

1.
 - I will talk about my thesis:
“Simulation of Simple Evolutionary System”
2.
 - I will give background, and computations involving our model in the simulations we did.
 - Then I will address these four questions, and make concluding remarks.
3. Part I
4.
 - Population is a collection of length ℓ binary strings
 - Population can be represented by a vector p ; the j th component is the proportion of string j in the population.
 - For example, when P is this, 3rd component of vector p is equal to this.
 - \mathcal{R} is the set of length ℓ binary strings and operations under \mathcal{R} are bitwise modulo 2 operations.
 - Here are examples of some operations under \mathcal{R}
5.
 - Crossover and mutation operators are defined using the bitwise operations in \mathcal{R} .
 - Crossover exchanges bits in parents u and v using crossover mask to produce children u' and v' using this
 - Here's an example. These are parents, these are offsprings.
 - Results depend on mask m .
 - χ_m gives probability of using crossover mask m .
 -
 - Mutation flips bits in x using mutation mask m .
 - In this example, this mutates to this using this mask.
 - μ_m gives probability of using mutation mask m

- The use of masks dates back to Geiringer, 1944
6.
 - This flowchart illustrates finite population genetic algorithm
 - We start from random initial population p .
 - Then randomly select parents u and v ,
 - And crossover to produce u' and v' according to randomly chosen crossover mask
 - We keep one of u' , v' and mutate using randomly chosen mutation mask to produce gamete g
 - We repeat above procedures to form next generation $\tau(p)$
 7.
 - Random Heuristic Search generalizes simple genetic algorithm
 - Given population p , τ is transition rule that maps p to the next generation p' where p and p' both belong to population space Λ_N . N is population size.
 - However, τ is stochastic function of crossover and mutation, and can not be predicted with certainty
 - Finite population evolution forms Markov chain
 8.
 - In infinite population model, population is modeled by vector p where p belongs to population space Λ .
 - \mathcal{G} is a function that maps p to the next generation p' where j th component is proportion of string j occurs in the next generation.
 - The sequence shows evolution of p under infinite population model.
 - \mathcal{G} is the expectation of $\tau(p)$
 - The variance of finite population in next generation is this.
 9.
 - This is our model setup for diploid population.
 - We consider diploid genome α with genome length l .
 - Population is modeled by vector q

- q_α is prevalence of diploid α
 - $t_\alpha(g)$ is transmission function which is probability of gamete g being produced from parent α
 - q' is next generation
 - This is the standard evolutionary model from population genetics.
- 10.
- Diploids can be determined in terms of haploid distributions.
 - Haploids can be determined in terms of diploid distributions.
 - And evolution equation can be expressed in terms of haploid distributions as
- $$\mathbf{p}'_{\gamma_0} = \sum_{\alpha_0, \alpha_1} \mathbf{p}_{\alpha_0} \mathbf{p}_{\alpha_1} t_{\langle \alpha_0, \alpha_1 \rangle}(\gamma_0)$$
- In the matrix form, evolution equation can be expressed as $\mathbf{p}'_g = \mathbf{p}^T M_g \mathbf{p}$
 - \mathbf{p}' is next generation.
 - Where entries in this matrix $M(g)$ is given by $M_g = t_{u,v}(g)$
- 11.
- This is mutation distribution we used. μ is mutation rate.
 - This is crossover distribution we use. χ is crossover rate.
 - This is transmission function.
 - Square brackets here are Iverson brackets which returns 1 if expression inside is true and returns 0 when expression inside is false.
 - This transmission function is expensive to compute because there are 3 sum terms in it.
- 12.
- W is Walsh matrix, $Z = 2^\ell$
 - Walsh transform of matrix A is given by this expression. and Walsh transform of vector w is given by this expression.
 - Here's the algorithm of computing Walsh transform.

- Using this algorithm, walsh transform can be computed in $O(Z \log Z)$ which is almost linear in Z
13. • Mixing matrix is M_0 and is given by the expression
- $$\widehat{M}_{u,v} = 2^{\ell-1} [uv = \mathbf{0}] \widehat{\mu}_u \widehat{\mu}_v \sum_{k \in \overline{u+v} \mathcal{R}} \chi_{k+u} + \chi_{k+v}$$
- This is evolution eqn in Walsh basis
- $$\widehat{p}'_g = 2^{\ell/2} \sum_{i \in g \mathcal{R}} \widehat{p}_i \widehat{p}_{i+g} \widehat{M}_{i,i+g}$$
14. • Now if we compare evolution eqn in Walsh basis to what we had before,
- we have single sum in computing p' compared to double sum from matrix multiplication before.
 - We need only one mixing matrix compared to 2^ℓ matrices for different g s.
 - Also calculating each mixing matrix in previous eqn required 3 sum terms, which is reduced to 1 sum term in walsh basis.
15. • So in summary, Reduction to haploid model and Walsh basis simplify 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
 - Consider $l = 14$, 2^{14} matrices would require 32 TB of memory, while one mixing matrix would require only 2 GB of memory
 - We think that is great optimization in resource
16. • In the 2nd part of this presentation, I talk about distance between finite population and infinite population.
- With naive computation as shown, there would be $2^\ell \cdot 2^\ell$ multiplication terms to be computed because α is diploid and have two components

- where f is finite population and q is infinite population
- We simplify it as shown in eqn (2) where it needs only $2^l + \text{cardinal value of } S_f$ terms
- S_f is set of diploids that are in finite populations
- Writing code to compute in the Walsh basis, and running simulations using the Walsh basis is a significant part of my thesis. It represents the "Efficient" in the thesis title.

17. Part II

18.
 - Our first question concerns about convergence of finite population to infinite population.
 - Chebyshev's inequality, Jensen's inequality and geometric point of view, all, suggest the distance might decrease as $1/\sqrt{N}$
 - But all of 3 implications are from inequalities. The distance might decrease much smaller than $1/\sqrt{N}$.
 - We investigate if the distance infact decreases like $1/\sqrt{N}$ in practice.
19.
 - We ran some simulations with $\chi = 0.1$ and $\mu = 0.001$ for different values of l
 - TThese graphs are in logarithmic scale.
 - This axis is the distance, (point to axis) This axis is population size, (point to axis) this axis is number of generations
 - The thing to notice about these graphs is how flat and planar they are.
20.
 - So we model the data by linear equation
 - Regression shows slope m is nearly equal to negative half $(-1/2)$.
 - This proves distance does decrease as $1/\sqrt{N}$
21.
 - $1/\sqrt{N}$ was theoretical upper bound but our simulaion shows it is really very good bound and the distance decreases as $1/\sqrt{N}$.

- 22. • Our 2nd question concerns about oscillation in finite populations.
- 23. • The infinite population sequence $\mathbf{p}, \mathcal{G}(\mathbf{p}), \mathcal{G}^2(\mathbf{p}), \dots$ may converge to a point, and we call that point a fixed point.
 - But under certain conditions, the sequence converges to a periodic orbit between two fixed points, say \mathbf{p}^* and \mathbf{q}^*
- 24. • And the conditions are: For some g

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

- 1st one is for mutation distribution and 2nd one is for crossover distribution
- We try to answer our 2nd question through simulations; that is do finite populations exhibit oscillations from random initial populations when infinite populations oscillate?
- 25. • Akin, Hastings, Wright, Bidwell and Agapie have studied oscillations in the past.
- 26. • Akin considers - continuous time model, we consider - discrete time model
 - Hastings' study is limited to two bits length, includes only crossover, but no mutation; we consider both crossover and mutation
 - Wright and Bidwell compute specific set of parameter values; there was particular relation between crossover, mutation and population; we use random crossover, mutation and population.
 - Wright and Agapie use dynamic mutation that depends upon where population is in the population space while we use static mutation
- 27. • Simulations were run for both haploid and diploid populations

- To visualize oscillations, distance to fixed points (p^* , q^*) are plotted
- 28.
- These are the results for haploid and diploid population of length 8
 - top row shows results for haploid, bottom row for diploids
 - Population size is in increasing order in columns
 - In the figure, Green line is distance of population to p^* , red line is distance to q^*
 - As population size increases, oscillation approaches the behavior exhibited by infinite population
- 29.
- So our answer to the 2nd question is
 - Yes, finite populations can exhibit approximate oscillation when infinite populations oscillate
- 30.
- Question 3 concerns the robustness of finite population oscillation under mutation-violation
- 31.
- We introduce violation ϵ as following
 - This means no periodic orbits for finite population
 - The modification in μ makes the Markov chain regular
 - This means no periodic orbits for infinite population
 - We study if finite population can exhibit approximate oscillations in that case
- 32.
- Simulations were run for different values of ϵ .
 - Distance of population to limits p and q without violation are plotted
- 33.
- These figures show results for haploid population behavior of string length 8
 - Graphs are arranged in rows for increasing ϵ and columns for increasing population size

- Graphs show convergence of finite population behavior to infinite population behavior as population increases
 - Results show oscillating behavior of population for smaller values of epsilon that diminishes with time.
 - As value of ϵ grows, oscillation diminishes
 - Oscillation dies out for infinite population.
 - Even though finite population also appears to be dying out, since Markov chain is regular, population must visit every population state infinitely. So these population will reoccur and oscillate infinitely often (for $\epsilon = 0.1$).
34. • Our conclusions from this simulation are
- Finite populations exhibit approximate oscillation even if Markov chain is regular when violation is small
 - If violation becomes larger, finite population oscillation decreases
 - As string length increases, oscillation degrades
35. • Our previous question concerns with the robustness of finite population oscillation under mutation-violation, our next question also concerns with the robustness of finite population but under crossover-violation
36. • We introduce violation ϵ in crossover distribution
- Crossover-violation means no periodic orbit exists for infinite population
 - We investigate if finite population can exhibit approximate oscillations in this case
37. • Simulations were run for different values of ϵ
- Distances of population to limits p and q without violation are plotted

38.
 - Graphs show results for haploid population behavior of string length 8
 - Results show similar behavior to that of violation in mutation case
 - However, we noticed that rate of damping of amplitudes of oscillation is slower than in mutation violation
39.
 - Conclusions from experiment on violation in crossover are
 - Finite populations can exhibit approximate oscillation if violation is small
 - If violation becomes larger, finite population oscillation decreases
40.
 - Overall conclusions from this research are
 - Vose's haploid model makes computation efficient in diploid case by reducing to haploid case
 - Distance between finite population and infinite population can decrease like $1/\sqrt{N}$
 - When infinite populations oscillate, finite populations exhibit approximate oscillation
 - Finite populations exhibit approximate oscillation for small mutation-violation
 - Finite populations exhibit approximate oscillation for small crossover-violation