- 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  $\mathcal R$  ar bitwise modulo 2 operations.
- 4. Crossover and mutation operators are defined using the bitwise operations in  $\mathcal{R}$ .
  - Given parents u and v, crossover produces children u' and v'.
  - x mutates to x + m.
- 5. This flowchart illustrates finite population genetic algorithm
  - We start from random initial population P.
  - Randomly select parents u and v
  - Crossover u and v to produce u' and v'
  - Keep one of u', v' and mutate
  - Repeat to form next generation and when next generation completes, replace it with new generation
  - The process is repeated until some threshold is meet
- 6. 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.

- Random Heuristic Search generalizes simple genetic algorithm and was presented in his book by Vose in 1999. Our work is largely based on this model
  - 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 hence,  $\tau(p)$  can not be predicted with certainty.
  - $\mathcal{G}(p)$  gives the expected next generation
  - The variance between finite population and infinite population is given by expression where r is population size
- 8. Our first question concerns about distance between finite population and 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 what happens 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.
  - $\bullet$   $q^n$  is population at generation n
  - $q_{\alpha}^{n}$  is prevalence of diploid  $\alpha$  at generation n
  - $t_{\alpha}(g)$  is transmission function which is probability of gamete g being produced from parent  $\alpha$
  - $q_{\gamma}^{n+1} = \sum_{\alpha} q_{\alpha}^{n} t_{\alpha}(\gamma_{0}) \sum_{\beta} q_{\beta}^{n} t_{\beta}(\gamma_{1})$  gives us next generation population.

- 10. Diploids are determined in terms of haploid distributions.
  - Haploids are determined in terms of diploid distributions.
  - Evolution equations can be expressed in terms of haploid distributions as
  - 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
  - Instead of using this transmission function, we want to compute mixing matrix in walsh basis.
- 12. W is walsh matrix
  - (hat) represents walsh transform and for matrix A,  $(\hat{A})$  is given by the expression  $\hat{A} = WAW$ , and for vector w,  $\hat{w}$  is by the expression  $\hat{w} = Ww$ .
  - 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

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

- 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.
  - d is the distance, N is population size, n is number of generations
  - Graphs show as population size increases, distance decreases, converge to infinite population
  - Graphs also show smoothing as genome length increases
  - Data shows a near linear dependence of log d on log N and that is what we are particularly interested in
- 16. So we tried to fit data in the linear equation
  - m is slope and b is y intercept
  - Regression shows m nearly equal to -0.5
  - This proves distance does decrease as  $1/\sqrt{N}$
  - Also graph for y intercept b shows,  $k = e^b$  decreases monotonically with genome length l, and increases monotonically with generation n
  - Increase in k for larger n seems to be a manifestation of the growing nonlinearity likely that the nonlinearity results partly from genetic drift experienced by finite populations

- and partly because predicted distance is for single step case as generation increases difference between finite population and infinite population accumulates non linearly
- 17. Conclusion from this simulation is that
  - Vose's infinite population model makes computation in diploid case efficient by reducing to the haploid case
  - $\bullet$  Distance between finite diploid population and infinite diploid population can decrease like 1/N
- 18. We move on to our 2nd question which concerns oscillation in finite populations.
- First I want to introduce term limit; we also call it fixed point interchangeably.
  - The infinite population sequence p,  $\mathcal{G}(p)$ ,  $\mathcal{G}^2(p)$ ,  $\cdots$  may converge to a point, that we call 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?
- 21. Other people in the past also have been interested in studying oscillations in populations.
  - 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 when cycles in an infinite haploid population model occur with crossover and mutation for 3 bit and 4 bit populations
- Wright and Agapie (2001) described cyclings in infinite populations for up to 4 bits, and also presented data for cyclings in finite populations
- 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
  10
  - top haploid, bottom diploids
  - $\bullet$  and for population size 4096, 40960, 81920
  - last column graphs show results for infinite population
  - 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.
- 25. Graphs show the results for haploid and diploid population of length12
  - We observe that increase in l degrades oscillation, and it is particularly noticeable in diploid case
  - We see an interesting behavior in this bottom left graph,
- 26. Here is zoomed in picture
  - We see oscillation between different levels
  - we observe this kind of behavior only for higher values of l in diploids and for small population size
  - It might be because there could be fixed points for other distributions in the vicinity of finite population trajectory and get attracted to those fixed points
  - And smaller populations do not follow infinite population path as closely as larger populations do; so as for larger populations, these behaviors were not observed

- We also plotted average amplitudes of oscillation in haploids and diploids
  - Graphs show
  - Oscillation amplitude increases with increase in population size
  - Amplitude of oscillation decreases with increase in l
- 28. Our conclusions from this simulation are
  - Finite populations exhibit approximate oscillation when infinite populations oscillate
  - 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 fixed points for diploid population of smaller size and larger l
- 29. Question 3 concerns the robustness of finite population oscillation under violation in mutation
- If Markov chain representing finite population is regular, positive steady state distribution exists
  - Which means no periodic orbit exists for finite population
  - We study if finite population can exhibit approximate oscillations in that case
- 31. 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
- 32. 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 for smaller values of epsilon that diminishes with time.
  - As value of epsilon grows, oscillation degrades
- 34. We observed oscillation also degrades as string length increases, that can be seen in results for diploids.
- 35. 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
- Question 4 also concerns the robustness of finite population oscillation, 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
- 38. We introduce violation  $\epsilon$  as following
- 39. Simulations were run for different values of  $\epsilon$ ,  $\ell$  and N
  - Distances of population to limits p and q without violation are plotted

- 40. Graphs show results for haploid population behavior of string length
  - 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
  - And, we see more randomness in population behavior than in mutation violation, especially for diploid case
- 41. 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
  - As string length increases, oscillation degrades
- 42. Overall conclusions from this research are
  - Vose's haploid model makes computation efficient in diploid case by reducing to haploid case
  - $\bullet$  Distance between finite population and infinite population can decrease like 1/N
  - When infinite populations oscillate, finite populations exhibit approximate oscillation
  - When Markov chain is regular, finite population exhibits approximate oscillation for small mutation violation
  - Finite populations exhibit approximate oscillation for small crossover violation