

simuPOP tutorial

Bo Peng, Ph.D.

What is simuPOP

An example

simuPOP components

Forward-time simulations using simuPOP, a tutorial

Bo Peng, Ph.D.

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



outline

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What is simuPOP

An example

simuPOP components

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



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What is simuPOP

An example

simuPOP components

A forward-time population genetics simulation environment



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An example

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A forward-time population genetics simulation environment

A population genetics simulation program



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An example simuPOP components

A forward-time population genetics simulation environment

- A population genetics simulation program
- Not coalescent-based



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What is simuPOP

An example

simuPOP components

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 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, ...



What simuPOP does

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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, ...
- 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 ...



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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 phenomina



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What is simuPOP

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



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An example simuPOP components

- demonstrate population genetics phenomina
- study the impact of genetic and demographic forces on the evolution of a population
- study the evolution of (complex) genetic diseases



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An example simuPOP components

- demonstrate population genetics phenomina
- 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



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An example simuPOP components

- demonstrate population genetics phenomina
- 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



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An example simuPOP components

- demonstrate population genetics phenomina
- 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
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- ...



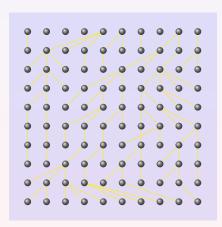
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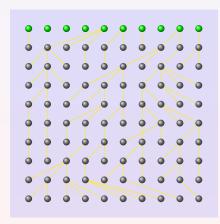


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An example simuPOP components



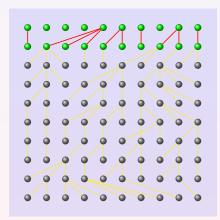
 Start from an initial population



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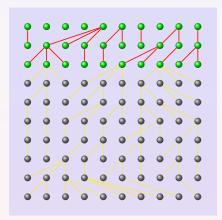
- Start from an initial population
- Evolve forward in time, generation by generation, subject to certain number of genetic and/or demographic effects



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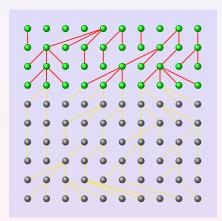
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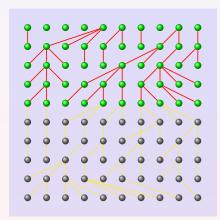
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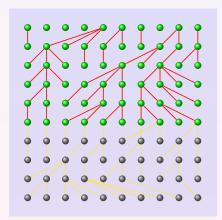
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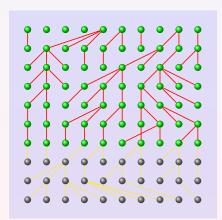
- Start from an initial population
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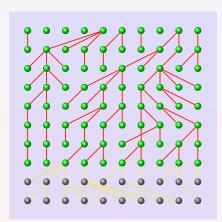
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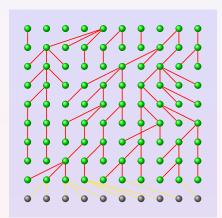
- Start from an initial population
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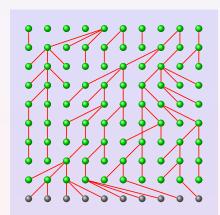
- Start from an initial population
- Evolve forward in time, generation by generation, subject to certain number of genetic and/or demographic effects



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- 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

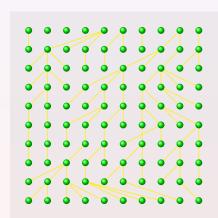


Backward-time simulation

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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

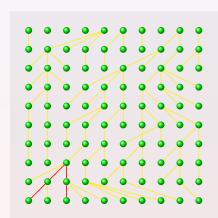


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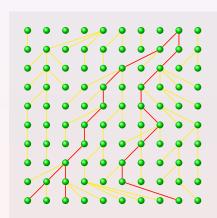


Backward-time simulation

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Backward-time

Sample based, efficient.

Forward-time

 Population based, inefficient.



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An example simuPOP components

Backward-time

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

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



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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

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



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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

- 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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An example

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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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An example simuPOP components

Backward-time

- Haploid simulation only
- Additive selection and penetrance models

- 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

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



On the simulations of complex human diseases

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What is simuPOP

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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

- 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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What is simuPOP

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

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



Output of the example

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An example

```
n
      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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What is simuPOP

An example

simuPOP components

```
>>> 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

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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



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What is simuPOP

An example

simuPOP components

```
>>> from simuPOP import *
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. . .
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. . .
       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
. . . )
```

initByValue is applied before evolution



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An example

simuPOP components

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            stat(LD=[0,1]),
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            pvEval(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



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An example

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            stat(LD=[0,1]),
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           pvEval(r"'%f ' % LD[0][1]", step=10),
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        end = 100
```

stat is applied to the offspring generation at every generation



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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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An example

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

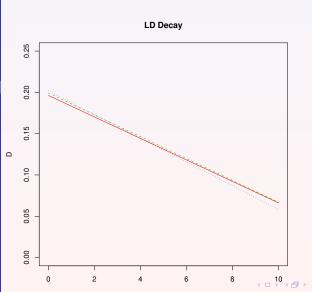


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An example



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

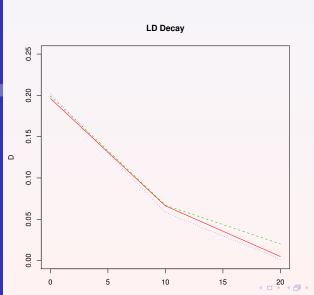


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An example



- Update at every 10 generations
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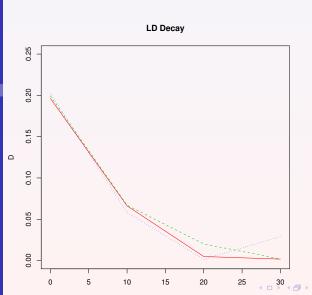


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- Update at every 10 generations
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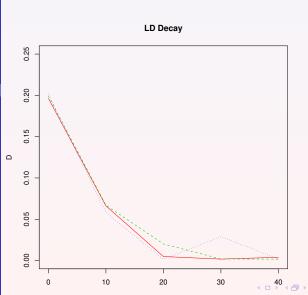


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An example



- Update at every 10 generations
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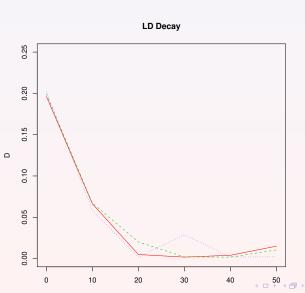


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An example



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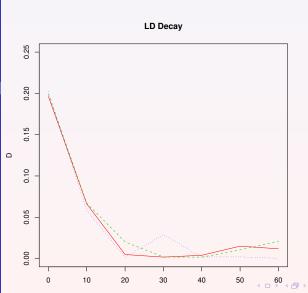


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An example



- Update at every 10 generations
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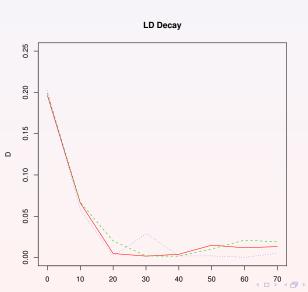


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An example



- Update at every 10 generations
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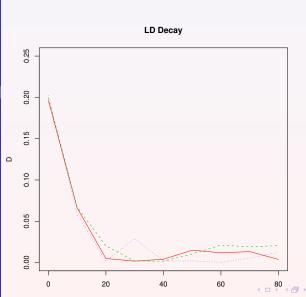


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- Update at every 10 generations
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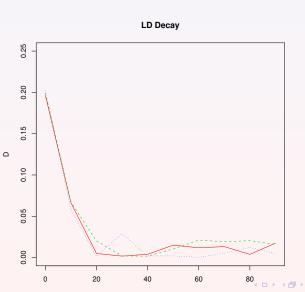


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- Update at every 10 generations
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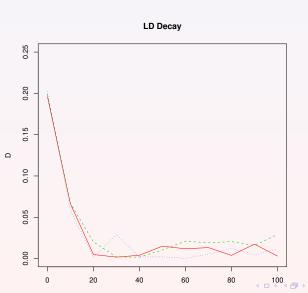


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An example



- 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

An example

All example

simuPOP components

Population

Individual
Operator
Mating scheme
Simulator

- 3 simuPOP components
 - Population
 - Individual
 - Operator
 - Mating scheme
 - Simulator

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What is simuPOP

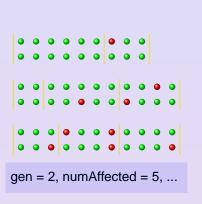
An example

simuPOP

components
Population

Individual
Operator
Mating scheme
Simulator

- Unaffected
- Affected



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What is simuPOP

An example

simuPOP component

components
Population
Individual

Individual
Operator
Mating scheme
Simulator



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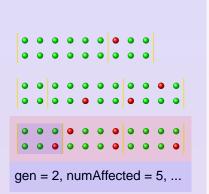
What is simuPOP

An example

simuPOP components

Population Individual Operator Mating scheme Simulator

- Unaffected
- Affected





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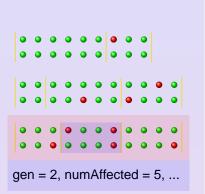
An example

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Population Individual Operator Mating scheme

Simulator

- Unaffected
- Affected



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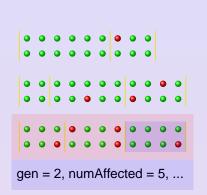
An example

simuPOP

components
Population
Individual

Individual
Operator
Mating scheme
Simulator

- Unaffected
- Affected



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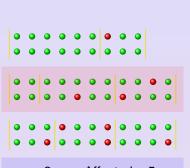
An example

simuPQP

components Population Individual

Operator Mating scheme Simulator

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

Ancestral generation 1

simuPOP tutorial

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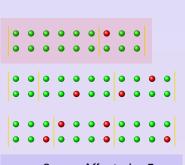
An example

simuPOP

components Population Individual

Operator Mating scheme Simulator

- Unaffected
- Affected



gen = 2, numAffected = 5, ...

Ancestral generation 2

Ancestral generation 1

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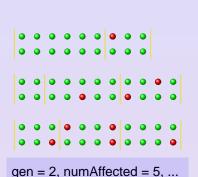
An example

simuPOP components

Population
Individual

Individual
Operator
Mating scheme
Simulator

- Unaffected
- Affected



Ancestral generation 2

Ancestral generation 1

Current generation

Population variables

```
THE UNIVERSITY OF TEXAS
MD ANDERSON
CANCER CENTER
Making Cancer History*
```

Create and manipulate populations

```
simuPOP
              >>> pop = population(size=10, loci=[2, 3])
  tutorial
              >>> Dump(pop)
 Bo Peng,
              Ploidy:
  Ph.D.
              Number of chrom:
              Number of loci:
What is
simuPOP
              Maximum allele state:
                                          255
An example
              Loci positions:
simuPOP
                                 1 2 3
components
              Loci names:
Population
Individual
                                 1001-1 1001-2
Operator
                                 loc2-1 loc2-2 loc2-3
Mating scheme
Simulator
              population size:
                                          10
              Number of subPop:
              Subpop sizes:
                                          10
              Number of ancestral populations:
              individual info:
              sub population 0:
                 0: MTT
                                          0
                    MU
                 2: MU
                                          0
```

MU



Genotypic structure

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An example

simuPOP components Population

Individual
Operator
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
>>>
```



simuPOP

tutorial

Population manipulation

>>> # make a copy of pop

```
>>> pop1 = pop.clone()
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            >>> # remove loci 2, 3, 4
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            >>> pop.removeLoci(keep=[0, 1])
            >>> # pop2 will have 3 chromosomes, with loci 2, 3, 2
What is
simuPOP
            >>> pop2 = MergePopulationsByLoci(pops=[pop, pop1])
            >>> # randomly assign alleles using given allele frequencies
An example
            >>> InitByFreq(pop2, [0.8, .2])
simuPOP
            >>> # calculate population allele frequency
components
            >>> Stat(pop2, alleleFreq=range(pop2.totNumLoci()))
Population
Individual
            >>> # print allele frequency
Operator
            >>> print pop2.dvars().alleleFreq
Mating scheme
Simulator
            [0.8066666666666664, 0.19333333333333], [0.796000000000000000]
            >>> # assign affection status using a penetrance model
            >>> MapPenetrance(pop2, locus=1,
                     penetrance={'0-0': 0.05, '0-1': 0.2, '1-1': 0.8})
            >>> # draw case control sample
            >>> (sample,) = CaseControlSample(pop2, cases=5, controls=5)
            >>> # save sample in Merlin OTDT format
            >>> from simuUtil import SaveOTDT
            >>> SaveQTDT(sample, output='sample', affectionCode=['U', 'A'],
                     fields=['affection'])
            . . .
                                                    4 T > 4 A > 4 E > 4 E > E 90 C
```



Population manipulation (cont.)

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An example

simuPOP components

Components
Population
Individual

Operator
Mating scheme
Simulator

```
>>> # have a look at the sample in Merlin-OTDT Format
>>> print open('sample.map').read()
CHROMOSOME MARKER POSITION
        loc1-1 1.000000
       loc1-2 3.000000
       loc1-1 1 1.000000
       loc1-2_1
                       3.000000
       1001-3 5.000000
3
       loc2-1 2.500000
       loc2-2 4.000000
>>> print open('sample.dat').read()
        affection
Α
М
       loc1-1
       1001-2
M
       loc1-1 1
M
М
       loc1-2 1
       1001-3
M
       loc2-1
М
       loc2-2
```



Population manipulation (cont.)

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An example

simuPOP components

component
Population
Individual

Operator
Mating scheme
Simulator

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

>>>



Population variables

```
simuPOP
tutorial
```

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An example

simuPOP components

Population
Individual

Operator Mating scheme Simulator

```
>>> pop = population(subPop=[5, 10], loci=[5])
>>> InitByFreg(pop, [.6, .3, .1])
>>> Stat(pop, alleleFreg=[1], genoFreg=[2])
>>> print pop.dvars().alleleFreg[1][0]
0.7
>>> from simuUtil import ListVars
>>> ListVars(pop.dvars(), useWxPvthon=False)
grp: -1
rep : -1
alleleNum :
  [1]
    [0]
               21
    [1]
    [2]
genoFreg :
  [2]
    [0]
      0 :
               0.2
               0.66666666667
      2:
               0.066666666667
    [1]
      1:
               0.066666666667
genoNum :
  [2]
    [0]
               3.0
               10 0
      2:
               1.0
    [1]
               1.0
                                               alleleFreq :
```



Population variables (cont.)

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An example

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components
Population

Population Individual Operator

```
subPop
  [0]
    alleleNum :
       [1]
         [0]
                 8
         [1]
                 1
         [2]
                 1
    genoNum :
       [2]
         [0]
                 2.0
                 2.0
         [1]
                 1.0
    genoFreg :
       [2]
         [0]
            0
                 0.4
                 0 4
         [1]
                 0.2
    alleleFreq :
       [1]
         [0]
                 0.8
         [1]
                 0.1
         [2]
                 0.1
```



Outline

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What is simuPOP

An example

An example

simuPOP components

Population Individual

Operator

Mating scheme Simulator

simuPOP components

- Population
- Individual
- Operator
- Mating scheme
- Simulator



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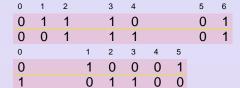
An example

simuPOP components

Population Individual

Operator
Mating scheme

Assume ploidy = 2, maxAllele = 1



Male

Affected

fitness father_id ...



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What is simuPOP

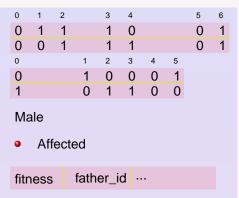
An example

simuPOP components

Population Individual

Operator
Mating scheme
Simulator

Assume ploidy = 2, maxAllele = 1



Chromosome 0



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What is simuPOP

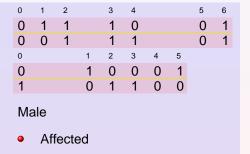
An example

simuPOP components

Population Individual

Operator Mating scheme Simulator Assume ploidy = 2, maxAllele = 1

fitness



father id ...

Chromosome 0

Chromosome 1



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What is simuPOP

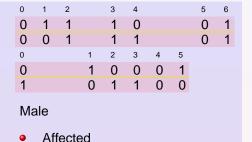
An example

simuPOP components

Population Individual

Operator Mating scheme Simulator Assume ploidy = 2, maxAllele = 1

fitness



father id ...

Chromosome 0

Chromosome 1

Sex



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What is simuPOP

An example

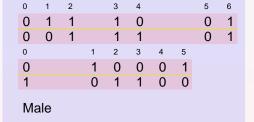
simuPOP components

Population Individual

Operator Mating scheme Simulator Assume ploidy = 2, maxAllele = 1

Affected

fitness



father id ...

Chromosome 0

Chromosome 1

Sex

Affection status



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What is simuPQP

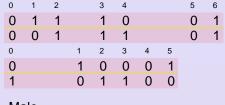
An example

simuPQP components

Population Individual

Operator Mating scheme Simulator

Assume ploidy = 2, maxAllele = 1



Male

Affected

fitness

father id ...

Chromosome 0

Chromosome 1

Sex

Affection status

Information fields



Individuals

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What is simuPOP

An example

simuPOP components

Population Individual

Operator

```
>>> 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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An example

simuPOP components

Population

Individual

Operator
Mating scheme

```
>>> 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
>>> print ind1.info('father_idx'), ind1.info('mother_idx')
```



Outline

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What is simuPOP

An example

All example

simuPOP components

Population

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Operator

Mating scheme Simulator

simuPOP components

- Population
- Individual
- Operator
- Mating scheme
- Simulator



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What is simuPOP

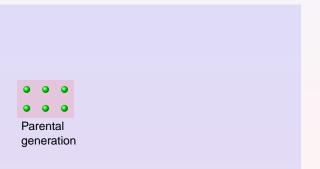
An example

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components

Population Individual

Operator





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What is simuPQP

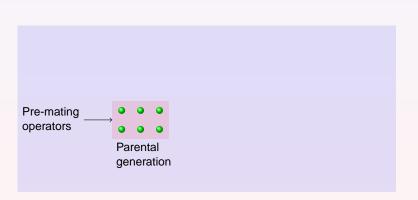
An example

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components

Population Individual

Operator





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What is simuPOP

An example

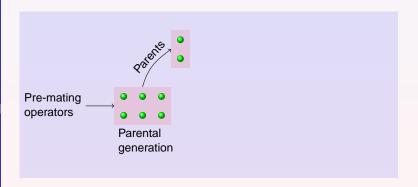
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components
Population

Population Individual

Operator

Mating scheme





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What is simuPOP

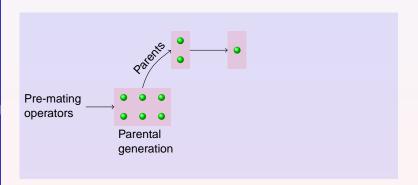
An example

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components
Population

Individual

Operator





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What is simuPOP

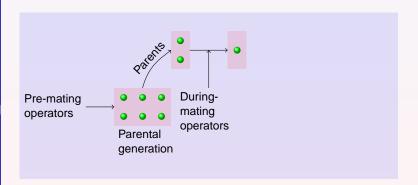
An example

simuPOP components

Components
Population

Population Individual

Operator





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What is simuPOP

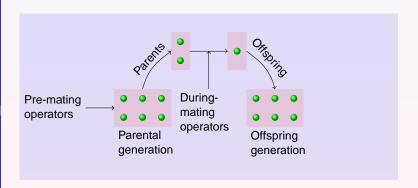
An example

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components
Population

Individual

Operator





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What is simuPOP

An example

simuPOP components

Population Population

Individual Operator

Mating scheme

Pre-mating operators

Parental generation

During-mating operators

Offspring generation

Post-mating operators

Offspring generation



Stages

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An example

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components
Population

Individual

Operator



Stages, an example

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components
Population

Individual

Operator



Output

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components
Population

Individual

Operator

Mating scheme
Simulator



Table-like output

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An example

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components
Population

Individual

Operator



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An example

simuPOP components

components

Population Individual

Operator

Mating scheme Simulator 3 simuPOP components

- Population
 - Individual
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Mating schemes

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components Population

Individual Operator



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Population Individual

Operator Mating scheme

Simulator

simuPOP components

- Population

- Mating scheme
- Simulator



Simulator

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An example

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Population Individual Operator