

# Self-Organizing Maps Which Utilize Imposed Tree-Based Topologies

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# Outline

- 1 Introduction
  - Kohonen's Self-Organizing Maps
  - Tree-Based Variants
- 2 The Tree-Based Topology-Oriented SOM (TTO-SOM)
  - Overview of the TTO-SOM
  - Input and Parameters
  - Declaration of the User-Defined Tree
  - Neural Distance
  - Bubble of Activity
- 3 Experiments and Results
  - Learning the Structure
  - The Hierarchical Representation
  - Skeletonization
- 4 Adaptive Data Structures
- 5 Merging ADS and TTO-SOM

## What is the **Goal** of this Research?

- Merge two very rich fields of Computer Science.
  - Neural Networks (**Self-Organizing Maps**)
  - Adaptive Data Structures
- **Question**: Can the data structure we use **Control** anything?
- **Question**: Can we **Modify** the data structure as we train?

# What is the **Goal** of this Research?

- **Question:** What is more important
  - The Neural Network?
  - The Data Structure?
  - The technique for Modifying the latter?
- **Open Issues...**
  - Other Neural Networks?
  - Other Data Structures?
  - Other techniques for **Modifying** these?



# What is a SOM? What Does it Do?

- Artificial Neural Networks.
- Maps high dimensional spaces to 2D (or 3D).
- Used in clustering and visualization.
- Learns **stochastic** distribution of the data.
- Preserves the **topology** of the data.

## How does it work?

- Operates in two modes: **Training** and **Mapping**.
- Training: Uses **Unsupervised** learning.
- Mapping: Automatically classifies a new input vector.

# Vector Quantization

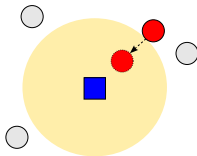
- Models probability density functions.
- Uses small subset of vectors – “**Prototypes**”.
- Useful for lossy data compression.
- Useful for density estimation/approximation.

# Winning Neuron

- Competitive Learning.
- Best Matching Unit (**BMU**).

$$s(x) = \arg \min_{c \in \mathcal{C}} \| x - v_c \|$$

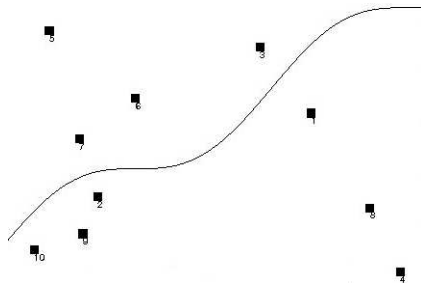
- BMU search may involve exploring all units.
- Neurons move towards the input point as below:



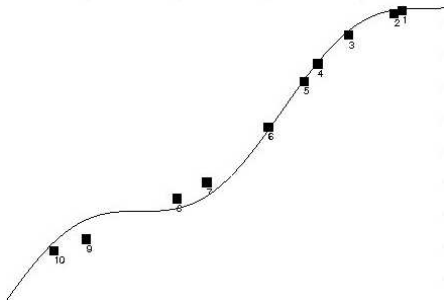
# Neighbors

- Units and edges constitute a network.
- A set of neurons “close” to the winner.
- Neighborhood function.
- Neighborhood “shrinks” with time.

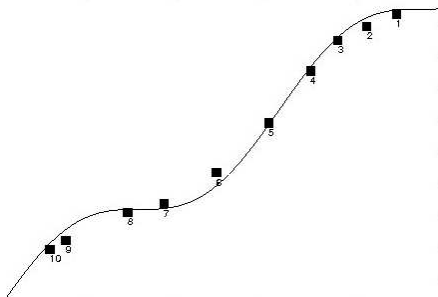
# SOM Example (1/5) – Initial Configuration



# SOM Example (2/5)

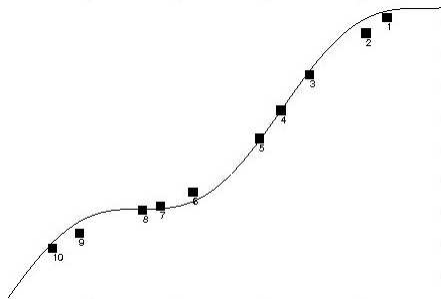


# SOM Example (3/5)

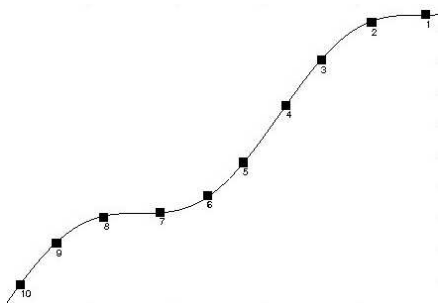




# SOM Example (4/5)



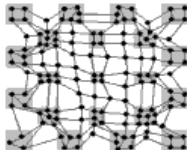
# SOM Example (5/5) – Final Configuration



Observe convergence: **Distribution** and **Topology**

## Known **Drawbacks** of the SOM.

- Nodes may converge to zero density areas.
- Finding the winner neuron is costly.
- Run many times to obtain suitable parameters.
- Few neurons often represent the data inaccurately.
- “Curse of Dimensionality”.



from L. Guan's paper

## Why Tree-Based Variants?

- Represent complicated data distributions more accurately.
- Speed up costly tasks (i.e., finding the winner neuron).

# Possible Properties of Tree-Based SOMs

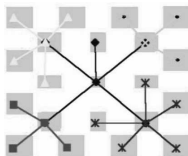
- **Dynamic/Static** tree.
- Distance in the **feature/tree** space.
- **Heuristic/Deterministic** winner search.
- “Frozen” neurons.
- SOMs arranged in layers.

# Tree-Based SOM Variants

- Self-Organizing Tree Maps (SOTM).
- Growing Hierarchical SOM (GHSOM).
- Tree Structured Vector Quantization (TSVQ).
- Evolving tree (ET).

# Self-Organizing Tree Maps (SOTM)

- Dynamic tree.
- Distance in the feature space.
- Distance threshold is used add nodes.



from L. Guan's paper

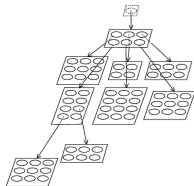
# Self-Organizing Tree Maps (SOTM)

- 1 Start with a single node
- 2 **Main Loop** (Repeat until Convergence)
  - 2.1 Obtain input
  - 2.2 Find BMU
  - 2.3.a If distance is greater than a threshold, create a new node
  - 2.3.b Else update BMU



# Growing Hierarchical SOM (GHSOM)

- Dynamic tree.
- SOMs arranged in layers.
- Error measure is used to add nodes.



GHSOM logo

# Growing Hierarchical SOM (GHSOM)

- 1 Start with a 2x2 SOM at layer-0
- 2 **Main Loop (Repeat until Convergence)**
  - 2.1 Train the SOM layer
  - 2.2 Calculate quantization error of each node ( $mqe$ )
  - 2.3 Calculate quantization error of the map (MQE)
  - 2.4.a If  $MQE > \text{threshold}$ , add row/column to SOM layer
  - 2.4.b If some unit contain  $mqe > \text{threshold}$ , create new SOM layer

# Tree Structured Vector Quantization (TSVQ)

- Static tree.
- “Frozen” neurons.
- Heuristic winner search.

# Tree Structured Vector Quantization (TSVQ)

- 1 Define tree structure
- 2 **Main Loop (Repeat until All Units are Frozen)**
  - 2.1 Find Best
    - 2.1.a If node is frozen select best child, call Find Best
    - 2.1.b Else return current node
  - 2.2 Update BMU
  - 2.3 If BMU is selected  $N$  times, it becomes frozen

# Evolving Tree (ET)

- Dynamic tree.
- Fixed number of children.
- “Frozen” neurons.
- Heuristic winner search.

# Evolving Tree (ET)

- 1 Start with a single node
- 2 **Main Loop (Repeat until All Units are Frozen)**
  - 2.1 Find Best Procedure
    - 2.1.a If node is frozen select best child, call Find Best Procedure
    - 2.1.b Else return current node
  - 2.2.a If node reaches threshold then Split
    - 2.2.a.1 node become frozen
    - 2.2.a.2 create/initialize  $k$  children
  - 2.3 Update BMU and neighbors

# Hierarchical SOM in the literature

- No clear winner.
- Opportunity for novel ideas is still open.

# The Tree-Based Topology-Oriented SOM (TTO-SOM)

- Static tree.
- Arbitrary **number** of children.
- Neighborhood based on tree space.
- Deterministic winner search.
- Winner search based on feature space.
- Infers both the data distribution and its structured topology.
- Generalization of the 1D SOM.



# Input and Parameters of the TTO-SOM

- Input
  - 1 Training sample set.
  - 2 Configuration of the  $k$ -ary tree.
- Parameters
  - 1 **Radius** of the Bubble of Activity.
  - 2 The SOM learning rate.

# The Radius

- The **Size** of the Bubble of Activity.
- Between 0 and the number of neurons.
- Its value should decrease as time proceeds.

# The Learning Rate

- Neurons should be moved toward the input signal.
- **Learning Rate**: The **Factor** of such a movement.
- Should decrease as convergence take place.

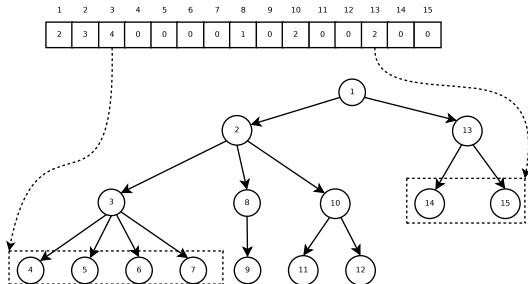
## Declaration of the User-Defined Tree

- The user describe the tree.
- Arbitrary number of children.
- Reflects *a priori* knowledge about the data distribution.
- Recursive definition.

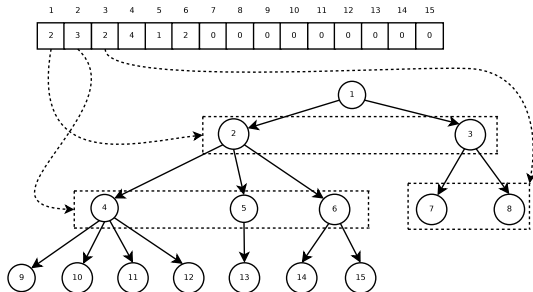
## Declaration of the User-Defined Tree

- Array specifying the number of children for each node.
- **Depth**-First/**Breadth**-First traversal.
- Index of the array: Node in the respective traversal.
- Content of the array: Number of children of each node.

# Example 1: Depth-First traversal



## Example 2: Breadth-First traversal



## Neural Distance Between Two Neurons...

### Definition

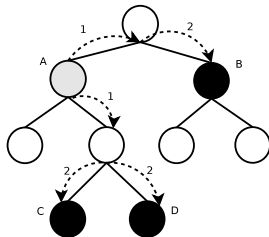
No. of edges in the shortest path connecting two given nodes.

- Depends on connections.
- Minimum Path.
- Includes non-leaf nodes.



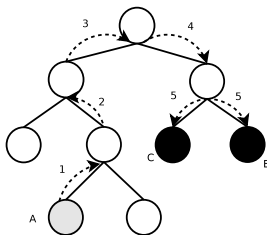
## Neural Distance: First example

- $B$ ,  $C$  and  $D$  are equidistant to  $A$ .
- $B$  and  $D$  are at different levels.
- $B$  is a non-leaf node.



## Neural Distance: Another example

- $B$  and  $C$  are at distance 5 to  $A$ .
- Distance from  $A$  to  $A$  is zero.



# The Bubble of Activity.

## Definition

Subset of nodes: Distance  $r$  away from the node examined.

- Intricately related to the notion of neural distance.
- Subset of nodes “close” to a given neuron.
- The **Radius** determines the size of the bubble.

# The Bubble of Activity.

## Formal Definition

$$B(v_i; T, r) = \{v | d_N(v_i, v; T) \leq r\}$$

Where,

$v_i$  The node currently being examined.

$v$  An arbitrary node in the tree  $T$ .

$d_N$  The neural distance.

$r$  The radius.

# The Bubble of Activity.

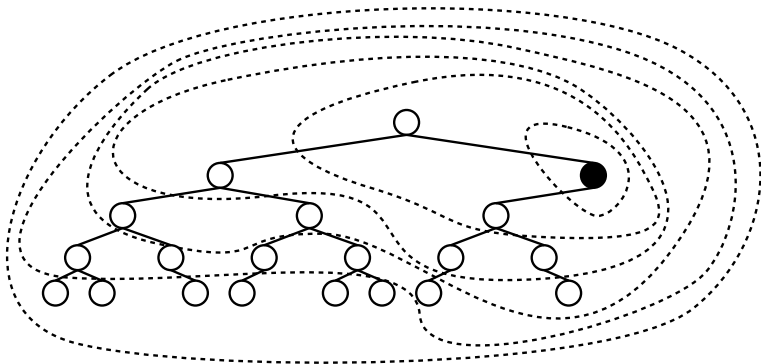
## Formal Definition

$$B(v_i; T, r) = \{v \mid d_N(v_i, v; T) \leq r\}$$

The Bubble of Activity also present the following properties:

- 1  $B(v_i, T, 0) = \{v_i\}$
- 2  $B(v_i, T, i) \supseteq B(v_i, T, i - 1)$
- 3  $B(v_i, T, |V|) = V$

# Bubble of Activity: An Example



# TTOSOM properties

- Static tree.
- Distance in the **Feature** space for winner search.
- Distance in the **Tree** space for bubble of activity.
- Deterministic winner search.

# TTOSOM Training Algorithm

- 1 Describe Topology
  - 1.1 Read next item in the array of children.
  - 1.2 Create children.
  - 1.3 Call Describe Topology recursively.
- 2 Main Loop (Repeat until Convergence)
  - 2.1 Receive input.
  - 2.2 Find BMU.
  - 2.3 Calculate Neighbors using neural distance.
  - 2.4 Move Neurons within the bubble of activity.
  - 2.5 Decrease radius/learning rate.



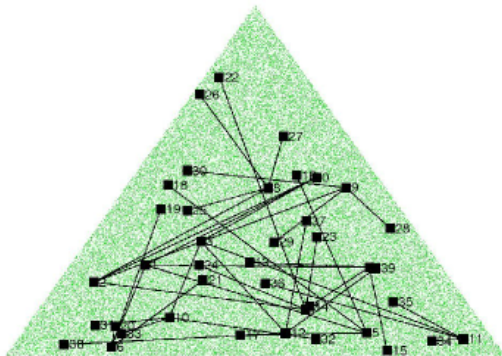
# TTOSOM Mapping Algorithm

- 1 Receive input.
- 2 Find BMU (in feature space).
- 3 Return BMU.

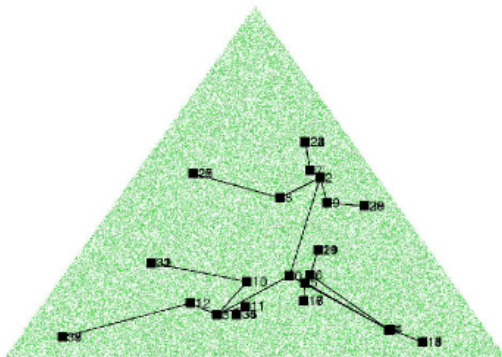
# Experiment 1: Triangular-Spaced Distribution

- Complete tree of 4 levels.
- Triangular shape.
- Capture essence of distribution.
- Define 3 children per node.

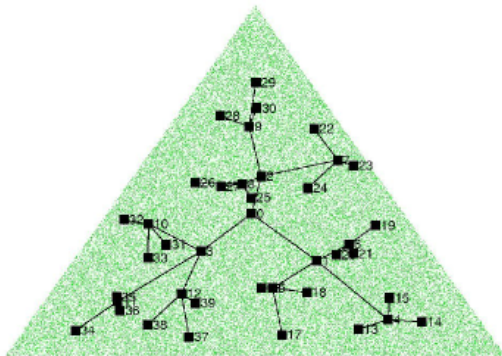
# Experiment 1: Triangular-Spaced Distribution



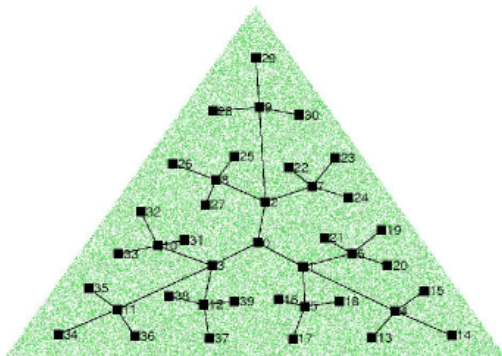
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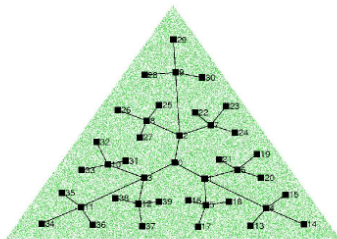


# Experiment 1: Triangular-Spaced Distribution



# Experiment 1: Triangular-Spaced Distribution

- The root roughly in the center.
- Each main branch towards a vertex.
- Sub-branches uniformly fill space around main branches.

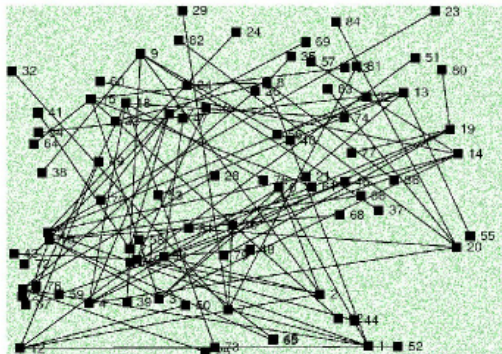


## Experiment 2: “Square-Shaped” Distribution

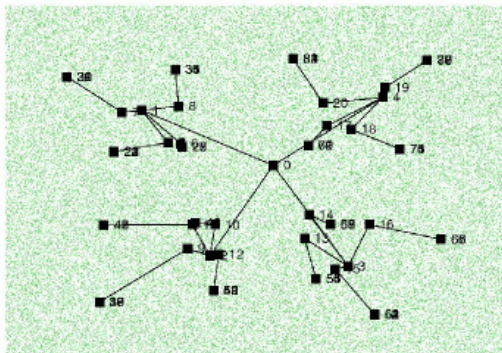
- Complete tree of depth 4.
- Rectangular shape.
- Capture essence of distribution.
- Define 4 children per node.



## Experiment 2: “Square-Shaped” Distribution

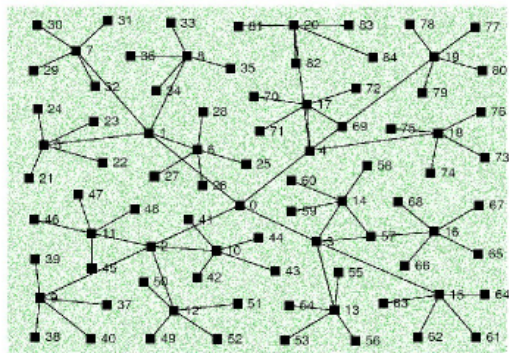


## Experiment 2: “Square-Shaped” Distribution



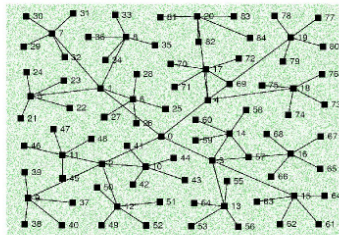


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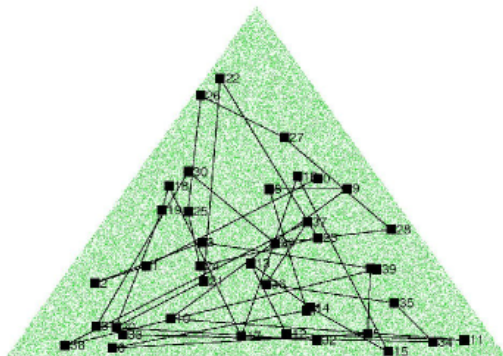
- Root near the center of mass.
- Main branches cover the principal diagonals.
- Sub-branches uniformly fill space around main branches.



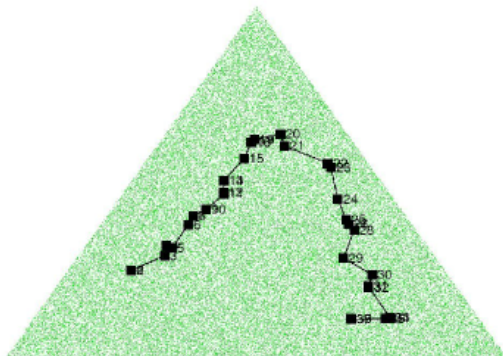
## Experiment 3: 1-ary tree

- Triangular shape.
- A list as the imposed topology.
- 1 children per node.

# Experiment 3: 1-ary tree

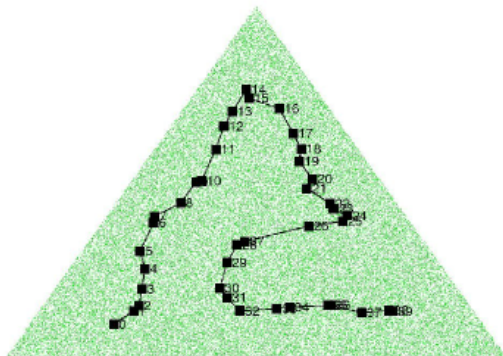


# Experiment 3: 1-ary tree

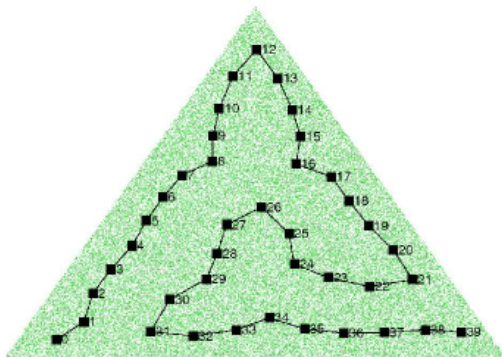




# Experiment 3: 1-ary tree

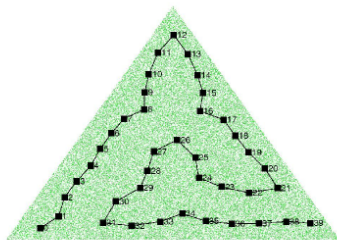


# Experiment 3: 1-ary tree



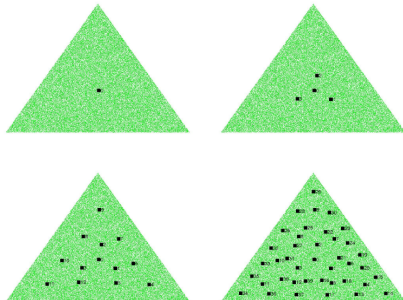
## Experiment 3: 1-ary tree

- The list represents the triangle effectively.
- Preserves “tree-like” topology.
- Generalization of 1D SOM.



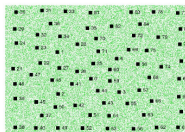
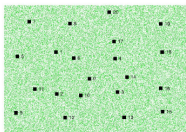
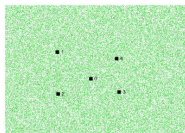
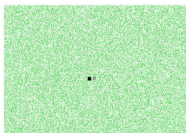
## Experiment 4: Multi-Resolution

- Hologram-like properties
- Not possessed by other SOM-based networks.
- Still represent the distribution and the structure.



## Experiment 5: Multi-Resolution

- Few level of the tree  $\rightarrow$  lower resolution.
- More levels of the tree  $\rightarrow$  finer resolution.



# Extracting the Skeleton of a Data Set

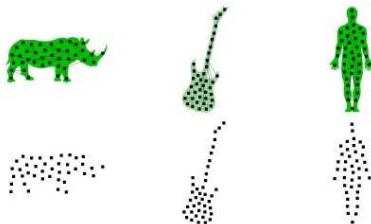
## Definition: Skeletonization

Process by which a 2D shape is transformed into 1D.

- Dimensionality reduction technique.
- Traditional skeletonization: Assumes pixel connectivity.
- SOM variations have been used to tackle this situation.
  - GNG-like approach.
  - MST calculated over neurons.

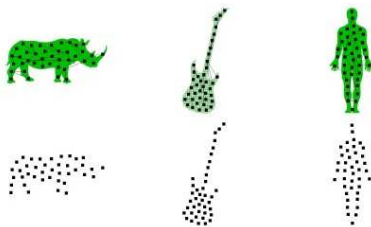
## Experiment 6: Skeletonization

- 3 objects processed using the same tree structure.
- Same schedule for parameters.
- No post processing of edges.



## Experiment 6: Skeletonization

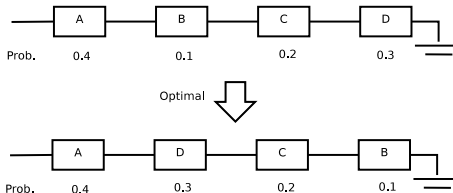
- Effectively represents 2D objects in 1D.
- Without any specific adaption.





# Adaptive Data Structures

- Optimal arrangement of nodes.
- Probability of accesses known  $\rightarrow$  Optimal Solution.
- We consider **unknown** probability of accesses.



## Adaptive Data Structures: Single Linked-List.

- Move-to-Head.
- Exchange Rule.

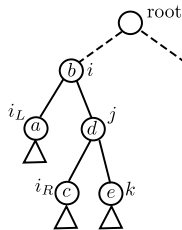
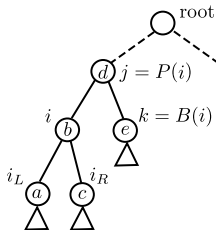
## Adaptive Data Structures: Trees.

- Move-to-Root.
- Exchange Rule.
- Conditional Rotations.
- Splay Trees.
- D-tree.
- Monotonic trees.

## Conditional Rotations

- Asymptotically produce an optimal tree.
- Rotations does not occur every step.
- **Only** if Weighted Path Length (WPL) is decreased.
- Rotation takes  $O(1)$ .
- Requires only 1 extra counter per node.

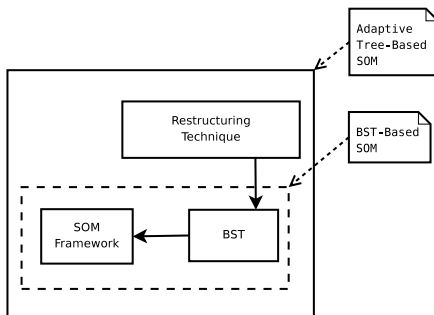
# Rotations for a Binary Search tree



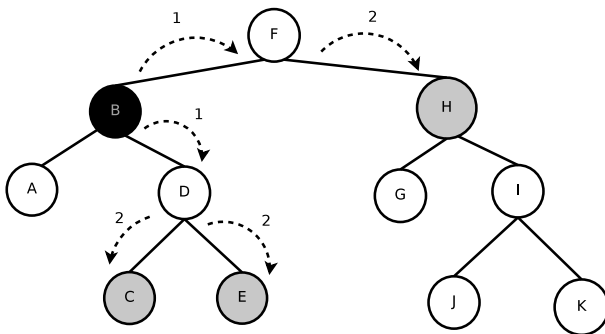
## Conditional Rotations: How?

- WPL is maintained for each node.
- On query: Update the visited nodes down on path.
- Stop once the node is found.
- Check if as a result of a rotation the WPL **Decreases**.
- Move node toward the root conditionally.

# ADS-TTOSOM Architecture

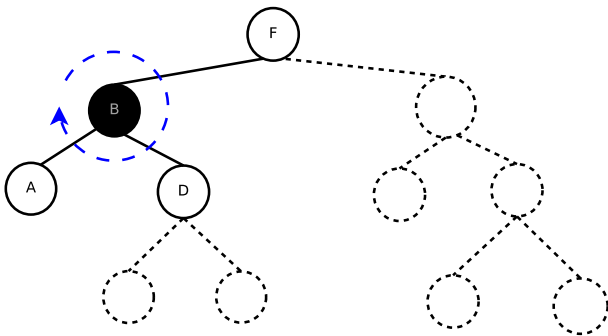


# Neural Distance – TTO-CONROT

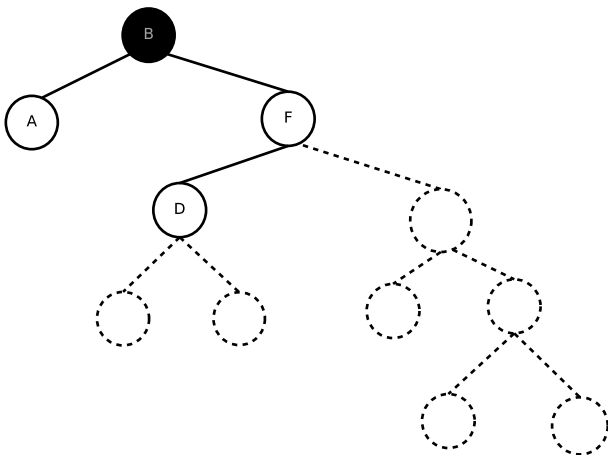




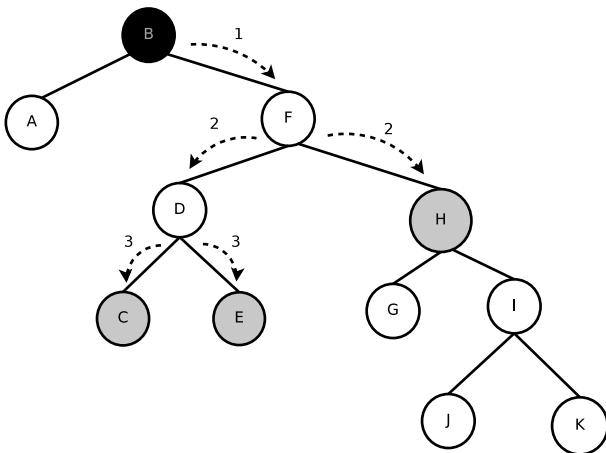
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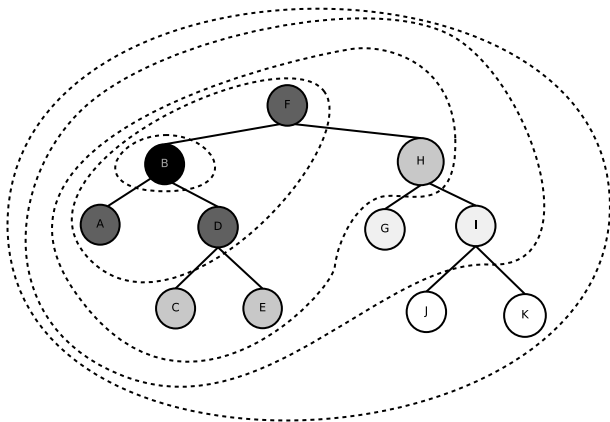
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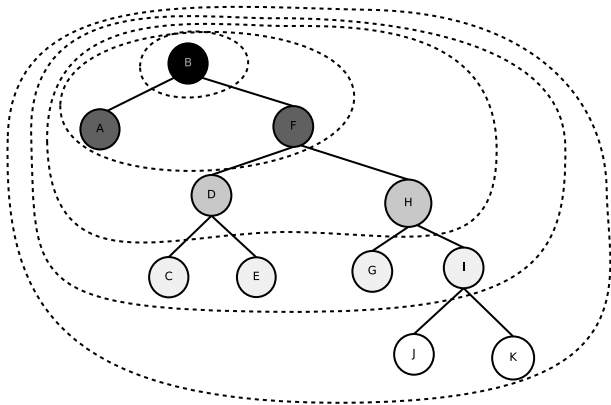
# Neural Distance – TTO-CONROT



# Bubble of Activity – TTO-CONROT



# Bubble of Activity – TTO-CONROT

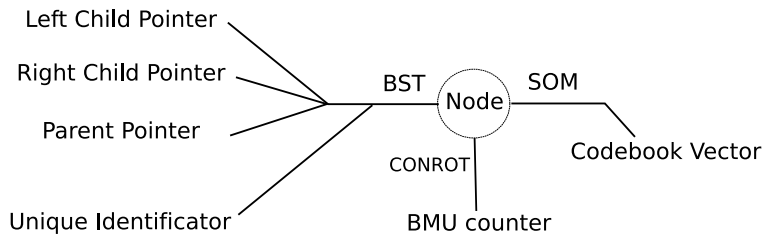


# Neuron Information

TTOSOM Neurons require fields for implementing:

- SOM
- BST
- ADS – CONROT

# Neuron Information



# Neural State

**Created** The new neuron is added to the tree.

**Initialized** The codebook vector assumes a value.

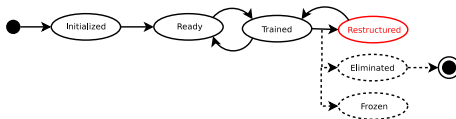
**Ready** Neuron is ready for training.

**Trained** The neuron is under training.

**Frozen** The neuron becomes static.

**Eliminated** The neuron is no longer useful.

**Restructured** The structure is modified (no deletion).





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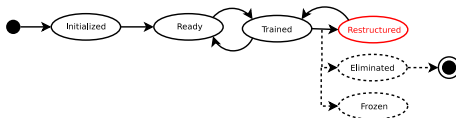
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**Created** The new neuron is added to the tree.

**Initialized** The codebook vector assumes a value.

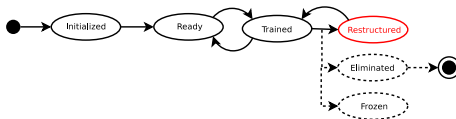
**Ready** Neuron is ready for training.

**Trained** The neuron is under training.

**Frozen** The neuron becomes static.

**Eliminated** The neuron is no longer useful.

**Restructured** The structure is modified (no deletion).



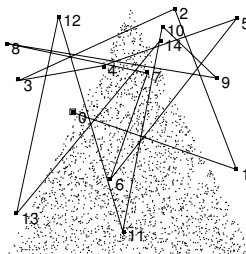
# TTO-CONROT Training Algorithm

- 1 Describe Topology
  - 1.1 Read next item in the array of children.
  - 1.2 Create children.
  - 1.3 Call Describe Topology recursively.
- 2 **Main Loop (Repeat until Convergence)**
  - 2.1 Get input.
  - 2.2 Find BMU.
  - 2.3 **Rotate BMU Conditionally.**
  - 2.4 Calculate Neighbors using neural distance.
  - 2.5 Move Neurons within the bubble of activity.
  - 2.6 Decrease radius/learning rate.

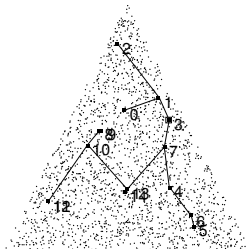
## Experiment 7: 1-ary tree – TTOSOM-CONROT

- List topology.
- Learns a Triangle distribution.
- Data structure is self-adapted.
- Most accessed nodes are moved to the root conditionally.
- BST property is also preserved.

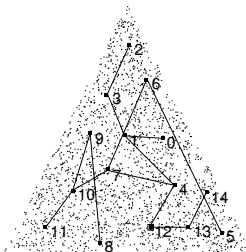
# Experiment 7: 1-ary tree – TTOSOM-CONROT



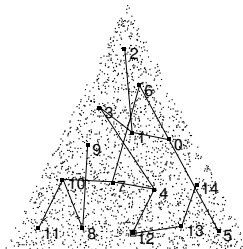
# Experiment 7: 1-ary tree – TTOSOM-CONROT



# Experiment 7: 1-ary tree – TTOSOM-CONROT



# Experiment 7: 1-ary tree – TTOSOM-CONROT

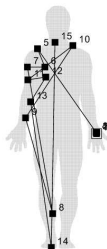




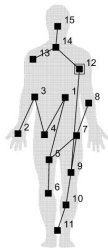
## Experiment 8: Human Shape – TTOSOM-CONROT

- Human Shape.
- Originally a list topology .
- Most accessed nodes are moved to the root conditionally.

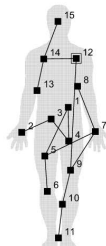
# Experiment 8: Human Shape – TTOSOM-CONROT



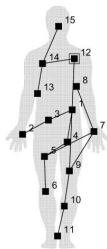
# Experiment 8: Human Shape – TTOSOM-CONROT



# Experiment 8: Human Shape – TTOSOM-CONROT



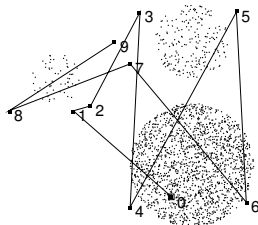
# Experiment 8: Human Shape – TTOSOM-CONROT



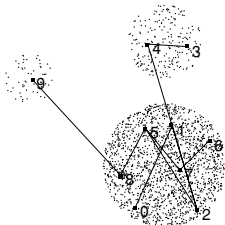
## Experiment 9: Circles – TTOSOM-CONROT

- Three cloud of Points.
- Originally a list topology.
- Number of codebook proportional to area.
- Most accessed codebook closer to the root.

# Experiment 9: Circles – TTOSOM-CONROT

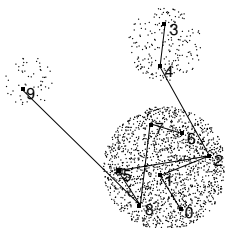


# Experiment 9: Circles – TTOSOM-CONROT

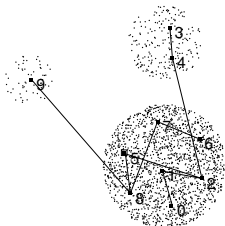




# Experiment 9: Circles – TTOSOM-CONROT



# Experiment 9: Circles – TTOSOM-CONROT



# Experiment 10: Sekeletonization – TTOSOM-CONROT

- Human, Rhinoceros.
- Originally a list topology.
- Still represent shape accurately.

# Experiment 10: Sekeletonization – TTOSOM-CONROT



# Experiment 10: Sekeletonization – TTOSOM-CONROT





# Experiment 10: Sekeletonization – TTOSOM-CONROT



# Summary

- **TTO-SOM** is able to determine:
  - Distribution of the data.
  - Structured topology.
- **TTO-SOM** can represent data in multiple granularity levels.
- **TTO-SOM** can extract a skeleton from the shape.
- **TTOSOM-CONROT** is able to determine:
  - Distribution of the data.
  - **Adaptive** Structure of topology.
- **TTOSOM-CONROT** merges Neural Nets and Adaptive DS.
- **TTOSOM-CONROT** has huge potential; Many open areas.