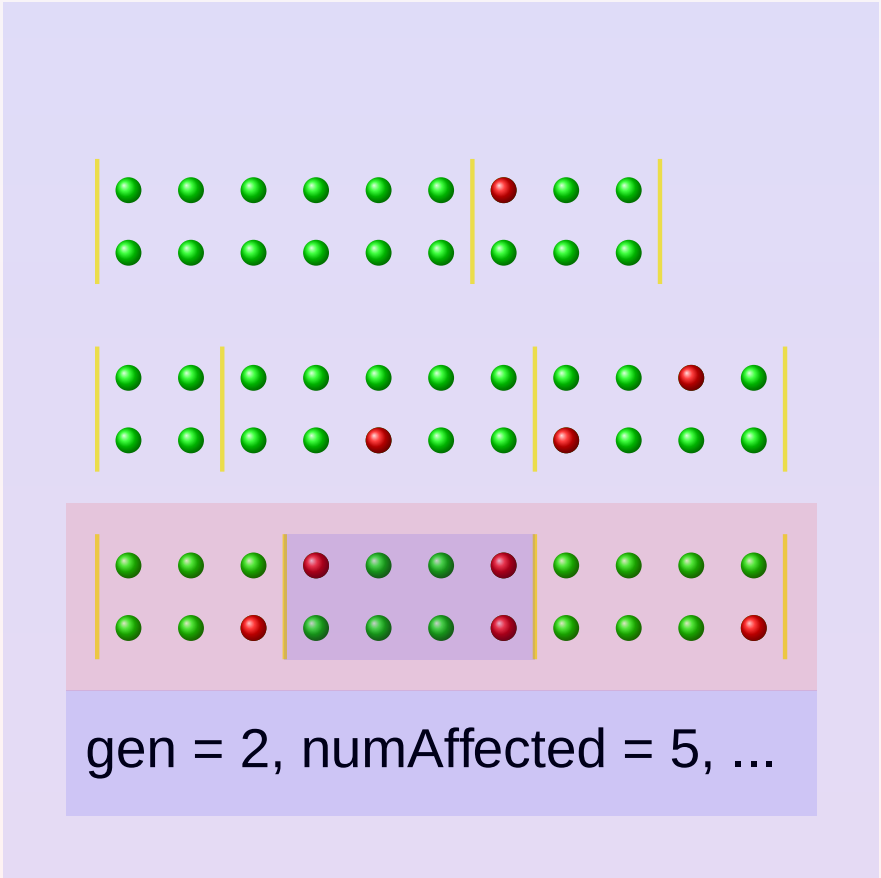

Current generation

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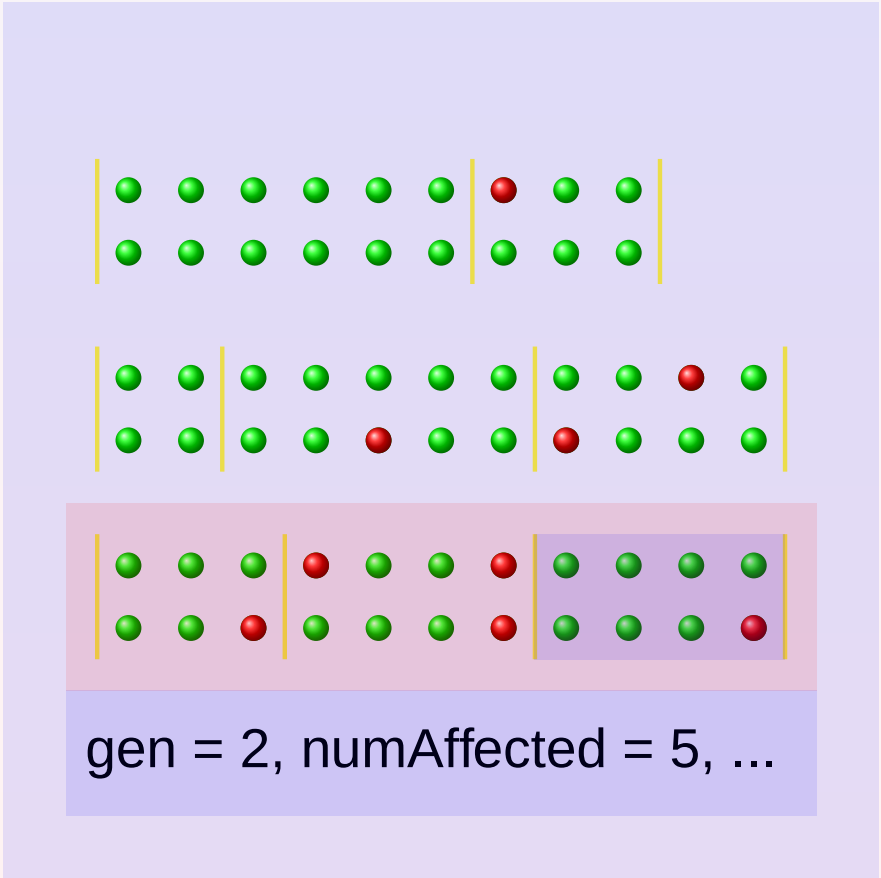

Current generation

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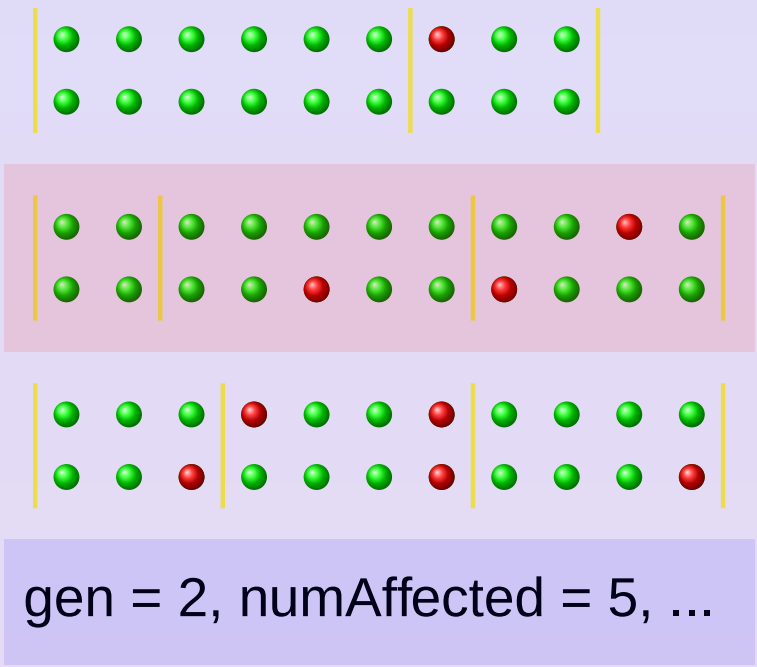

Ancestral generation 1

Current generation

Structure of a population

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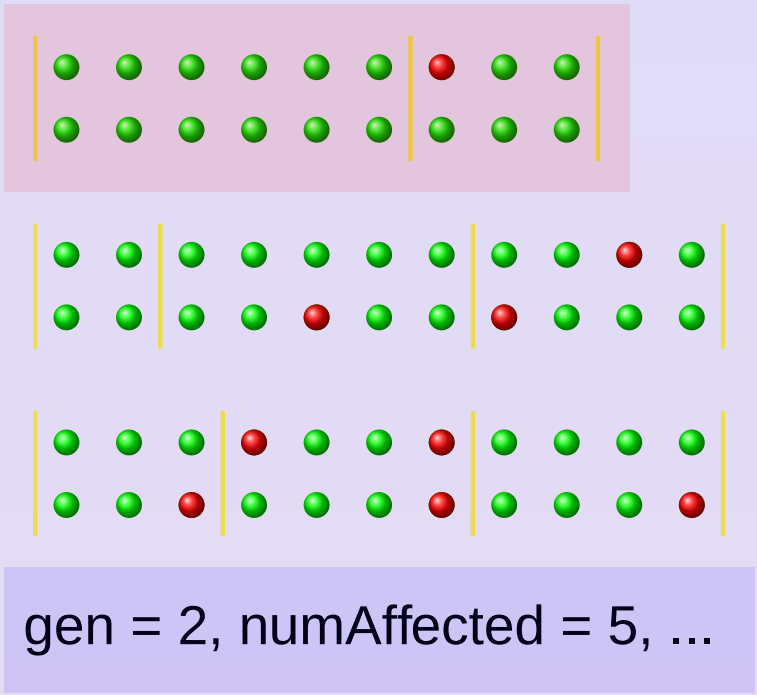

Structure of a population

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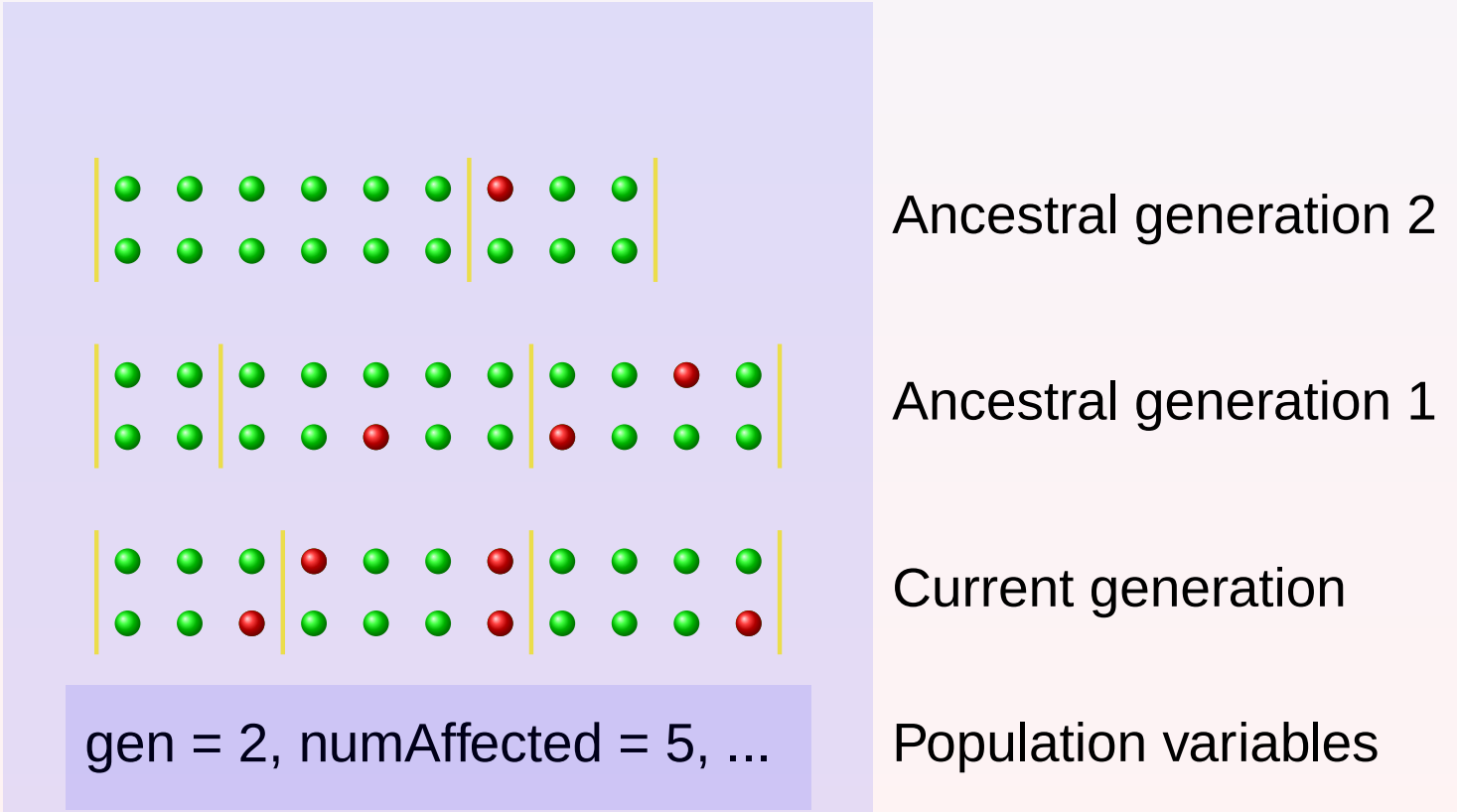

Create and manipulate populations

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What is simuPOP

An example

simuPOP components

Population

Individual

Operator

Mating scheme

Simulator

```
>>> 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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Individual

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Mating scheme

Simulator

```
>>> 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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Population

Individual

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Mating scheme

Simulator

```
>>> # 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
[[0.8066666666666664, 0.1933333333333333], [0.7960000000000000
>>> # 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


```
>>> 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 :      0.666666666667
       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

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

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

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

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

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

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

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 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: 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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Stages, an example

Output

Table-like output

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Mating schemes

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Simulator