Finding the number of local optima in the 2-spin fitness landscape model

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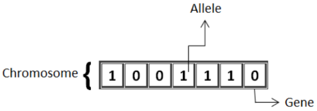
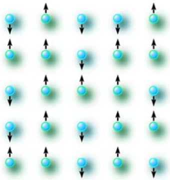
Overview

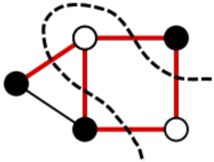
1. Motivation.
2. Definition.
3. Properties.
   - Local Optima.
4. Random Field models for fitness landscapes.
   - Properties of Random Fields
   - Covariance matrix
5. Landscapes Models
6. Number of local optima
   - Local optima for the NK-model
   - Local optima for the 2-spin model

Discrete Problems

- Evolution and Genetic Algorithms.
- Physics of disordered systems.
- Discrete optimization problems.



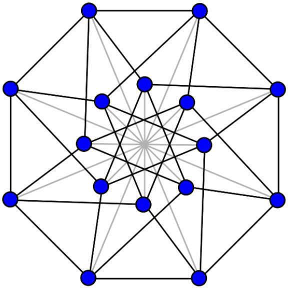




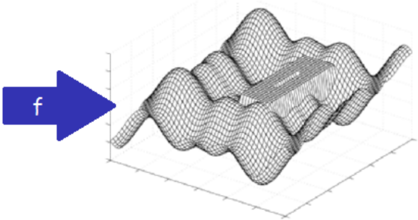
Landscapes

A **landscape** consists of:

A set V of configurations together with a notion of **neighborhood**:



And a '**cost**' or '**fitness**' **function** $f : V \rightarrow \mathbb{R}$



Therefore we can see V as a graph Γ with each vertex corresponding to one configuration and an edge between any two neighbors.

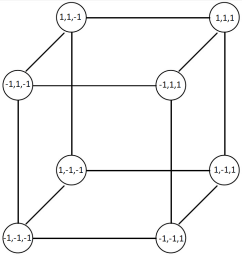
Landscapes

Configurations

We will denote a configuration $x \in V$ as $x = (x_1, x_2, \ldots, x_n)$. We will call the entry x_i a **locus**, and it can only take the values +1 or -1. Therefore $x \in \{\pm 1\}^n$

Neighborhood

There is an edge between two configurations $x, y \in V$ if they differ only in one entry. This makes our configuration space a Hamming graph $\mathbb{H}_2^n$.



H_2^3

Properties

Local and Global Optima

- The goal in landscapes problems is to find the **'best' value** of the cost function f, which represent the fittest of individuals, the best tour in the TSP, or the lowest energy for spin glass. However **local optima** are obstacles in the way.
- A configuration $x \in V$ is a **local minimum** if $f(x) \leq f(y) \;\; \forall y$ neighbor of x.
- And the minimum x is called **global** if $f(x) \leq f(y) \;\; \forall y \in V$

Ruggedness

The **number of local optima** is a measure for the ruggedness of a landscape. In general, it's hard to calculate.

Random Field models for fitness landscapes

- We cannot hope to describe landscapes from their underlying biological and chemical structure, therefore one approach taken is to consider probabilistic models of fitness landscapes.

Definition

The set $\{f : V \to \mathbb{R}\}$ together with a measure $\mu\{f\}$ form the probability space Ξ, which we call a **random field** on the graph Γ. This measure can be seen as the form $P(c_1, c_2, \ldots, c_{|V|})$ which is the probability that for all configurations x_i holds simultaneously $f(x_i) \leq c_i$, where $c_i \in \mathbb{R}$.

Properties of Random Fields

Expected values

The expected value of a random variable X defined on the random field is given by

$$\mathbb{E}[X] := \int_{\mathbb{R}^{|V|}} X \mathrm{d}P(c_1, \ldots, c_n)$$

Covariance matrix

The covariance matrix C of a random field is defined componentwise as

$$C_{x,y} = \mathrm{Cov}[f(x), f(y)] = \mathbb{E}[f(x)f(y)] - \mathbb{E}[f(x)]\mathbb{E}[f(y)]$$

and is symmetric and non-negative definite.

Landscapes Models

House of Cards (HoC)

One of the simplest models. The fitness values $f(x)$ for each configuration x are assigned independently at random from some probability distribution.

Sherrington Kirkpatrick (or 2-spin model)

This models a spin glass of n particles with 2 spin states, represented by $\{+1, -1\}$:

$$H_{SK}(x) := \sum_{i<j} J_{ij} x_i x_j$$

where the coupling constants J_{ij} are i.i.d. Gaussian random variables with mean 0 and variance 1.

P-spin model

A generalization of the Sherrington Kirkpatrick model in which each locus interacts with another p-1 locus.

NK Model: Different interactions between loci

NK Model

In this model, the fitness $f(x)$ of a configuration x is given by

$$f(x) = \sum_{i=1}^{n} f_i(x_{b_{i,1}}, x_{b_{i,2}}, \ldots, x_{b_{i,K}})$$

where f_i is an independent HoC landscape for the locus i, depending on K loci and the indices $b_{i,j}$ represent which K loci are being considered.

Interaction between loci (NK model)

Note that the values for all the $\mathbf{b}_i$ were left undefined, and exactly these values model the interaction scheme between loci. For instance:

Adjacent neighborhood

Each sub-landscape f_i depends on the i-th locus and its $K - 1$ following neighbors. That is,

$$\mathbf{b}_i = (x_i, x_{i+1}, \ldots, x_{i+K})$$

each element modulo n.

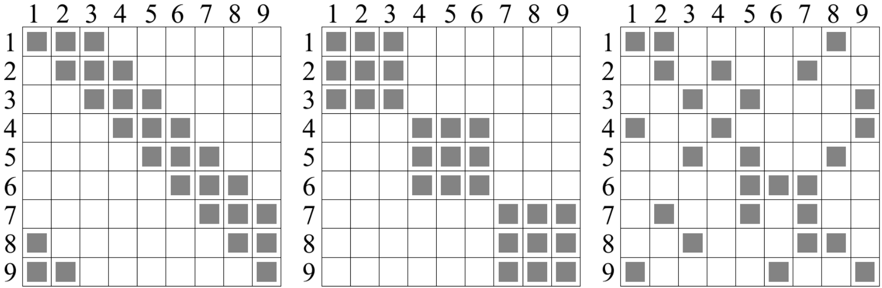
Random neighborhood

The neighborhood set b_i contains i and $K - 1$ other numbers, which are chosen at random from $\{1, 2, \ldots, n\}$.

Interaction between loci (NK model)

Block neighborhood

With n an integer multiple of K, n is divided into n/K disjoint K-subsets and each block effectively behaves as an independent HoC landscape.



Adjacent neighborhood   Block neighborhood   Random neighborhood

How to find the number of local optima?

The idea is to find the probability π_{max} that a randomly chosen configuration x is a maximum, and the actual number of maxima $\#_{max}$ is just

$$\#_{max} = 2^n \pi_{max}$$

For the NK-model we will try to find $1/2 \leq \lambda_k^{model} \leq 1$ such that

$$\#_{max} = (2\lambda_k^{model})^n$$

where the factor 2 is introduced just as a reminder that the search space ($\mathbb{H}_2^n$) increases as 2^n.

Calculating the local optima

The easiest example is the House of Cards model. Since $f(x)$ is random for every configuration, π_{max} is just the probability that x is the maximum among $n + 1$ random values, which is

$$\pi_{max} = \frac{1}{n+1}$$

However, there is a general formalism for computing π_{max} in the HoC and other models. Let us define the operator $\Delta_l : \mathbb{H}_2^n \leftarrow \mathbb{H}_2^n$ for all $l \in \{1, 2, \ldots, n\}$ as

$$(\Delta_l x)_m = (1 - 2\delta_{lm})x_m$$

which changes the l-th entry of the configuration x.

Calculating the local optima

Let h_0 and h_l be the fitness values for x and $\Delta_l x$ respectively, i.e., $h_0 = f(x)$ and $h_l = f(\Delta_l x)$. Then, x is a local maximum if $h_0 > h_l$ or $u_l \equiv h_0 - h_l > 0$ for all $1 \leq l \leq n$. With vector notation, $\mathbf{u} \equiv (u_1, u_2, \ldots, u_n)$, the **joint probability density** of the u_l is given by

$$P(\mathbf{u}) = \int \prod_{l=0}^{n} dh_l p_f(h_l) \prod_{l=1}^{n} \delta(u_l - (h_0 - h_l)),$$

and the characteristic function

$$\Phi(\mathbf{q}) = \int dy\ p_f(y) \left(\prod_{l=1}^{n} \phi_f(-q_l) \right) \exp\left(iy \sum_{l=1}^{n} q_l \right)$$

where $\phi_f(-q_l)$ is the individual characteristic function of $p_f(h)$.

Calculating the local optima

By performing the inverse Fourier transform of $\Phi(q)$ and then integrating over only positive values of u_l (condition for x to be maximum and represented by $\theta(\mathbf{u} > 0)$), we obtain:

$$\pi_{max} = \prod_{l=1}^{n} \int_0^{\infty} du_l \; P(\mathbf{u}) = \int \frac{DuDq}{(2\pi)^n} e^{-i\mathbf{q}\cdot\mathbf{u}} \theta\,(\mathbf{u} > 0)\,\Phi(\mathbf{q})$$

With these expresions one can recover the number of local optima for the HoC model and more importantly, one can get the number of maximum for some neighborhood models of the NK- model.

Local optima for the 2-spin model

The idea:

1. The NK-model with $K = 2$ and the adjacent neighborhood is the 2-spin model. Find the number of maxima for this case.
2. Calculate the covariance matrix of the 2-spin model.
3. Compare the covariance values with the number of maxima and try to find a relation between them.

Part 1. Local maxima for the NK model

In the NK model, the total fitness $F(x)$ of a configuration x is a sum of individual HoC fitness values defined on each particular block or neighborhood.

Since a characteristic function is the natural object when dealing with sums of independent random variables, the approach will be based on the characteristic function of the NK blocks, and using the notation from previous slides, it has the form

$$\Phi(\mathbf{q}) = \prod_{r=1}^{N} \Phi_r(\mathbf{q})$$

Where $\Phi_r(\mathbf{q})$ denotes the characteristic function of $\mathbf{u}$ within the NK block B_r.

Part 1. Local maxima for the NK model

With the help of an incidence matrix notation $b_{l,r}$ that indicates the presence (absence) of a locus l in a neighborhood set r, i.e. $b_{l,r} = 1(0)$ if $l \in B_r (l \notin B_r)$; the characteristic function ϕ_r can be rewritten as:

$$\Phi_r(\mathbf{q}) = \int dy_r \; p_f(y_r) \prod_{l=1}^{n} \left[\phi_f(-q_l) e^{i y_r q_l}\right]^{b_{l,r}}$$

Then, once the full characteristic function has been derived, π_{max} is readily calculated by inverse Fourier transform the same way as before, and for the Adjacent Neighborhood reads as:

$$\pi_{max}^{AN} = \int D\mathbf{y} P(\mathbf{y}) \frac{D\mathbf{u} D\mathbf{q}}{(2\pi)^n} e^{-i\mathbf{q}\cdot\mathbf{u}} \theta(\mathbf{u} > 0) \prod_{l=1}^{n} \phi_f(-q_l)^k \, e^{i q_l \sum_{r=0}^{k-1} y_{(l+r) \bmod (n)}}$$

TODO

- Simplify for $k = 2$, and compare with other results for 2-spin.
- Compare with covariance matrix.

Thank you.