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Statistical Mechanics Theory of Genetic Algorithms

Part I — Overview

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Preview of Coming Attractions

The statistics mechanics theory of genetic algorithms:

- Describes the *average dynamics* of genetic algorithms acting on specific problems.
- Requires approximations and assumptions, mostly controllable.
- Includes finite population effects.
- Dynamical equations can be difficult to solve, but the computation is independent of the population size and of the string size.
- Leads to accurate predictions

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Example: Subset Sum — A weakly NP hard problem:

Reference: (Rattray '96)

- There are L files with sizes f_i for the ith file.
- The back-up disk has size D and is not big enough to hold all of the files.
- Find the subset of the files which comes closest to filling the disk.

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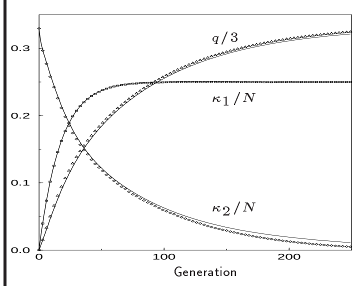
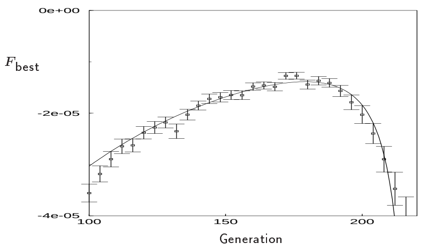
κ_1 is the mean amount stored on the disk; κ_2 is the variance, q is a measure of the similarity of the solutions in the population.





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What system will we study

- Dynamics of a finite population of strings
- Undergoing mutation + selection + crossover
- Many components in each string
- Complex ("realistic") selection models — problems with some characteristics of realistic problems.

Mostly interested in applied (directional) selection.
Natural selection also of interest

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A simple genetic algorithm

Representation: fixed length string of L bits. $x_i \leftarrow \{0,1\}$. E.g.

$$\mathbf{x} = 1001110$$

Quantity to be optimized: *Objective-function* or *trait*; a function of the strings, $E(\mathbf{x})$.

Population: of N strings. Fixed size.

Selection weight: N parents are chosen from the current population; probability of selection string α is

$$p^{\alpha} = \frac{W(\mathbf{x}^{\alpha})}{\sum_{\gamma} W(\mathbf{x}^{\gamma})}.$$

Recombination/Crossover: This operation produces offspring from a pair of parents by *randomly* combining parts of each parent.

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Single-point crossover:

$$A_1 = 1111111|1111111 \quad \rightarrow \quad A_1' = 0000000|1111111$$
$$A_2 = 0000000|0000000 \quad \rightarrow \quad A_2' = 1111111|0000000$$

Multi-point crossover:

$$A_1 = 111|111111|11111 \quad \rightarrow \quad A_1' = 000|111111|00000$$
$$A_2 = 000|000000|00000 \quad \rightarrow \quad A_2' = 111|000000|11111$$

Uniform crossover: Each site is independently chosen em at random from parent 1 or parent 2.

Mutation: This operation simply changes characters in the offspring string at random. Each character is changed with a small probability.

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Goals of the Theory

To answer questions such as:

- How do GAs work (insight)?
- On what problems do GAs excel?
- How can genetic algorithm search be optimized?

By solving the dynamics of evolutionary search on specific problems: To do this, we must

- Derive a *deterministic* set of equations describing the evolution
- Solve it for the specific problem.

We have to find a set of equations of motion which are deterministic and simple enough to solve.

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Aside — Schema theory does not achieve this

- Does not produce equations of motion which can be iterated.

expectation value = actual values in particular population

Usual approach is to (implicitly) assume infinite population so that both sides of equation involve expectation values.

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Basic Idea

To get simple equations: Describe the population in terms of a few *macroscopic* quantities — statistics of the population.

To get deterministic equations: Describe the population in terms of average behaviour of the macroscopics.

To close the loop: Use a statistical inference method (maximum entropy).

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Levels of Description

Microscopic description: Describe the system in terms of the actual details of the constituents.

Macroscopic description: Describe the system in terms of a few statistical, and large scale properties of the system.

Example — electrons in a circuit **Microscopic description:** The quantum-mechanical wave function of the 10^{24} conduction elections interacting with themselves, the other elections, the nuclei, etc.

Macroscopic description: $V = IR$.

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Points about microscopic description:

- It is potentially rigorous, but ...
- It is extremely difficult to solve,
- Were a solution to exist, it would be extremely complicated; difficult to obtain useful information.

Points about the macroscopic description:

- It is approximate,
- It is easy to solve and directly related to the useful information,
- There is missing information. A method of inference may be required.

Statistical Mechanics = macroscopic description + MaxEnt inference

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Elements of Statistical Mechanics

Image a system which can be in states: $s_1, s_2, \ldots, s_{N_\Omega} \in \Omega$.

(Huge number of states) E.g.

- Molecules in a glass of H_2O,
- genes in a population of genotypes.

Dynamics — stochastic, at least in initial conditions.

Remove the stochasticity by considering an *ensemble* of systems. Goal is to predict behaviour on average over the ensemble.

Microscopic knowledge: Probability of finding a member of the ensemble in state $s_i, P(s_i)$. N_Ω numbers.

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Our actual knowledge: Some average (macroscopic) quantity Q.

$$Q = \sum_{s_i \in \Omega} Q(s_i) P(s_i).$$

Problem: Suppose you want to know about some other quantity, G,

$$G = \sum_{s_i \in \Omega} G(s_i) P(s_i)$$

if we don't know the P's, how can we do it.

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Maximum Entropy Inference: Choose the assignment of the $\{P(s_i)\}$ which is consistent with Q and otherwise has the most "uncertainty" (or assumes the least information).

Uncertainty of a distribution: Given by the entropy

$$H = -\sum_{s_i \in \Omega} P(s_i) \log P(s_i),$$

determines the amount of information required to remove the uncertainty.

Maximum Entropy Distribution: Optimize

$$H = -\sum_{s_i \in \Omega} P(s_i) \log P(s_i) + \lambda \sum_{s_i \in \Omega} Q(s_i) P(s_i)$$

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$$\boxed{P(s_i) = \frac{e^{-\lambda Q(s_i)}}{\sum_{s'_i \in \Omega} e^{-\lambda Q(s'_i)}}}$$

The Lagrange multiplier, λ is chosen so that

$$\frac{\sum_{s_i \in \Omega} e^{-\lambda Q(s_i)} Q(s_i)}{\sum_{s'_i \in \Omega} e^{-\lambda Q(s'_i)}} = Q.$$

Statistical Mechanics = describe system by

- Considering averages over ensembles
- Using maximum entropy distribution to infer other quantities.

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Maximum Entropy Inference

Maximum Entropy Distribution:

- Occupies almost all of probability distribution space, as $N_\Omega \to \infty$,
- Is an assumption (of microscopic chaos).

Works well if

- Q is "self-averaging; averages of Q are similar to typical ones,
- Q explains most of the non-random aspects of the system (otherwise further macroscopic quantities will be required).

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Application to Evolutionary Dynamics

Microscopic approach: Markov chain and quadratic dynamical systems methods.

Microscopic approach:

- Predict average statistics of E, e.g. mean standard deviation, best, etc. (Called $\kappa_1, \kappa_2, \ldots$).
- Predict average configurational statistics, e.g. a measure of how similar the strings in the population are q.
- **Problem:** It is not possible to relate configurational statistics to objective function statistics.

Maximum Entropy inference is used to close this loop.

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Closing the loop