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Evolutionary escape from local fitness peaks through inversion mutations

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Model of molecular evolution

Adaptive molecular evolution is often conceptualised as adaptive walks on rugged fitness landscapes that are driven by changes in the genome (mutations).

The problem

Once a local fitness peak is reached there are no more selectively accessible pathways by the mechanism of single nucleotides (point) mutations. Then, the evolutionary dynamics get stuck in a suboptimal peak, hindering any possibility to reach other higher peaks.

Inversion mutations operation

\[ f(x') = f(x) + \Delta \]

where the complementary value is determined by \( x' = (x_1, x_2, \ldots, x_N) \) and \( \Delta \) is the difference between the fitness value of the parent sequence and its offspring.

The model

We simulate artificial molecular evolution of digital organisms (replicas), each of which contains a single piece of DNA. We engineer a computational model to cartoon the double-stranded structure of DNA, and simulate inversion-like mutations: a permutation of the complementary strand, which are then exchanged with the main strand within the segment where the inversion occurs. We model digital genotypes made up of a binary alphabet \( \{0, 1\} \). In analogy with DNA primary sequence, the bits represent (artificial) binary nucleotides. We also assume that genomes are arranged in circular strings with constant number of base-pairs. For the sake of simplicity, our model does not consider non-coding regions, mimicking the molecular evolution of some viruses and mitochondrial DNA with compact genomes and closed double-stranded DNA circles. It is important to emphasise that our computational model simulates intragenic-like mutations. We do not include recombination, so we are modelling asexual replication.

Enumeration of accessible mutants

Examples of the number of neighbouring sequences \( D \) per genotype of size \( N \) (subscripts numbers are the occurrence frequencies of \( 1 \) and \( 0 \)).

Accessible-mutants graphs

Representative examples for \( N = 4, 7 \) and 10. Colours indicate the nodal degree. The reported values correspond to the true mean degree \( \langle k \rangle \) and the maximum. The upper row shows the point mutation case, verifying that the accessible-mutants' graphs are isomorphic to the Hamming graphs \( H(2, 2N) \) and \( H(2, 2N+1) \) (i.e. the hypercubes \( 2^N \) ) (the genotype space). The lower graphs correspond to the inversion mutations cases, where we can appreciate that the accessible mutants graphs are not isomorphic to their respective genotype space (hypercubes).

Example of accessible mutants (genotypes with \( N = 4 \))

Fitness and epistatic interaction

Behaviour of the mean fitness of genotypes with size \( N = 100 \) for different rugged landscapes, tuned through \( K = 0, \ldots, 99 \). For adjacent (+) and random (\( \times \)) neighbourhood interactions. Red color corresponds to inversion mutants and blue to point mutations.

Summary

This work provided computational evidence that once an adaptive walk reaches a local fitness peak, then inversion mutations can redirect the evolutionary process towards genotypes with higher fitness values. The way our model was conceived, also proves that escape from a local peak of fitness can occur in constant environments without contingencies. Our model for inversion mutations not only elucidated an escape mechanism, but have also made it possible to uncover interesting aspects about the combinatorics of inversion mutations. We have been able to contrast the isomorphism of mutational graphs for point mutations and their isomorphism with the genotype space. Finally, it was possible to verify that for a very simple model of population genetics in the strong weak mutation limit—with rugged landscapes simulated with the well known NK model—our adaptive walks simulations showed that when the evolutionary dynamics is driven by inversions, higher fitness values can be reached.

Bibliography