

Efficient Simulation Of A Simple Evolutionary System

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Outline

Background

Question 1: Distance between finite and infinite population

Question 2: Oscillation in finite population

Question 3: Oscillation in finite population under violation in mutation

Question 4: Oscillation in finite population under violation in crossover

Conclusion

Terms

Population P : a collection of length ℓ binary strings

Population vector \mathbf{p} : \mathbf{p}_j is the proportion of string j in the population

If $P = 00, 01, 01, 10, 11, 11$, then $\mathbf{p}_3 = 2/6 = 1/3$

\mathcal{R} denotes a set binary strings of length ℓ

Addition and multiplication of elements in \mathcal{R} are bitwise operations modulo 2

$$x = 1101, y = 1010$$

$$x + y = 1101 + 1010 = 0111$$

$$xy = 1101 \cdot 1010 = 1000$$

$$\bar{x} = 0010$$

Crossover & Mutation

Crossover : Choose parents u and v , exchange bits using crossover mask m :

$$u' = um + v\bar{m}, v' = u\bar{m} + vm$$

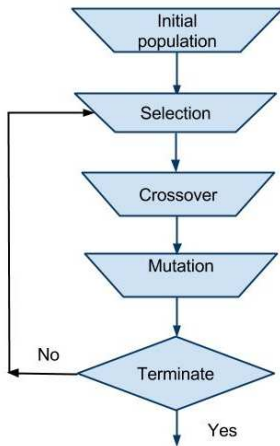
$$u = \mathbf{11001011}, v = 11011111, m = 11110000$$

$$\{\mathbf{11001011}, 11011111\} \rightarrow \{\mathbf{1100}0000 + 00001111, 0000\mathbf{1011} + 11010000\} \rightarrow \{\mathbf{1100}1111, 1101\mathbf{1011}\}$$

Mutation: Flip bits using mutation mask:

$$x \rightarrow x + m$$

Finite Population GA



Randomly select parents u and v

Crossover u and v to produce u' and v'

Keep one of u' , v' , and mutate

Repeat above to form next generation

Repeat whole process until system stops to improve or threshold is reached

Infinite Population Model

Population is modeled as a vector \mathbf{p}

\mathcal{G} maps \mathbf{p} to the next generation

$\mathcal{G}(\mathbf{p})_j$ = probability that string j occurs in the next generation

The infinite population model is the sequence

$$\mathbf{p} \rightarrow \mathcal{G}(\mathbf{p}) \rightarrow \mathcal{G}(\mathcal{G}(\mathbf{p})) \rightarrow \cdots$$

Random Heuristic Search

τ is a stochastic transition rule that maps \mathbf{p} to \mathbf{p}

For a finite population, sequence $\mathbf{p}, \tau(\mathbf{p}), \tau^2(\mathbf{p}), \dots$ forms Markov chain

$\tau(\mathbf{p})$ cannot be predicted with certainty

$\mathcal{G}(\mathbf{p})$ is the expected next generation $\mathcal{E}(\tau(\mathbf{p}))$

The variance in the next generation is

$$\mathcal{E}(\|\tau(\mathbf{p}) - \mathcal{G}(\mathbf{p})\|^2) = \frac{1 - \|\mathcal{G}(\mathbf{p})\|^2}{r}$$

Question 1: Distance Between Finite and Infinite Population

Chebyshev's inequality \rightarrow

$$\|\tau(\mathbf{p}) - \mathcal{G}(\mathbf{p})\| \leq \frac{k}{\sqrt{r}}$$

Jensen's inequality \rightarrow

$$\mathcal{E}(\|\tau(\mathbf{p}) - \mathcal{G}(\mathbf{p})\|) \leq \frac{\sqrt{1 - \|\mathcal{G}(\mathbf{p})\|^2}}{\sqrt{r}}$$

Geometric point of view \rightarrow

$$\|\tau(\mathbf{p}) - \mathcal{G}(\mathbf{p})\| = O(r)$$

Does the distance decrease in practice like $1/\sqrt{r}$?

Diploid Population Model

Diploid genome: $\alpha = \langle \alpha_0, \alpha_1 \rangle$

$\mathbf{q}^n \rightarrow$ population at generation n

$\mathbf{q}_\alpha^n \rightarrow$ prevalence of diploid α

$t_\alpha(g) \rightarrow$ probability that gamete g is produced from parent α

$$\mathbf{q}_\gamma^{n+1} = \sum_{\alpha} \mathbf{q}_\alpha^n t_\alpha(\gamma_0) \sum_{\beta} \mathbf{q}_\beta^n t_\beta(\gamma_1)$$

Diploid Model Reduction to Haploid Model

Diploid distribution in terms of haploids

$$q_{\langle \gamma_0, \gamma_1 \rangle}^n = p_{\gamma_0}^n p_{\gamma_1}^n$$

Haploid distribution in terms of diploids

$$\mathbf{p}_g^n = \frac{1}{2} \sum_{\alpha_0, \alpha_1} \mathbf{q}_{\langle \alpha_0, \alpha_1 \rangle}^n ([g = \alpha_0] + [g = \alpha_1])$$

Evolution equation in terms of haploid distributions \mathbf{p} ,

$$\mathbf{p}_{\gamma_0}^{n+1} = \sum_{\alpha_0, \alpha_1} \mathbf{p}_{\alpha_0}^n \mathbf{p}_{\alpha_1}^n t_{\langle \alpha_0, \alpha_1 \rangle}(\gamma_0)$$

Matrix form:

$$\mathbf{p}'_g = \mathbf{p}^T M_g \mathbf{p}$$

where

$$(M_g)_{u,v} = t_{\langle u,v \rangle}(g)$$

Specialization to Vose's Haploid Model

Mutation:

$$\mu_i = (\mu)^{\mathbf{1}^T i} (1 - \mu)^{\ell - \mathbf{1}^T i}$$

Crossover:

$$\chi_i = \begin{cases} \chi c_i & \text{if } i > 0 \\ 1 - \chi + \chi c_0 & \text{if } i = 0 \end{cases}$$

For uniform crossover, $c_i = 2^{-\ell}$

$$t_{\langle u, v \rangle}(g) = \sum_{i \in \mathcal{R}} \sum_{j \in \mathcal{R}} \sum_{k \in \mathcal{R}} \mu_i \mu_j \frac{\chi_k + \chi_{\bar{k}}}{2} [k(u + i) + \bar{k}(v + j) = g]$$

where $u, v \in \mathcal{R}$

Walsh Basis

$$W_{n,t} = N^{-1/2}(-1)^{n^T t} \text{ where } N = 2^\ell$$

$$\hat{A} = WAW$$

$$\hat{w} = Ww$$

Mixing matrix in Walsh basis

$$\hat{M}_{u,v} = 2^{\ell-1} [uv = \mathbf{0}] \hat{\mu}_u \hat{\mu}_v \sum_{k \in \overline{u+v}\mathcal{R}} \chi_{k+u} + \chi_{k+v}$$

Evolution eqn in Walsh basis

$$\hat{\mathbf{p}}'_g = 2^{\ell/2} \sum_{i \in g\mathcal{R}} \hat{\mathbf{p}}_i \hat{\mathbf{p}}_{i+g} \hat{M}_{i,i+g}$$

where $g\mathcal{R} = \{gi \mid i \in \mathcal{R}\}$

Computational Advantages

Specialization simplifies computation, which otherwise for diploid case would have been impractical

Only one mixing matrix as opposed to 2^ℓ is needed to compute next generation

For $\ell = 14$, using 2^{14} mixing matrices with each having $2^{14} \cdot 2^{14}$ entries would require 32 TB of memory, whereas one mixing matrix requires only 2 GB

Distance Computation

Naive computation

$$\|\mathbf{f} - \mathbf{q}\|^2 = \sum_{\alpha} (\mathbf{f}_{\alpha} - \mathbf{q}_{\alpha})^2 \longrightarrow 2^{\ell} \cdot 2^{\ell} \text{ terms}$$

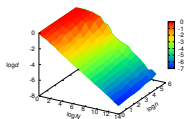
Our implementation

$$\begin{aligned} \|\mathbf{f} - \mathbf{q}\|^2 &= \sum_{\alpha \notin S_{\mathbf{f}}} (\mathbf{f}_{\alpha} - \mathbf{q}_{\alpha})^2 + \sum_{\alpha \in S_{\mathbf{f}}} (\mathbf{f}_{\alpha} - \mathbf{q}_{\alpha})^2 \\ &= \sum_g^2 (\mathbf{p}_g)^2 + \sum_{\alpha \in S_{\mathbf{f}}} \mathbf{f}_{\alpha} (\mathbf{f}_{\alpha} - 2\mathbf{q}_{\alpha}) \rightarrow 2^{\ell} + |S_{\mathbf{f}}| \text{ terms} \end{aligned}$$

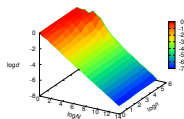
$$S_{\mathbf{f}} = \{\alpha \mid \mathbf{f}_{\alpha} > 0\}$$

Convergence

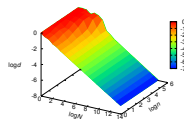
$$\chi = 0.1, \mu = 0.001$$



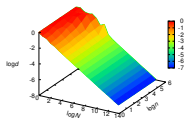
(a) $\ell = 4$



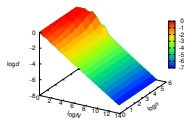
(b) $\ell = 6$



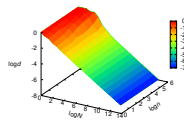
(c) $\ell = 8$



(d) $\ell = 10$



(e) $\ell = 12$

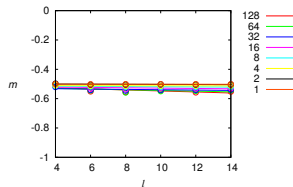


(f) $\ell = 14$

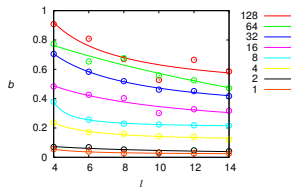
Figure : Convergence of finite population behaviour

Regression

$$\log d = m \log N + b$$



(a) Slope m



(b) Intercept b

Figure : Regression parameter for generation $n \in \{1, 2, 4, 8, 16, 32, 64, 128\}$

$$d \approx N^m e^b$$

From figure (a) above, $m \approx -0.5$

$$d \approx k/N$$

Conclusion 1

Vose's infinite population model makes computation in diploid case efficient by reducing to the haploid case

Distance between finite diploid population and infinite diploid population can decrease like $1/\sqrt{N}$

Question 2

Oscillations in Finite Population Evolution

Limits

The sequence $\mathbf{p}, \mathcal{G}(\mathbf{p}), \mathcal{G}^2(\mathbf{p}), \dots$ may converge to a fixed point

$$\mathcal{G}(\omega) = \lim_{n \rightarrow \infty} \mathcal{G}^n(\mathbf{p}) = \omega$$

But under some circumstances, the sequence converges to a periodic orbit that oscillates between two fixed points, \mathbf{p}^* and \mathbf{q}^*

Periodic Orbit: Necessary and Sufficient Conditions

For some $g \in \mathcal{R}, g \neq 0$

$$\begin{aligned}-1 &= \sum_j (-1)^{g^T j} \mu_j \\ 1 &= \sum_{k \in \bar{g}\mathcal{R}} \chi_{k+g} + \chi_k\end{aligned}$$

Infinite populations converge to a periodic orbit

Do finite populations also exhibit oscillation from random initial populations?

Previous Works on Oscillation

Akin (1982) proved existence of cycling for continuous-time 2-bit diploid model

Hasting (1981) studied cycling in populations with infinite 2-bit diploid population model

Wright and Bidwell (1997) provided examples of cycling in an infinite haploid model with crossover and mutation for 3 bit and 4 bit populations

Wright and Agapie (2001) described cycling in infinite population for up to 4 bits, and also presented data for cycling in finite population

Akin considered continuous time model and we consider discrete time model
Hastings' study was limited to two bits length, and includes only crossover but not mutation

Examples provided by Wright and Bidwell were for specific set parameter values for crossover, mutation and fitness

Wright and Agapie used dynamic mutation that depends upon where population is in the population space

Another difference between Wright and Agapie's work and ours is fitness

We study cyclic behavior for:

- fixed fitness function and random: initial population, mutation and crossover distribution

- higher bit length (up to 14)

- both haploid and diploid populations, and for both finite and infinite populations

We also visualize oscillation

Simulation

Simulations were run for both haploid and diploid populations

Random initial population

$\ell \in 8, 10, 12, 14$

$N = 4096, 40960, 81920$

To visualize oscillation, distance between fixed points and population are plotted

Oscillation

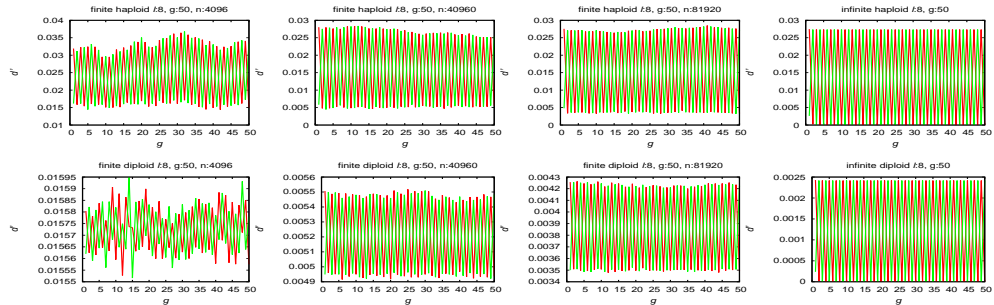


Figure : Infinite and finite population behavior for genome length $\ell = 8$

Oscillation

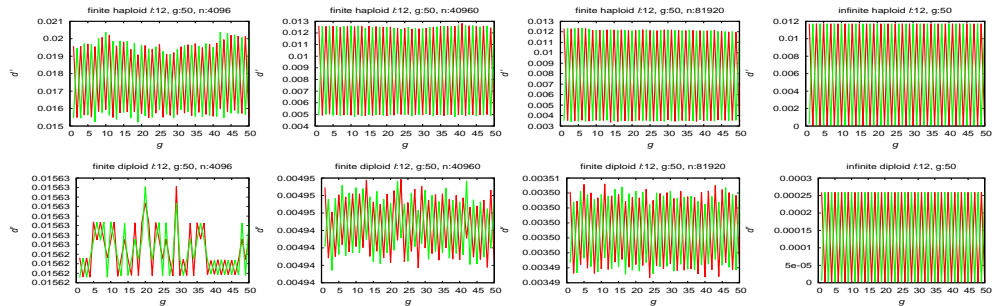
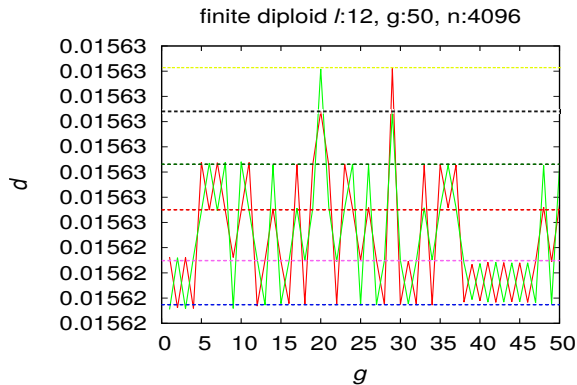


Figure : Infinite and finite population behavior for genome length $\ell = 12$

Oscillation: Unusual Behavior

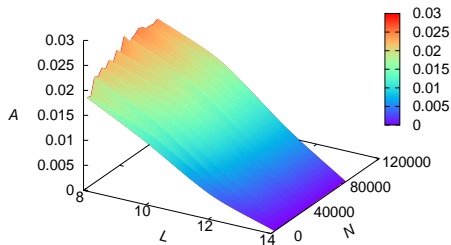


(a)

Figure : Oscillation between different points

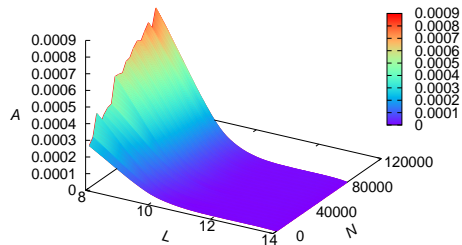
Oscillation Amplitude

Average oscillation amplitude (haploid)



(a)

Average oscillation amplitude (diploid)



(b)

Figure : Average oscillation amplitude

Conclusion 2

Finite population evolution exhibits approximate oscillations

As ℓ increases, oscillation amplitude decreases

As population size increases, oscillation amplitude increases and randomness decreases

Finite population can also oscillate between different pairs of points for diploid population of smaller size and larger ℓ

History

Haldane, in 1932, summarized basic population genetics models : Wright, Fisher and Haldane

Several people working with evolution-inspired algorithms in the 1950s and the 1960s Box (1957), Friedman(1959), Bledsoe (1961), Bremermann (1962), and Reed, Toombs and Baricelli (1967)

In 1960s and 1970s, Holland and colleagues formalized and promoted population based algorithms with crossover and mutation

Vose (1999) presented efficient methods for computing with a haploid model using mask-based operators introduced by Geiringer (1944)