Elementary Landscape Decomposition of Combinatorial Optimization Problems

Francisco Chicano

Work in collaboration with L. Darrell Whitley
Motivation

• Landscapes’ theory is a tool for analyzing optimization problems

• Peter F. Stadler is one of the main supporters of the theory

Towards a Theory of Landscapes

Peter F. Stadler

Institut für Theoretische Chemie, Universität Wien.
Währingerstraße 17, A-1090 Wien, Austria

Santa Fe Institute.
1399 Hyde Park Rd., Santa Fe, NM 87501, USA

• Applications in Chemistry, Physics, Biology and Combinatorial Optimization

• Central idea: study the search space to obtain information

  • Better understanding of the problem
  
  • Predict algorithmic performance
  
  • Improve search algorithms
A landscape is a triple \((X,N,f)\) where:

- \(X\) is the solution space
- \(N\) is the neighbourhood operator
- \(f\) is the objective function

The pair \((X,N)\) is called configuration space.

The neighbourhood operator is a function \(N : X \rightarrow \mathcal{P}(X)\).

Solution \(y\) is neighbour of \(x\) if \(y \in N(x)\).

Regular and symmetric neighbourhoods:

- \(d = |N(x)| \quad \forall x \in X\)
- \(y \in N(x) \iff x \in N(y)\)

Objective function:

\(f : X \rightarrow R\) (or \(N, Z, Q\)).
An elementary function is an eigenvector of the graph Laplacian (plus constant)

Adjacency matrix

\[ A_{xy} = \begin{cases} 
1 & \text{if } y \in N(x) \\
0 & \text{otherwise} 
\end{cases} \]

Degree matrix

\[ D_{xy} = \begin{cases} 
|N(x)| & \text{if } x = y \\
0 & \text{otherwise} 
\end{cases} \]

Graph Laplacian:

\[ \Delta = A - D \]

Depends on the configuration space

Elementary function: eigenvector of \( \Delta \) (plus constant)

\[ \Delta (f - b) = \lambda (f - b) \]

Eigenvalue
• An elementary landscape is a landscape for which

\[
\text{avg}\{ f(y) \} = \alpha f(x) + \beta \quad \forall x \in X
\]

where

\[
\text{avg}\{ f(y) \} = \frac{1}{d} \sum_{y \in N(x)} f(y)
\]

• Grover’s wave equation

\[
\text{avg}\{ f(y) \} = f(x) + \frac{k}{d} (\bar{f} - f(x)) \quad \forall x \in X
\]

Characteristic constant: \( k = -\lambda \)
Some properties of elementary landscapes are the following

\[ f(x) < \min_{y \in N(x)} \left\{ \text{avg}\{f(y)\}, f(y) \right\} \quad \text{or} \quad f(x) > \max_{y \in N(x)} \left\{ \text{avg}\{f(y)\}, f(y) \right\} \]

where \( f(x) \neq \bar{f} \)

- **Local maxima and minima**
## Elementary Landscapes: Examples

<table>
<thead>
<tr>
<th>Problem</th>
<th>Neighbourhood</th>
<th>d</th>
<th>k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Symmetric TSP</td>
<td>2-opt</td>
<td>n(n-3)/2</td>
<td>n-1</td>
</tr>
<tr>
<td></td>
<td>swap two cities</td>
<td>n(n-1)/2</td>
<td>2(n-1)</td>
</tr>
<tr>
<td>Antisymmetric TSP</td>
<td>inversions</td>
<td>n(n-1)/2</td>
<td>n(n+1)/2</td>
</tr>
<tr>
<td></td>
<td>swap two cities</td>
<td>n(n-1)/2</td>
<td>2n</td>
</tr>
<tr>
<td>Graph α-Coloring</td>
<td>recolor 1 vertex</td>
<td>(α-1)n</td>
<td>2α</td>
</tr>
<tr>
<td>Graph Matching</td>
<td>swap two elements</td>
<td>n(n-1)/2</td>
<td>2(n-1)</td>
</tr>
<tr>
<td>Graph Bipartitioning</td>
<td>Johnson graph</td>
<td>n^2/4</td>
<td>2(n-1)</td>
</tr>
<tr>
<td>NEAS</td>
<td>bit-flip</td>
<td>n</td>
<td>4</td>
</tr>
<tr>
<td>Max Cut</td>
<td>bit-flip</td>
<td>n</td>
<td>4</td>
</tr>
<tr>
<td>Weight Partition</td>
<td>bit-flip</td>
<td>n</td>
<td>4</td>
</tr>
</tbody>
</table>
Landscape Decomposition

- What if the landscape is not elementary?
- Any landscape can be written as the sum of elementary landscapes

There exists a set of eigenfunctions of $\Delta$ that form a basis of the function space (Fourier basis)

Elementary functions (from the Fourier basis)

Non-elementary function

Elementary components of $f$
• If $X$ is the set of binary strings of length $n$ and $N$ is the bit-flip neighbourhood then a Fourier basis is

$$\{\psi_w\} \quad w \in \{0, 1\}^n$$

where

$$\psi_w(x) = (-1)^{bc(w \land x)} = \prod_{i=1}^{n}(-1)^{x_i w_i}$$

• These functions are known as Walsh Functions

• The function with subindex $w$ is elementary with $k = 2 \ bc(w)$

• In general, decomposing a landscape is not a trivial task → methodology required
### Landscape Decomposition: Examples

<table>
<thead>
<tr>
<th>Problem</th>
<th>Neighbourhood</th>
<th>d</th>
<th>Components</th>
</tr>
</thead>
<tbody>
<tr>
<td>General TSP</td>
<td>inversions</td>
<td>$\frac{n(n-1)}{2}$</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>swap two cities</td>
<td>$\frac{n(n-1)}{2}$</td>
<td>2</td>
</tr>
<tr>
<td>QAP</td>
<td>swap two elements</td>
<td>$\frac{n(n-1)}{2}$</td>
<td>3</td>
</tr>
<tr>
<td>Frequency Assignment</td>
<td>change 1 frequency</td>
<td>$(\alpha-1)n$</td>
<td>2</td>
</tr>
<tr>
<td>Subset Sum Problem</td>
<td>bit-flip</td>
<td>n</td>
<td>2</td>
</tr>
<tr>
<td>MAX k-SAT</td>
<td>bit-flip</td>
<td>n</td>
<td>k</td>
</tr>
<tr>
<td>NK-landscapes</td>
<td>bit-flip</td>
<td>n</td>
<td>$k+1$</td>
</tr>
<tr>
<td>Radio Network Design</td>
<td>bit-flip</td>
<td>n</td>
<td>max. nb. of reachable antennae</td>
</tr>
</tbody>
</table>
Selection operators usually take into account the **fitness value** of the individuals.

We can improve the selection operator by selecting the individuals according to the **average value** in their neighbourhoods.
In elementary landscapes the traditional and the new operator are the same!

Recall that...

$$\text{avg}\{f(y)\} = \alpha f(x) + \beta \quad \forall x \in X$$

However, they are not the same in non-elementary landscapes. If we have $n$ elementary components, then:

$$\text{avg}\{f(y)\} = \alpha_0 + \alpha_1 f(x) + \sum_{i=2}^{n} \alpha_i f_i(x) \quad \forall x \in X$$

The new selection strategy could be useful for plateaus.
Let \( \{x_0, x_1, \ldots\} \) a simple random walk on the configuration space where \( x_{i+1} \in N(x_i) \).

The random walk induces a time series \( \{f(x_0), f(x_1), \ldots\} \) on a landscape.

The autocorrelation function is defined as:

\[
r(s) = \frac{\langle f(x_t) f(x_{t+s}) \rangle_t - \langle f \rangle^2}{\langle f^2 \rangle - \langle f \rangle^2}
\]

The autocorrelation length is defined as:

\[
l = \sum_{s=0}^{\infty} r(s)
\]

Autocorrelation length conjecture:

The number of local optima in a search space is roughly

\[
M \approx \frac{|X|}{|X(x_0, l)|}
\]

Solutions reached from \( x_0 \) after \( l \) moves
The higher the value of $l$, the smaller the number of local optima and the better the performance of a local search method.

$l$ is a measure of the ruggedness of a landscape.

### Autocorrelation Length Conjecture

<table>
<thead>
<tr>
<th>Length</th>
<th>Ruggedness</th>
<th>Nb. steps (config 1)</th>
<th>Nb. steps (config 2)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>% rel. error</td>
<td>nb. steps</td>
</tr>
<tr>
<td>10 ≤ $\zeta$ &lt; 20</td>
<td>0.2</td>
<td>50500</td>
<td>0.1</td>
</tr>
<tr>
<td>20 ≤ $\zeta$ &lt; 30</td>
<td>0.3</td>
<td>53300</td>
<td>0.2</td>
</tr>
<tr>
<td>30 ≤ $\zeta$ &lt; 40</td>
<td>0.3</td>
<td>58700</td>
<td>0.2</td>
</tr>
<tr>
<td>40 ≤ $\zeta$ &lt; 50</td>
<td>0.5</td>
<td>62700</td>
<td>0.3</td>
</tr>
<tr>
<td>50 ≤ $\zeta$ &lt; 60</td>
<td>0.7</td>
<td>66100</td>
<td>0.4</td>
</tr>
<tr>
<td>60 ≤ $\zeta$ &lt; 70</td>
<td>1.0</td>
<td>75300</td>
<td>0.6</td>
</tr>
<tr>
<td>70 ≤ $\zeta$ &lt; 80</td>
<td>1.3</td>
<td>76800</td>
<td>1.0</td>
</tr>
<tr>
<td>80 ≤ $\zeta$ &lt; 90</td>
<td>1.9</td>
<td>79700</td>
<td>1.4</td>
</tr>
<tr>
<td>90 ≤ $\zeta$ &lt; 100</td>
<td>2.0</td>
<td>82400</td>
<td>1.8</td>
</tr>
</tbody>
</table>

Angel, Zissimopoulos. *Theoretical Computer Science* 264:159-172
Autocorrelation and Landscapes

- If $f$ is a sum of elementary landscapes:

  \[ r(s) = \sum_{i \neq 0} \frac{a_i^2}{\sum_{j \neq 0} a_j^2} \left( 1 - \frac{k_i}{d} \right)^s \]

  \[ l = \sum_{i \neq 0} \frac{d a_i^2}{k_i \sum_{j \neq 0} a_j^2} \]

- For elementary landscapes:

  \[ r(s) = \left( 1 - \frac{k}{d} \right)^s \]

  \[ l = \frac{d}{k} \]

- Using the landscape decomposition we can determine \textit{a priori} the performance of a local search method.
Conclusions & Future Work

Conclusions

• Elementary landscape decomposition is a useful tool to understand a problem
• The decomposition can be used to design new operators
• We can exactly determine the autocorrelation functions
• It is not easy to find a decomposition in the general case

Future Work

• Methodology for landscape decomposition
• Search for additional applications of landscapes’ theory in EAs
• Design new operators and search methods based on landscapes’ information
Thanks for your attention !!!