Landscape Families

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Outline

- Fitness Landscapes
- Spin Glasses
- N-K landscapes
- Optimisation problems
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Fitness Landscapes: Introduction

- The concept of 'fitness landscapes' stems from Wright's studies in theoretical biology in the 1930s.
- The concept was used to explain the evolution and fitness of genotypes.
- More resently it has been applied to the understanding of combinatorial problems.
- Especially interesting is what landscape features characterise hard problems.

Fitness Landscapes: Example

More formally, the key ingredients of a fitness landscape are

1. a set X of configurations,
2. a notion of neighbourhood, nearness, distance, or accessibility on X, and
3. a fitness function $f : X \longrightarrow \mathbb{R}$

Spin Glasses: Introduction

- Spin glasses are magnetic substances which have complicated magnetic interactions.
- They can both exhibit so called ferromagnetic and anti-ferromagnetic interaction.
- Spin glasses are amorphous substances which show structure only for a few tens atom lengths.
- Amorphous substances are usually 'transparent' for some wavelengths of light.
- The spin glass model tries to model the magnetic interaction and properties of the substancess.

Spin Glasses: General Model

- a crystal lattice with N lattice sites

- Each site i is assigned a vector quantity $\mathbf{s}_i$, the *magnetic spin*.

- The sites interact according to a *coupling constant* J_{ij}.

- A *configuration* of the system is a assignment to the N magnetic spins.

- The energy, or the *Hamiltonian*, of the system at particular state $\mathbf{s}$ is

$$H(\mathbf{s}) = -\sum_{i>k} J_{ij}\mathbf{s}_i \cdot \mathbf{s}_k$$

Spin Glasses: Ground States

- One of the most interesting problems for a spin glass is finding the minimum energy configuration, the *ground state*.

- **Definition.** The problem GROUND STATE is to find the minimum energy configuration given the necessary input to compute the Hamiltonian of the system.

- The model presented above is usually too general for analysis in any manner, which is why simpler forms are usually analysed.

Spin Glasses: Ising Models

- In the ising model the spins s_i are restricted to $s_i = \pm 1$.

- Consider a graph $G_N = (V, E)$ with N vertexes.

- Each vertex $i \in V$ is associated with magnetic spin s_i.

- Each edge $\{i, j\}$ is labelled with a coupling constant J_{ij}.

- The energy of a state $s = (s_1, s_2, \ldots, s_N)$ is given by:

$$H(s) = -\sum_{\{i,j\} \in E} J_{ij} s_i s_j.$$

Ising Models: Relation to Cuts

- Let $C^+ = \{i | s_i = 1\}$ and $C^- = \{i | s_i = -1\}$.

- Let E^+ be the edges with endpoints only in C^+ and E^- in C^- respectively. The edges which go between the two partitions are denoted $E^{\pm}$.

- The *weight* of a cut $C = (C^+, C^-)$ is defined as

$$weight(C) = \sum_{\{i,j\} \in E^{\pm}} J_{ij}$$

Ising Models: Relation to Cuts

- Using $weight(C)$ the Hamiltonian can be rewritten

$$
\begin{aligned}
H(C) = & \quad - \sum_{\{i,j\} \in E^+} J_{ij} - \sum_{\{i,j\} \in E^-} J_{ij} - \sum_{\{i,j\} \in E^\pm} J_{ij} = \\
= & \quad - \sum_{\{i,j\} \in E} J_{ij} + 2 weight(C)
\end{aligned}
$$

- MINIMUM WEIGHT CUT is NP-complete $\rightarrow$ GROUND STATE is NP-complete.

Ising Models: Partition Functions

- Physicists are also interested in the so called *partition function*. It is defined as

$$Z = \sum_{\{s\}} exp(-\beta H(s)).$$

- The partition function in one sense completely characterises the system.

- With knowledge of the partition function the ground state among other things can effectively be computed.

- Consequently it is at least as hard as finding the ground state.

- A naive approach to solving to compute the partition function would require 2^N summations.

Ising Models: Partition Functions

- Analytical exact solutions are available for 1-D and planar 2-D geometries.

- Finding generalisations turned out to be impossible.

- MINIMUM WEIGHT CUT problem is polynomial when the graph is planar

- **Theorem. (Istrail)** Finding the partition function is NP-hard for every non-planar crystal lattice.

Ising Models: Limit Solutions

- By assigning a probability distribution to the set of states in the system, the methods of statistical mechanics (S& M ;))are available.

- $$P(s) = exp(-\beta H(s))/Z$$

- Results apply in the limit $N \rightarrow \infty$ (*thermodynamical limit*).

- The coupling constants adhere to some probability distribution

- Example result: if J_{ij} is 1 or -1 with equal probability the minimum of the Hamiltonian takes on the value $-.7633N^{3/2}$.

N-K Landscapes: Introduction

- Introduced by Stuart Kauffmann.
- A family of landscapes where the ruggedness – the number of local optima – could easily be tuned.
- Applications: protein folding, evolutionary computation, models of genotype evolution, etc.

N-K Landscapes: Definitions

- The N-K model can be seen as a simple way of generating a tunable fitness function on bit strings, $\mathbf{x} = x_1 x_2 \ldots x_N$.

- A fitness function f is constructed by generating N component functions f_i.

- Each f_i depends on $K + 1$ bits.

- The fitness function f is the average of the component functions.

$$f(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^{N} f_i(x_{i_1}, x_{i_2}, \ldots, x_{i_{K+1}})$$

- Moving in the landscape is done by flipping a single bit of the input string.

N-K Landscapes: Variations

- In the *adjacent* model f_i depends on i:th bit and K adjacent bits.

- In the *random* model f_i depends on the i:th bit and K other randomly chosen bits.

- In the *arbitrary* model f_i depends on $K + 1$ randomly chosen bits.

- The values for the component functions are constructed by for each function sampling 2^{K+1} values from a random distribution, which usually is Gaussian.

N-K Landscapes: Properties

- For the case K=0, each component function is independent of the other functions. A simple hill climbing algorithm will find the unique optimum.

- In case when $K = N - 1$ each component function is dependent an all of the bits of the string.

- Each bit string is statistically independent of its neighbours.

- - The probability that a random bit string is a local optimum is $\frac{1}{N+1}$.
  - The expected number of local optima is $\frac{2^N}{N+1}$.
  - A hill climbing algorithm is expected to hit a local optimum in $ln(N-1)$ steps.

N-K Landscapes: Properties

- When $1 \leq K < N-1$ the component functions depend on some but not all bits in the string.
  - When K is small, many of the bits are the same for the highest local optima. This correlation decreases when K is increased.
  - The average Hamming distance between local optima is approximately

$$\frac{N log_2(K+1)}{2(K+1)}.$$

N-K Landscapes: Complexity

- **Theorem. (Weinberger)** The N-K optimisation problem with adjacent neighbourhoods is solvable in $O(2^K N)$ steps and is thus in $\mathcal{P}$.

- For arbitrary neighbourhoods, i.e. when f_i can depend on any bits, the problem is difficult for $K \geq 1$. The problem can be reduced to the NP-complete problem MAX2SAT. **Theorem.** The N-K optimisation problem with random neighbourhoods is polynomial for $K = 1$.

- **Theorem.** The N-K optimisation problem with random neighbourhoods is NP-complete for $K \geq 2$. (Reduction to MAX2SAT possible again)

- **Theorem.** The approximation threshold for the algorithm with $K \geq 2$ is at most $1 - \frac{1}{2^{K+1}}$.

N-K Landscapes: Approximation

function N-K-OPTIM () : (bit string) $=$

for i **from** 0 **to** $N-1$ **do**

$S_0 \leftarrow$ subset of S where the i:th bit is 0

$M_0 \leftarrow$ average of f over S_0

$S_1 \leftarrow$ subset of S where the i:th bit is 1

$M_1 \leftarrow$ average of f over S_1

if $M_0 > M_1$ **then**

$s[i] \leftarrow 0$

$S \leftarrow S_0$

else

$s[i] \leftarrow 1$

$S \leftarrow S_1$

od

return s //Return the approximate string

Optimisation Problems: Introduction

- In the following we will discuss two well-known optimisation problems: travelling salesman (TSP) and ASSIGNMENT.

- The problems are in many ways similar but they have crucial difference.

- TSP is NP-complete while ASSIGNMENT is in P.

Optimisation Problems: TSP

- An instance of the travelling salesman problem is an $n \times n$ matrix (a_{ij}), where each $a_{ij} \geq 0$.

- The problem is to find the permutation π of $\{1, \ldots, N\}$ such that $C(\pi) = \sum_{i=1}^{n} a_{\pi(i),\pi(i+1)}$ (where by $\pi(n+1)$ we mean $\pi(1)$) is minimised.

- TSP belongs to the category problems for which no polynomial approximation scheme is possible unless $P = NP$

TSP: Spin Glass Analysis

- TSP was one the first combinatorial optimisation problems to which the probabilistic methods developed for spin glasses were applied.

- The links a_{ij} are considered as uniformly distributed random variables on $[0, 1]$

- The cost function $C(\pi)$ is interpreted as the Hamiltonian.

- The tours have a probability according to the formula above.

- Result: the length of the tour, with probability one, is in the large limit $l = 2.08$.

- The result has been corroborated with numerical simulations.

TSP: Landscape

- Stadler and Schnabl have studied statistical properties of the TSP landscape for both the symmetric and the asymmetric case.

- Two different neighbourhoods are studied: transpositions and inversions.

- The study used random walks and other statistical analysis to examine the landscapes

- Symmetric case: TSP generates an AR(1) landscape.

- Asymmetric case: When transpositions are used it is once again an AR(1) landscape. With inversion it is more complex.

ASSIGNMENT: Definition

- An instance of ASSIGNMENT is a $n \times n$ matrix (a_{ij}) where $a_{ij} \geq 0$.

- The problem is to find a permutation π on $\{1, 2, \ldots, n\}$ such that

$$E_n^* = \sum_{i=1}^{n} ai, \pi(i)$$

  is minimised.

- The formulation is very similar to TSP.

ASSIGNMENT: Spin Glass Analysis

- Let the a_{ij} be drawn from a common probability density $\rho(a)$
- E_n^* corresponds to the Hamiltonian.
- It has been proved that

$$lim_{n\to\infty}\langle E_n^*\rangle = \frac{\pi^2}{6}.$$

- When the a_{ij} are drawn from an exponential distribution it has been shown that in the finite case the average optimum is

$$\langle E_n^*\rangle = \sum_{k=1}^{n} \frac{1}{k^2}.$$

ASSIGNMENT: Landscape

- As the permutation can be arbitrary in matching there several possibilities for neighbourhoods.

- Examples include transposition, composition with another permutation, etc.

- The correlation of the landscape is the same as for TSP.