Saddles and Barriers in Lanscapes of Generalized Search Operators

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Characterization of Landscapes

A landscape is a triple $(\mathbb{X}, N, f)$

$\mathbb{X}$	set of configurations.
$N : \mathbb{X} \to P(\mathbb{X})$	neighborhood function.
$f : \mathbb{X} \to \mathbb{R}$	cost or fitness function.

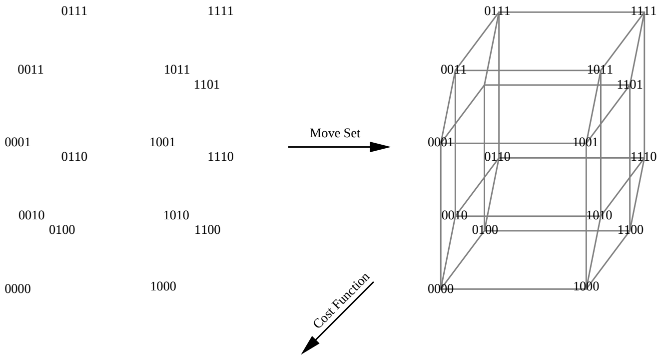
The neighborhood function is typically defined by a move set.

Speed of optimization depends on the roughness of the Landscape.

Measures of roughness suggested in the literature:

- Number of local optima
- Correlation lengths (e.g. along a random walk)
- Lengths of adaptive walks
- Folding temperature vs. glass temperature T_f / T_g
- Energy barriers between the local optima. Especially, the maximum barrier height ("depth" in SA literature)

From Configurations to a Landscape



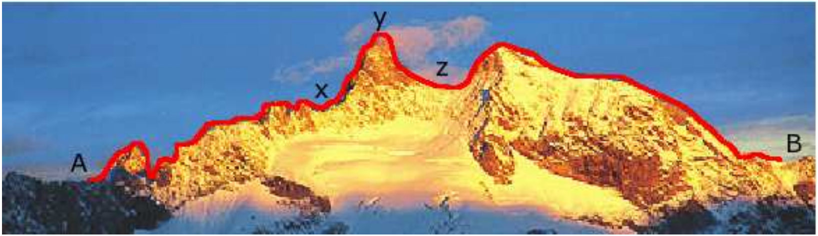
Move set:	point mutation
Cost function:	spin-glas hamiltonian

A Path in a Landscape

A path in a landscape is a ordered list of configurations.

$$\pi = \{x_1, x_2, \ldots, x_n\} \text{ such that } x_j \in \mathbb{X} \wedge x_{j+1} = N(x_j); \forall j$$

Note that a path depends on the neighborhood function!

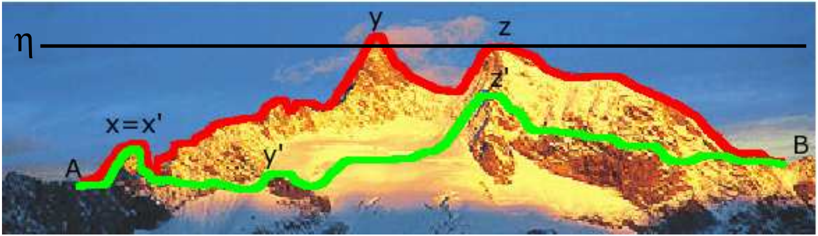


Example (path)

1. $N(y) = \{x, y, z\}$
2. path from A to B $\pi = \{A, \ldots, x, y, z, \ldots, B\}$

Path-Connectedness: Accessibility in a Landscape

A configuration y is accessible from x on level η if there is a path $\pi \in P_{xy}$ such that $f(z) \leq \eta; \forall z \in \pi$



Example ($A \overset{\eta}{\leftrightarrow} B$)

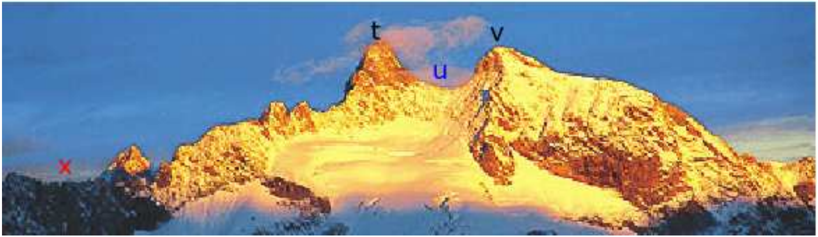
$\pi = \{A, x, y, z, B\}$
$f(x) < \eta$
$f(y) > \eta$

$\Rightarrow$ B is not accessible from A

$\pi = \{A, x', y', z', B\}$
$f(x') < \eta$
$f(y') < \eta$
$f(z') \leq \eta$
$\Rightarrow$ B is accessible from A

Minima in a Landscape

- x is a **local minimum** if $f(x) \leq f(y); \forall y \in N(x)$
- x is a **global minimum** if $f(x) \leq f(y); \forall y \in \mathbb{X}$



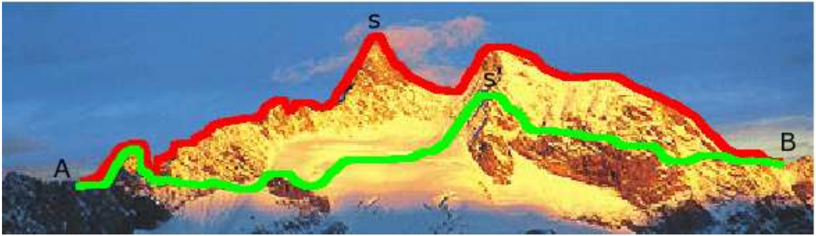
Example (local/global minimum)

$f(u) \leq f(t) \wedge f(u) \wedge f(v)$ $f(u) \leq f(n); \forall n \in N(u)$ $\Rightarrow$ u is a local minimum $\exists\ f(x) < f(u)$ $\Rightarrow$ not a global minimum!	$f(x) \leq f(n); \forall n \in \mathbb{X}$ $\Rightarrow$ x is the global minimum

Saddle Points in a Landscape

A **saddle point** between two minima is the highest cost configuration on the lowest cost path between the two minima.

$$\widehat{f}[x, y] = \min_{\pi \in P_{xy}} \max_{s \in \pi} f(s)$$



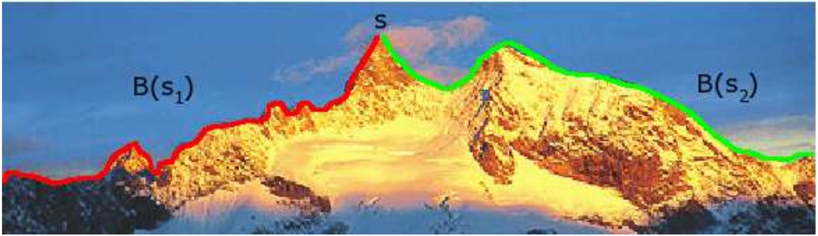
Example ($\widehat{f}[A, B]$)

1. find the $\max_{s \in \pi} f(s)$ of each path from A to B
   $\Rightarrow$ s and s'
2. take the min path (lowest saddle point) between A and B
   $\Rightarrow$ s' is the saddle point between A and B

Basin of Attraction in a Landscape

To each saddle point S there is a unique collection of configurations $B(S)$ reachable by a path that never exceeds $f(S)$.

$$B(s) = \{x \in \mathbb{X} | x \overset{f(S)}{\longleftrightarrow} S \text{ and } f(x) < f(S)\}$$

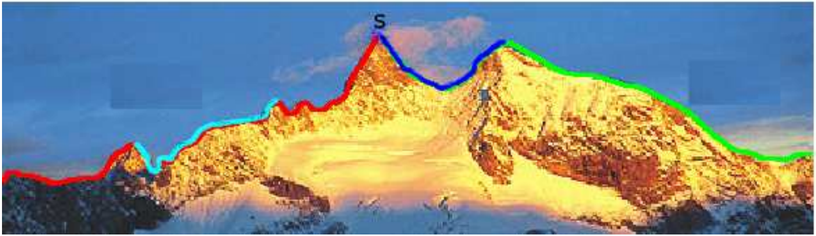


Note: the configurations in a basin of attraction $B(s)$ are mutually connected by paths that never go higher than f(s)!

From Basins to a Hierarchical Structure

Two situations can arise for any two saddle points S and S' with $f(S) < f(S')$:

1. $B(S)$ is a sub-basin of $B(S')$
2. The two basins are disjoint.

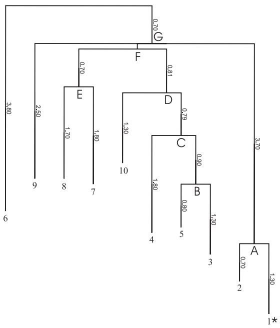


This property arranges the minima and saddle points in a unique hierarchical structure termed barrier tree.

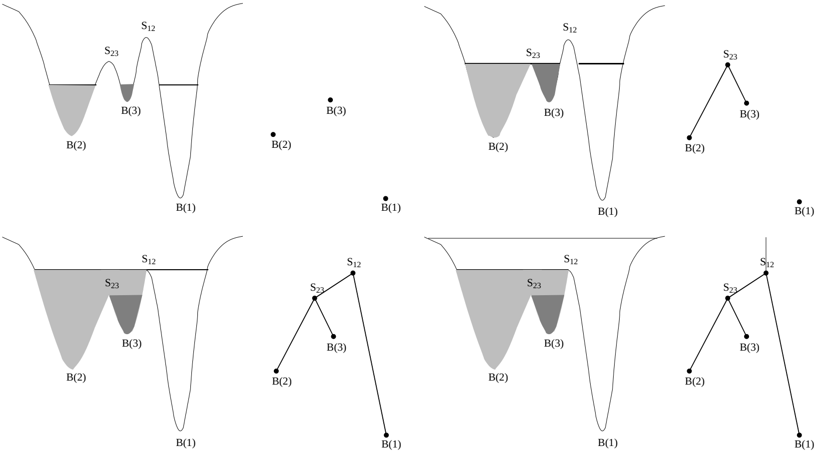
Energy Barriers and Barrier Trees

Some topological definitions:
A configuration is a

- local minimum if its cost is lower than the cost of **all** neighbors
- local maximum if its cost is higher than the cost of **all** neighbors
- saddle point if there are at least two local minima that can be reached by a downhill walk starting at this point



The Flooding Algorithm: Construction of Barrier Trees



Information from the Barrier Trees

- Local minima
- Saddle points
- Barrier heights
- Gradient basins
- Partition functions and free energies of (gradient) basins
- Depth and Difficulty of the landscape

A gradient basin is the set of all initial points from which a gradient walk (steepest descent) ends in the same local minimum.

Depth and Difficulty

$$\mathrm{D} = \max\left\{ B(s) \middle| s \text{ is not a global minimum } \right\}$$

$$\psi = \max\left\{ \frac{B(s)}{f(s) - f(\min)} \middle| s \text{ is not a global minimum} \right\}$$

Recombination Spaces

The search space for variation operators that depand on a single parent has the structure of a graph.

The analog of the adjacency relation for variation operators that depend on two parents is the *recombination set*.

$\mathcal{R}(x, y)$ is defined as the set of all possible recombinants of two parents x and y.

1. $\{x, y\} \in \mathcal{R}(x, y)$
2. $\mathcal{R}(x, y) = \mathcal{R}(y, x)$
3. $\mathcal{R}(x, x) = \{x\}$
4. $\mathcal{R}(x, y) \subseteq \mathrm{span}\{x, y\}$

Closure Function

The set of points in X that are **accessible** from A can be described by a closure function $\mathrm{cl} : \mathcal{P}(X) \to \mathcal{P}(X)$

$$c_{\mathcal{R}}(A) = \bigcup_{x,y \in A} \mathcal{R}(x, y)\,.$$

Axioms for Topological Spaces:

(K0) $\mathrm{cl}(\emptyset) = \emptyset$.

(K1) $A \subseteq B$ implies $\mathrm{cl}(A) \subseteq \mathrm{cl}(B)$ (isotonic).

(K2) $A \subseteq \mathrm{cl}(A)$ (expanding).

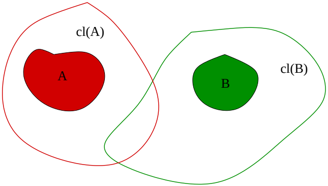
(K3) $\mathrm{cl}(A \cup B) \subseteq \mathrm{cl}(A) \cup \mathrm{cl}(B)$ (sub-additive).

(K4) $\mathrm{cl}(\mathrm{cl}(A)) = \mathrm{cl}(A)$ (idempotent).

Neighborhood Spaces satisfy K0 - K2. (recombination spaces)
Finite Graphs satisfy K0 - K3. (mutation only models)

Connectedness in Neighborhood Spaces

Two sets $A, B \in \mathcal{P}(X)$ are **semi-seperated** if $\text{cl}(A) \cap B = \text{cl}(B) \cap A = \emptyset$



A subset A of X is **connected** if it cannot be decomposed into two non-empty semi-separated sets.

1. Individual points $\{x\}$ are always connected.
2. If A, B are connected and $A \cap B \neq \emptyset$ then $A \cup B$ is connected.
3. If A is connected then $\text{cl}(A)$ is connected.
4. Let $A_\imath$ be a collection of of connected sets with $x \in A_\imath$ for all $\imath$, than $\bigcup_\imath A_\imath$ is also connected.

The unique maximally connected subset of A that contains point x

$$A[x] = \bigcup \{ Z \subseteq A \big| x \in Z \text{ and } Z \text{ is connected} \}$$

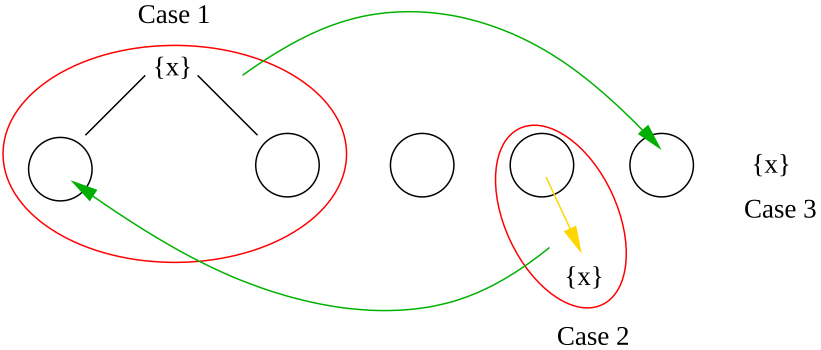
Structure of in Neighborhood Spaces

The collection $\{A[x] | x \in X\}$ defines a partition of the set A in terms of maximally connected components.

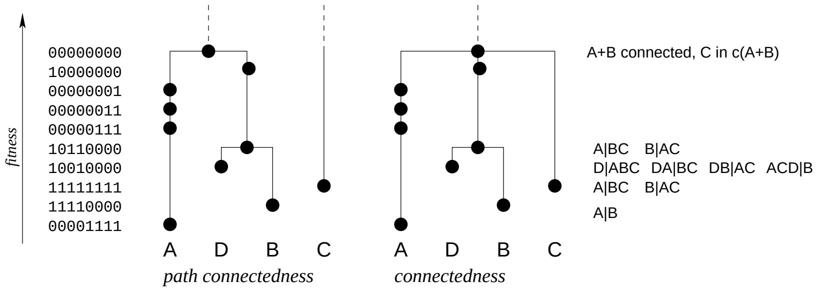
The closer space $(X, c_{\mathcal{R}})$ is disconnected i.e $X[x] = \{x\}$.

If the closure function is a superpositon of mutation and recombination the closure space is a **digraph**.

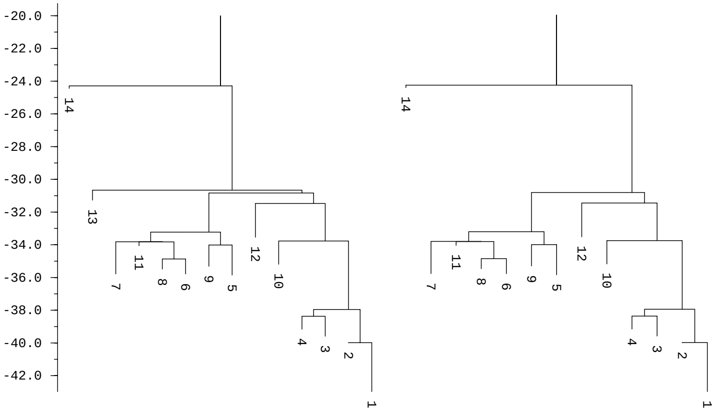
Modified Flooding Algorithm



Schematic Example



Example I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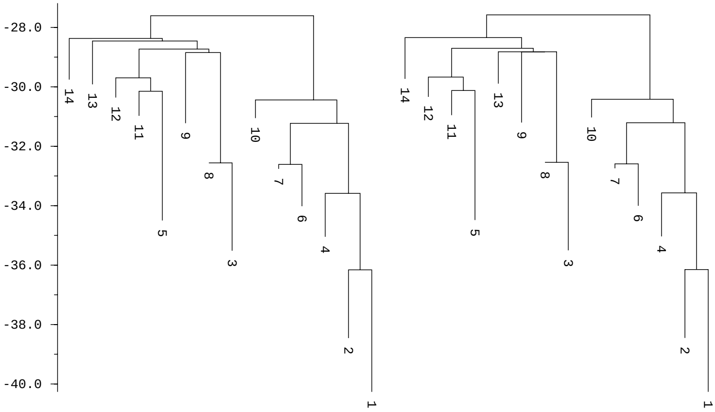
Example II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