- I will talk about my thesis:
   "Simulation of Simple Evolutionary System"
- 2. I will give background, then address four questions, and make concluding remarks.
- 3. Population is a collection of length l binary strings
  - A population can be represented by a vector; the *j*th component is the proportion of string j in the population.
  - $\mathcal{R}$  is the set of length  $\ell$  binary strings and operations under  $\mathcal{R}$  are bitwise modulo 2 operations.
- 4. 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 the rule  $u' = um + v\bar{m}, v' = u\bar{m} + vm$
  - Mutation flips bits in x using mutation mask m according to rule x to x + m.
- 5. This flowchart illustrates finite population genetic algorithm
  - Start from random initial population p.
  - Randomly select parents u and v
  - Crossover u and v to produce u' and v' according to randomly chosen crossover mask
  - Keep one of u', v' and mutate using randomly chosen mutation mask to produce gamete g
  - Repeat to form next generation  $\tau(p)$
- 6. In Random Heuristic Search,
  - Given population p,  $\tau$  is transition rule that maps p to the next generation p'.

- The sequence shows finite population evolution which forms Markov chain
- However,  $\tau$  is stochastic function of crossover and mutation, and crossover masks and mutation masks are randomly chosen. So,  $\tau(p)$  can not be predicted with certainty
- $\chi_i$  is probability of choosing crossover mask i
- $\mu_i$  is probability of choosing mutation mask i
- 7. In infinite population model, population is modeled as by a vector  $\boldsymbol{p}$ 
  - $\mathcal{G}$  is a function that maps p to the next generation where  $\mathcal{G}(p)_j$  is probability that string j occurs in the next generation.
  - The sequence shows evolution of p under infinite population model.
  - The variance between next generation finite population and infinite population is given by expression where N is population size
- 8. Our first question concerns about convergence of finite population to infinite population
  - Chebyshev's inequality, Jensen's inequality and geometric point of view, all, suggests the distance might decrease as  $1/\sqrt{r}$
  - But all of 3 implications are from inequalities. So the distance might decrease much smaller than  $1/\sqrt{r}$ .
  - We investigate if the distance in fact decreases like  $1/\sqrt{r}$  in practice. For this we set up simple diploid model.
- 9. It is infinite population model.
  - We consider diploid genome  $\alpha$  with genome length 1.
  - q is current generation population
  - $q_{\alpha}$  is prevalence of diploid  $\alpha$
  - $t_{\alpha}(g)$  is transmission function which is probability of gamete g being produced from parent  $\alpha$

- q' is next generation
- 10. Diploids can be determined in terms of haploid distributions.
  - Haploids can be determined in terms of diploid distributions.
  - Evolution equation can be expressed in terms of haploid distributions as

$$m{p}_{\gamma_0}' \, = \, \sum_{lpha_0,\,lpha_1} m{p}_{lpha_0} \, m{p}_{lpha_1} \, t_{\langlelpha_0,\,lpha_1
angle}(\gamma_0)$$

- In the matrix form, evolution equations can be expressed as
- Where M(g) is mixing matrix
- 11. This slide shows computation of crossover and mutation distributions, and transmission function
  - Transmission function is computed with this expression
  - There are 3 sum terms in in it, which is expensive
- 12. W is walsh matrix
  - (A) is walsh transform of matrix A, and  $\hat{w}$  is walsh transform of column vector w.
  - Mixing matrix is given by the expression

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

• And evolution eqn in Walsh basis is

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

- Now if we compare evolution eqn in Walsh basis to what we had before, we got rid of matrix multiplication to compute next generation.
- We don't need to refer to  $2^{\ell}$  mixing matrices either, only one mixing matrix is required in walsh basis computation.
- Calculating each mixing matrix in previous eqn required 3 sum terms, which is reduced to 1 sum term in walsh basis.

- Reduction to haploid model and computing in Walsh basis simplified computations and made it efficient
  - 3 sum terms in transmission function is reduced to only one sum terms for computing mixing matrix in walsh basis
  - We only need one mixing matrix as opposed to  $2^{l}$
  - Consider l = 14,  $2^{14}$  mixing 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
- 14. With naive computation as shown in equation (1), there would be  $2^l \cdot 2^l$  multiplication terms to be computed
  - where f is finite population and q is infinite population
  - We simplify it as shown in eqn (2) where it needs only  $2^l$  + cardinal value of  $S_f$  terms
  - $S_f$  is set of diploids that are in finite populations
- 15. We ran simulations with  $\chi = 0.1$  and  $\mu = 0.001$  for different values of l
  - These graphs show the results in logarithmic scale.
  - (point to axis) d is the distance, (point to axis) N is population size, (point to axis) n is number of generations
  - Data shows as population size increases, distance decreases and converge to infinite population
  - Graphs show flat surface so we model the data by linear equation
- 16. Regression shows slope m is nearly equal to -0.5
  - This proves distance does decrease as  $1/\sqrt{N}$
- 17.  $1/\sqrt{N}$  was theoretical upper bound but our simulation shows it is really very good bound and the distance decreases as  $1/\sqrt{N}$ .

- 18. Our 2nd question concerns about oscillation in finite populations.
- 19. First I want to introduce term limit; we also call it fixed point.
  - The infinite population sequence p,  $\mathcal{G}(p)$ ,  $\mathcal{G}^2(p)$ ,  $\cdots$  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 p\* and q\*
- 20. And the conditions are: For some g

$$-1 = \sum_{j} (-1)^{g^{T} j} \boldsymbol{\mu}_{j}$$
$$1 = \sum_{k \in \bar{g}\mathcal{R}} \boldsymbol{\chi}_{k+g} + \boldsymbol{\chi}_{k}$$

- So our 2nd question is do finite populations also exhibit oscillations from random intial populations when infinite population oscillate?
- 21. Akin, Hasting, Wright, Bidwell and Agapie have studied oscillations in the past.
- 22. Akin considered continuous time model, we consider discrete time model
  - Hastings' study limited to two bits length, includes only crossover, not mutation
  - Wright and Bidwell compute a specific fitness function and a specific initial population for randomly generated mutation and crossover distributions in an attempt to find cyclic behavior
  - Wright and Agapie used dynamic mutation that depends upon where population is in the population space while we use static mutation
  - We study oscillation for
  - fixed fitness function and random: initial population, mutation and crossover distribution

- higher bit length (up to 14), and actually oscillation conditions for infinite populations are independent of string length
- both haploid and diploid populations, and for both finite and infinite populations
- We also visualize oscillation
- 23. Simulations were run for both haploid and diploid populations
  - for different string lengths l
  - and for population size 4096, 40960, 81920
  - $\bullet$  To visualize oscillations, distances between fixed points  $(p^*\;,\,q^*)$  and population are plotted
- Graphs show the results for haploid and diploid population of length
  - top haploid, bottom diploids
  - Population size 4096, 40960, 81920 is in increasing order in columns
  - As population size increases, oscillation approaches the behavior exhibited by infinite population
  - We observe more randomness in diploids than in haploids for same string length and population size.
- Graphs show the results for haploid and diploid population of length
  - We observe that increase in 1 degrades oscillation (particularly in diploids)
- 26. Our conclusions from this simulation are
  - Finite populations exhibit approximate oscillation when infinite populations oscillate
  - As population size increases, randomness decreases

- 27. Question 3 concerns the robustness of finite population oscillation under violation in mutation
- 28. We introduce violation  $\epsilon$  as following
  - ullet The modification in  $\mu$  makes the Markov chain regular
  - This means no periodic orbits for finite population and no periodic orbits for infinite population
  - We study if finite population can exhibit approximate oscillations in that case
- 29. Simulations were run for different values of  $\epsilon$ ,  $\ell$  and N
  - Distances of population to limits p and q without violation are plotted
- Graphs show results for haploid population behavior of string length
  - Graphs are arranged in rows for increasing  $\epsilon$  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.
  - Oscillation dies out for infinite population.
  - Even though finite population also appears to be dying out, since Markov chain is regular, finite population will oscillate infinitely often.
  - As value of epsilon grows, oscillation diminishes
- 31. Graphs show results for diploid population behavior of string length 12
  - We observed oscillation also degrades as string length increases. It
    is seen in both haploid and diploid cases, but particularly noticeable
    in diploids.

- 32. 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
- 33. Our last 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 violation in crossover
- Violation in crossover means no periodic orbit exists for infinite population
  - But we don't know if Markov chain is regular in this case
  - We investigate if finite population can exhibit approximate oscillations in this case
- 35. We introduce violation  $\epsilon$  as following
- 36. Simulations were run for different values of  $\epsilon$ ,  $\ell$  and N
  - Distances of population to limits p and q without violation are plotted
- Graphs show results for haploid population behavior of string length
  - Results show similar behavior to that of violation in mutation case
- 38. Graphs show results for diploid population behavior of string length 12
  - However, we noticed that rate of damping of amplitudes of oscillation is slower than in mutation violation
  - And, we see more randomness in population behavior than in mutation violation, especially for diploid case
- 39. Conclusions from experiment on violation in crossover are

- Finite populations 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 population exhibits approximate oscillation for small mutation violation
  - Finite populations exhibit approximate oscillation for small crossover violation