Neural Networks for Structured Knowledge

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Course Overview

Introduction

Knowledge Representation

Knowledge Processing

Neural Networks and Structured Knowledge

Generalized Recursive Neuron

Computational and Complexity Issues

Conclusions

Terminology

Knowledge, Data and Information

Knowledge:

definition:[1] Information and understanding about a subject which a person has in his or her mind or which is shared by all human beings

similar terms:[2] *learning, lore, scholarship, wisdom, instruction, book-learning, enlightenment, expertise, intelligence, light, theory, science, principles, philosophy, awareness, insight, education, substance, store of learning, know-how*

important aspects: possibly complex structure (relations between items)

[1] [Sinclair, 1987]
[2] [Laird, 1982]

Data:

definition:[1] Information, usually in the form of facts or statistics that you can analyse, or that you use to do further calculations

similar terms:[2] *evidence, reports, details, results, notes, documents, abstracts, testimony, matters of direct observation, facts, raw materials, memorandums, statistics, figures, measurements, conclusions, information, circumstances, experiments*

important aspects: rigid, simple structure (tables)

[1] [Sinclair, 1987]
[2] [Laird, 1982]

Information:

definition:[1]

1. knowledge acquired through experience or study
2. knowledge of specific and timely events or situations; news
3. the act of informing or the condition of being informed
4. an office, agency, etc. providing information
5. a charge or complaint made before justice of the peace
6. the results derived from the processing of data according to programmed instructions
7. another word for data

[1] [Hanks, 1979]

similar terms:[1] *derived knowledge, acquired facts, evidence, knowledge, reports, details, results, notes, documents, testimony, facts, figures, statistics, measurements, conclusions, deductions, plans, field or laboratory notes, learning, erudition; news, report, notice, message*

important aspects:

rather vague usage in common language, precise definition in information theory

[1] [Laird, 1982]

Knowledge Hierarchy

Structured Knowledge

information items and their relationships

information items

objects, concepts, features, attributes

relationships

hierarchical, membership, component, similarity, location, ...

Knowledge Representation

formalisms to describe information items and their relationships

adequate
: are essential aspects captured?

comprehensible
: is the represented knowledge understandable?

transferable
: can the knowledge be communicated?

uniform
: is identical information consolidated?

composite
: can components be grouped into ensembles?

reliable
- belief / truth
- consistency

verifiable
- objective / subjective
- facts
- derived knowledge
- basic assumptions

efficient
- usage of space
- execution time for basic operations

Requirements

on a knowledge model

unambituity

no confusion between objects
no mixing of properties (cross talk)
orthogonality

content-oriented access

addressing of objects via features
similarity

arbitrary complexity

depth
dimensionality

context

application of operations according to the current context

structure sensitivity

processing is guided by the internal structure of an object

graceful degradation

no complete breakdown under stress
e.g. memory limitation, execution errors

parallel processing

simple elementary operations

statistical relevance

acquisition and preparation of knowledge according to statistical properties of the real environment

statistical inference

conclusions based on statistical relevance

Basic Functionalities

important constructs for dealing with knowledge

new concepts

extension and organization of knowledge
natural / real or formal / nominal causes

identification of individuals

assignment of properties to individuals (concrete, uniquely identifiable objects)

classification

arraignment of individual into classes
comparison and abstraction of features

definition

specification of necessary and sufficient constraints for an individual to belong to a certain class

relations

relationships between objects must be representable and interpretable

systems

structured grouping of individuals
e.g. aggregation of objects with a certain relation

roles

extraction of an element from a relation

events

systems with temporal aspects as an important property (state)

actions

subject-oriented sequence of events

Knowledge Representation

with Neural Networks

representation methods

local / distributed

symbol-oriented / subsymbolic

knowledge types

Which types of NNs are best suited for which types of knowledge?

Representation Methods

important principles independent of NN types

local

each unit represents one particular concept or object

distributed

the representation of a single concept or object is carried by several units

symbol-oriented

concepts and their properties are only accessible via symbols

subsymbolic

access via features of a concepts

Symbol

sign or token used to represent an object or concept

- unambiguous identification
- loclized
- arbitrary shape
- needs explanation or mapping

Symbol & NN

arbitrary mapping from symbol to object

associative memory
learning of the relation between object and symbol

Icon

also: *Simile*, simplified picture

- inherent similarity to the object to be represented
- not necessarily unambiguous
- localized
- obvious mapping

Icon & NN

retains essential properties of the object to be represented

associative memory
learning of the relation between object and representation

only feasible if the icon is already defined

Index

indicator

- elicits an important feature of the object
- usually unambiguous
- localized
- inherent mapping

Index & NN

direct representation of one essential aspect of the object

simple network
computation of a function from input to output

Object & Properties

mapping of an object and its properties

hetero-associative memory

learning of the relation between an object and its properties

Structured Objects

objects are composed from components (compositionality)

recursive auto-associative memory

a reduced representation of the input layer in the hidden layer
this reduced representation is recursively used as part of the input layer

Symbol Grounding

establishment of a mapping between a symbol and the object to be represented

- emergence of the mapping
- causal correlation?
- basis for a good model

Binding-Problem

simultaneous unambiguous mapping for several objects in one network

tensor-product
: matrix with entries where object and properties meet
problem: quadratic space requirements

synchronicity
: associated elements are identified by simultaneous activity
problem: limited by available phases

signatures
: different objects use different signals problem: signatures are essentially symbols

Symbols and Formal Systems

semantics for a formal system based on concrete experiences with a real environment, not only in reference to other symbol structures

- meaning often assigned by the programmer / designer
- "parasitic" mapping (not intrinsic, but interpreted)
- possibility of errors due to interpretation of symbols ("concept" vs. string)
- often not plausible as a model for cognitive phenomena

Extreme Positions

about knowledge and its representation

formalistic assumption
: knowledge can be represented by finite structures composed of discrete atomic symbols in accordance with a finite number of syntactic relations [1]

relativistic assumption
: knowledge can only be described in a meaningful way with respect to a framework incorporating non-quantitative aspects like experience, belief, expectation, feelings, ...
as a consequence, knowledge cannot be described in absolute terms [2]

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[1] [MacLennan, 1994]
[2] Joseph Weizenbaum

Physical Symbol Systems Hypothesis

A *Physical Symbol System* consists of symbols and structures that have to be realized physically; it has the necessary and sufficient conditions for an intelligent system [1]

[1] [Newell and Simon, 1976]

Knowledge Processing Methods

- knowledge recall
- identification of structures or patterns
- content-based access
- similarity-based access
- search
- generalization
- (logical) inference
- probabilistic, evidential, fuzzy, analogical, ... reasoning
- metaphors
- planning
- ...

Neural Network Models

used for knowledge processing

- simulated annealing
- distributed production rules
- syllogistic reasoning
- reflexive reasoning
- spreading activation
- evidential reasoning

Logic and Simulated Annealing

satisfiability of a logical formula is checked via energy minimization

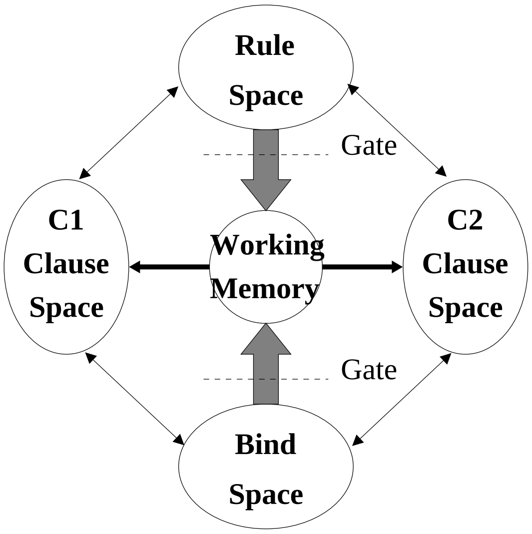
- transformationof the formula into an equivalent network
  äquivalentes Netzwerk
- energy minimization via simulated annealing

Distributed Production Rules

Distributed Connectionist Production System

- many simple, neuron-like units
- rule interpreter for production rules
- distributed representation

DCPS Architecture



Syllogistic Reasoning

modeling of higher cognitive functions through mental models

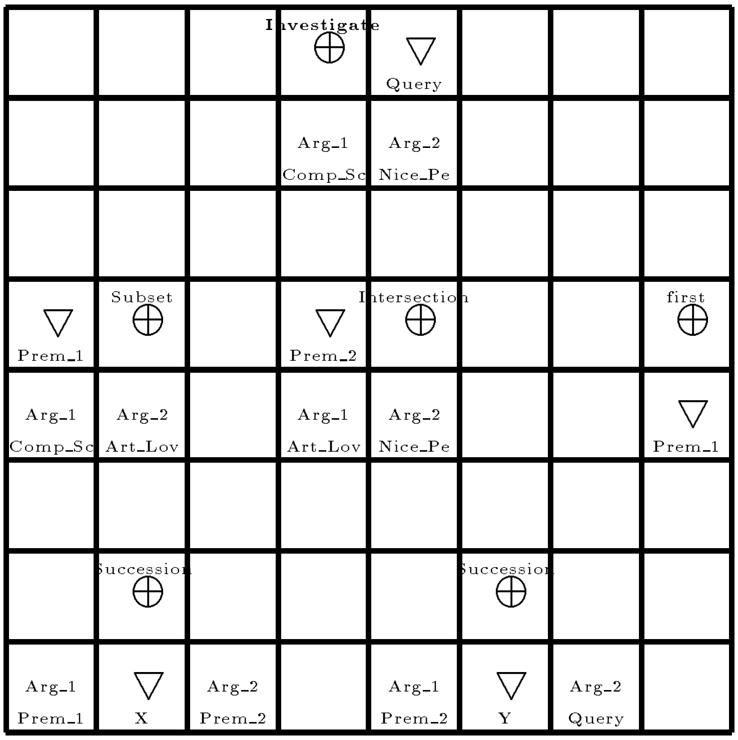
- abstract example situations
- generation and evaluation of hypotheses
- short-term memory for several co-existing objects and hypotheses
- similarity-based access
- similar concepts are represented in spatial proximity
- similarly structured concepts are processed in a similar way
- encoding via relative positions in the network
- association between common activity patterns in relevant substructures

Conposit: *An Example*

`(Query:)`	`Computer scientists, nice people?`
`(Premise 1:)`	`Some computer scientists are art lovers.`
`(Premise 2:)`	`All art lovers are nice people.`
`(Conclusion:)`	`Some computer scientists are nice.`

Notation:

bold typeface	action / relation	e.g. **Investigate**
italics typeface	type / role	e.g. Arg_1
SMALLCAPS TYPEFACE	name / object	e.g. ART_LOV
$\bigoplus$	class	
$\bigtriangledown$	instance	



Advantages and Problems

of CONPOSIT

+ cognitively plausible reasoning patterns
+ similarity-based processing techniques
- essentially sequential method

Reflexive Reasoning

modeling of reasoning techniques through structured networks

- many simple, neuron-like units
- fast
- large number of rules
- limited expressiveness

Spreading Activations

reasoning process is modeled through spreading activation in a network

- based on semantic networks
- local representation
- variable bindings through signatures
- disambiguation
- access to similar events

CONSYDERR

CONnectionist SYstem with Dual representation for Evidential Robust Reasoning

- two-level architecture:
  local (concepts)
  distributed (features)
- based on vague, evidential reasoning (fuzzy evidential logic)
- able to deal with
  partial information
  similarity-based unification
  inheritance of properties
  Inconsistencies

CONSYDERR Architecture

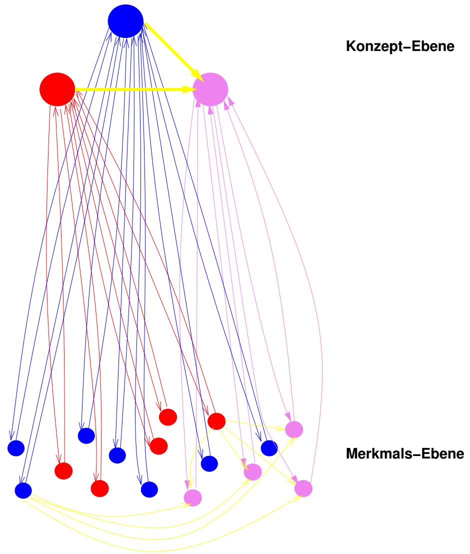
local layer

reasoning over *concepts*
rules are represented via directed edges from premise nodes to conclusion nodes
specific mechanism for variable bindings (transmission and representation of signatures)

distributed layer

reasoning over *features*
similarity appears as overlap in features

CONSYDERR Layers



Evaluation Model

- links between nodes of the local and the distributed layer
- concept nodes in the local layer have connections to those nodes in the distributed layer that represent the same concept
- rule connections from the local layer are duplicated diffusely in the distributed layer
- interaction between the two layers according to a fixed cycle:

  Phase I links from local to distributed are active (top down)

  Phase II links within both layers are active

  Phase III links from distributed to local are active (bottom up)

Advantages and Problems

of CONSYDERR

+ different types of reasoning
+ connectionist evaluation model
- complex, biologically implausible neuron model
- rigid interaction scheme
- limited similarity notion

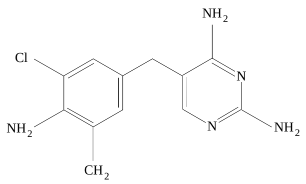
PART II

Neural Networks for Structured Domains

MOTIVATION

Extension of neural networks to structured domains

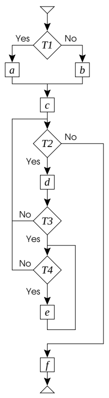
Example 1: Chemistry



- Quantitative Structure-Activity Relationship (QSAR)
- Quantitative Structure-Property Relationship (QSPR)
- DNA Analysis

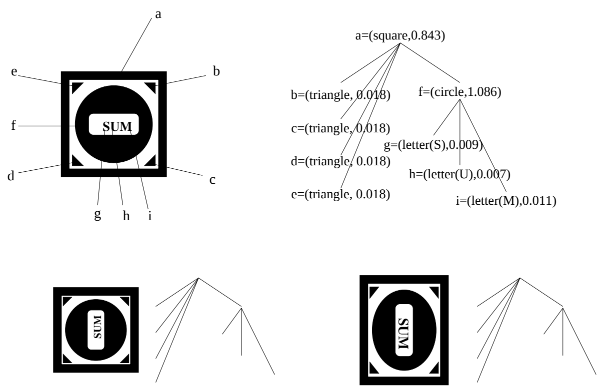
Example 2: Software Engineering

```
program  name (list);
var
 . . .
begin
if  T1 then
        a
else
        b;
c;
while T2 do
        begin
        d;
        if  T3 then
        while T4 do
                e
        end;
f
end.
```



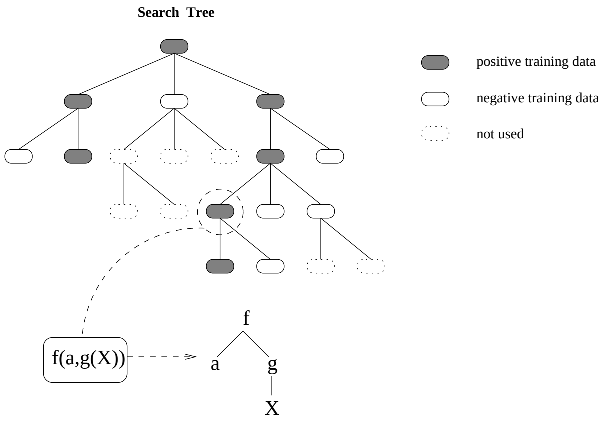
- Software Quality: metric for quality, reusability, maintainability, etc.

Example 3: Pattern Recognition



- Recognition of structured patterns

Example 4: Problem Solving



- Learning Heuristics

WHY NEURAL NETWORKS ?

Because

- Universal Approximators
- Automatic Inference (Learning)
- Nice Classification Capability
- Robust to Noise
- Can Deal with Real Valued Information

PROBLEMS

- PROBLEM 1
  how can we represent a structure **in** a neural network ?
- PROBLEM 2
  how can we classify a structure **by** a neural network ?
- PROBLEM 3
  how can we store **in** and recall a structure **by** a neural network ?

Representation of Structures in NN

- **PROBLEM 1**: Representing Structures in NN
- Reduced Descriptions
- RAAM Family Models

Representing Structures in NN

Structures can be represented in NN by using:

- **Local Representation**
  - spatial encoding
  - time encoding
- **Distributed Representation**

Local Representation

In a local representation

- each neuron represents a component of the structure
- each connection represents a relation between components
- trivial and not efficient

Examples

- MPP (Waltz and Pollack, 1985), PPN (Selman and Hirst, 1985)
- Parsing Network (Charniak and Santos, 1987)
- ACME (Holyoak and Thagard, 1989)
- μKLONE (Derthick, 1990)
- SHRUTI (Ajjanagadde and Shastri, 1991)

Distributed Representation

- each component of the structure is represented by a set of units
- each unit contribute to the representation of a set of components

Examples

- DCPS (Touretzky and Hinton, 1988)
- Tensor Products (Smolensky, 1990)
- RAAM (Pollack, 1990), LRAAM (Sperduti, 1994)
- Convolution-based models:
  TODAM (Murdock, 1983), CHARM (Metcalfe, 1991), TODAM2 (Murdock, 1993), **Holographic Reduced Representations** (Plate, 1991)

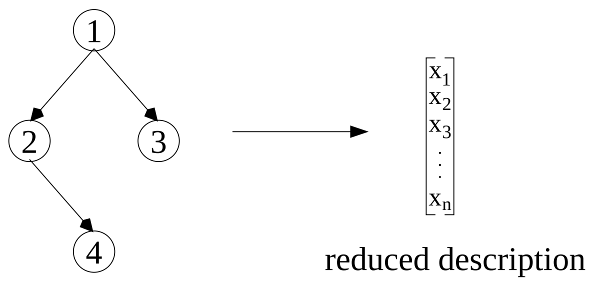
Distributed Representations (cont.)

Reduced Descriptions (Hinton, 1987; 1990)

- Encoding of complex conceptual structure in distributed representations
- Four desiderata
  1. **Representational adequacy:** reconstruct the full representation from the reduced description
  2. **Reduction:** fewer units
  3. **Systematicy:** related in a systematic way to the full representation
  4. **Informativeness:** tell us something about the concept that it refers to, without it being necessary to reconstruct the full representation

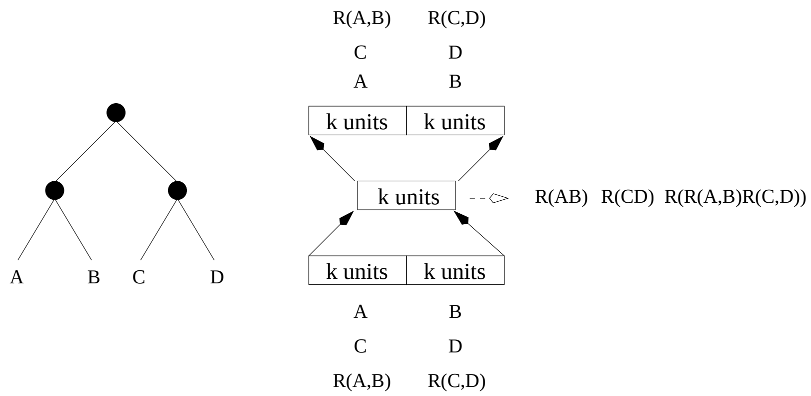
Distributed Representations (cont.)

Both **RAAM** and **Holographic Reduced Representations** implement reduced descriptions

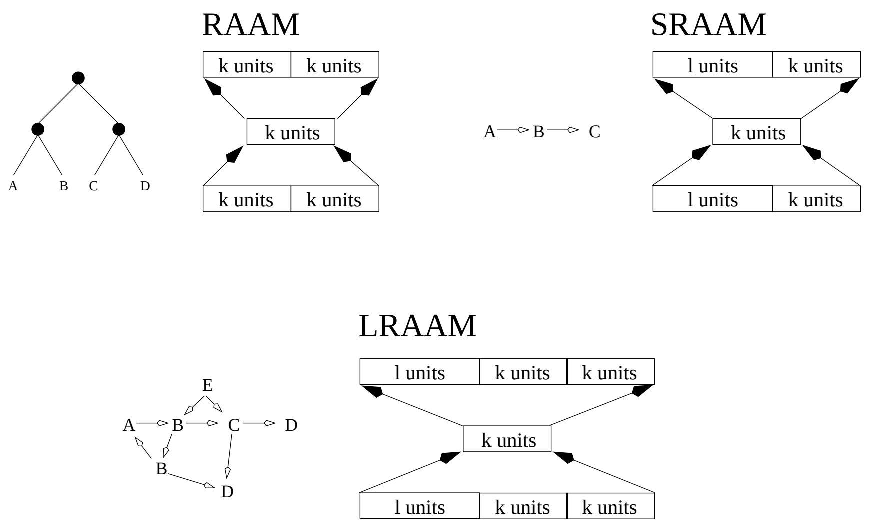


Recursive Auto-Associative Memory

- Tree with labeled leaves → Numeric vector
- Small sets of fixed-width trees encoded in patterns all of the same size



RAAM Family

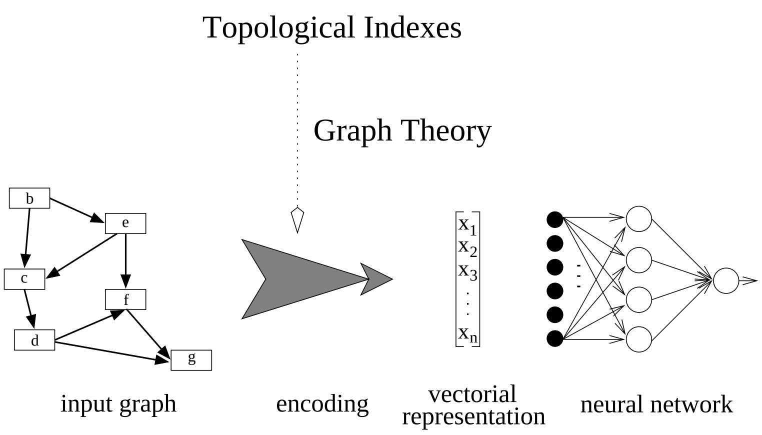


Classification of Structures by NN

Outline

- **PROBLEM 2**: Classification
- Generalized Recursive Neuron
- Models of Recursive Neural Networks
- Computing the Gradient

Classification with Standard NN



PROBLEM:

a priori definition of the encoding process

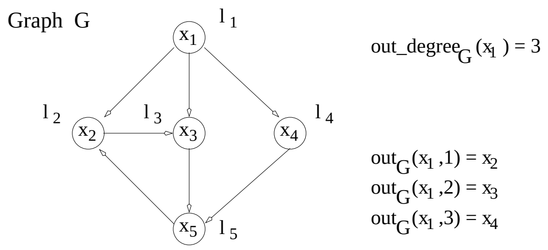
- the relevance of different features of the graphs may change dramatically for different classification tasks

- the encoding process has to work for any classification task ($\rightarrow$ representations difficult to classify)

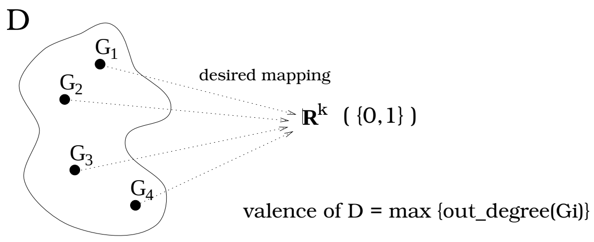
SOLUTION:

encoding performed by a NN

PRELIMINARIES

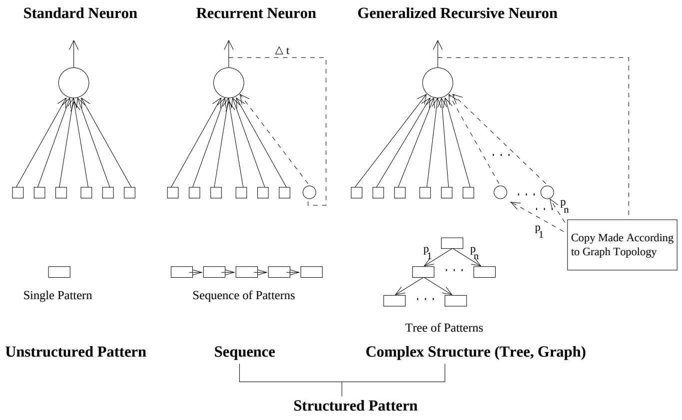


STRUCTURED DOMAIN



Generalized Recursive Neuron

- standard and recurrent neurons are not suited to dealing with labeled structures
- to solve this inadequacy we introduce the *generalized recursive neuron*



Generalized Recursive Neuron (def.)

The output $o^{(g)}(x)$ of a generalized recursive neuron

$$o^{(g)}(x) = f(\sum_{i=1}^{N_L} w_i l_i + \sum_{j=1}^{out\_degree_X(x)} \hat{w}_j \, o^{(g)}(out_X(x,j)))$$

where

x is a vertex of graph X

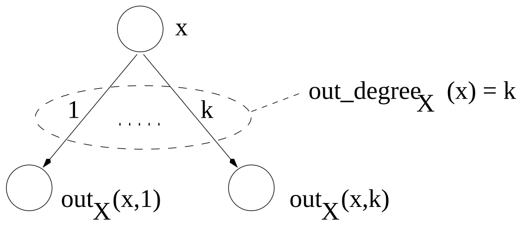
f is a sigmoidal function

N_L is the number of units encoding the label $\mathbf{l} = \phi_X(x)$ attached to the current input x

$\hat{w}_j$ are the weights on the recursive connections

Generalized Recursive Neuron (cont.)

- the output is computed recursively on the offsprings

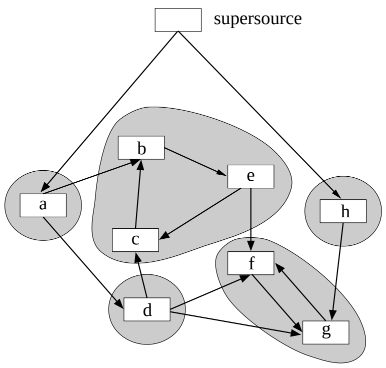


- the following two conditions must hold:
  - Number of Connections: as many recursive connections as the domain valence;
  - Supersource: graph X must have a reference *supersource*.

Supersource

graph without a supersource $\rightarrow$ add an extra vertex s

- with a minimal number of outgoing edges
- such that s is a supersource for the new graph



EXAMPLES (Generalized Recursive Neuron)

Sequence: $x_k \to x_{k-1} \to \ldots \to x_1$

- Generalized recursive neuron

$$o(x_1) = f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(1)})$$

$$o(x_i) = f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(i)} + \hat{w}_1 o(x_{i-1})) \quad i = 2, \ldots, k$$

- Standard recurrent neuron (time t of processing explicit)

$$o(t=1) = f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(1)})$$

$$o(t) = f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(t)} + \hat{w}_1 o(t-1)) \quad t = 2, \ldots, k$$

EXAMPLES (Generalized Recursive Neuron)

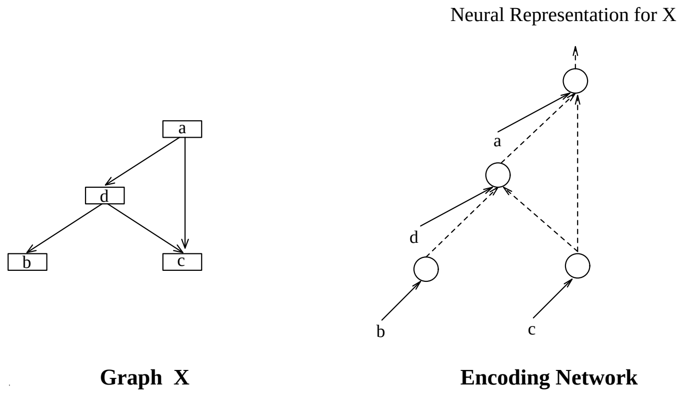
Graph with cycle

$$\begin{array}{ccccc} x_6 & \rightarrow & x_5 & \leftarrow & x_4 \\ & & \downarrow & & \uparrow \\ & & x_3 & \rightarrow & x_2 & \rightarrow & x_1 \end{array}$$

$$\begin{aligned}
o(x_1) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(1)}) \\
o(x_2) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(2)} + \hat{w}_1 o(x_1) + \hat{w}_2 o(x_4)) \\
o(x_3) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(3)} + \hat{w}_1 o(x_2)) \\
o(x_4) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(4)} + \hat{w}_1 o(x_5)) \\
o(x_5) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(5)} + \hat{w}_1 o(x_3)) \\
o(x_6) &= f(\textstyle\sum_{j=1}^{N_L} w_j l_j^{(6)} + \hat{w}_1 o(x_5))
\end{aligned}$$

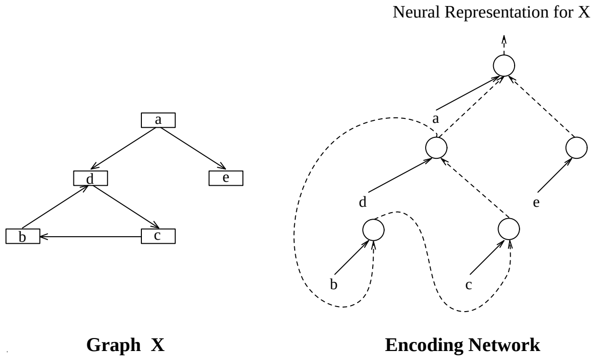
ENCODING NETWORK

since each graph X has a supersource s, then we can see $o(s)$ as computed by an **Encoding Network** obtained by replicating the (set of) generalized recursive neuron(s) according to the graph topology



ENCODING NETWORK (cont.)

if the graph X contains a cycle, then the **Encoding Network** is recurrent

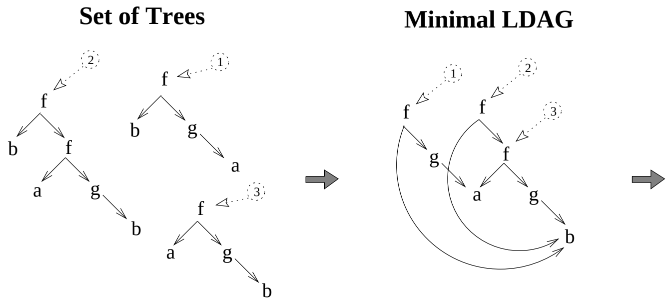


WARNING: there is no guarantee that the Encoding Network is convergent

OPTIMIZATION TRAINING SET

if we only have DAGs, then the training set can be optimized:

1. all the DAGs in the training set are merged into a single minimal DAG, i.e., a DAG with a minimal number of vertices
2. a topological sort on the vertices of the minimal DAG is performed to determine the updating order on the vertices for the network



Sorted Training Set

#	label	left	right
0	b	nil	nil
1	a	nil	nil
2	g	nil	0
3	g	nil	1
4	f	1	2
5	f	0	3
6	f	0	4

NEURAL NETWORKS FOR STRUCTURES

- Back-Propagation Networks
- Simple Recurrent Networks (Elman-Style)
- Cascade-Correlation
- Neural Trees
- Real-Time Recurrent Networks

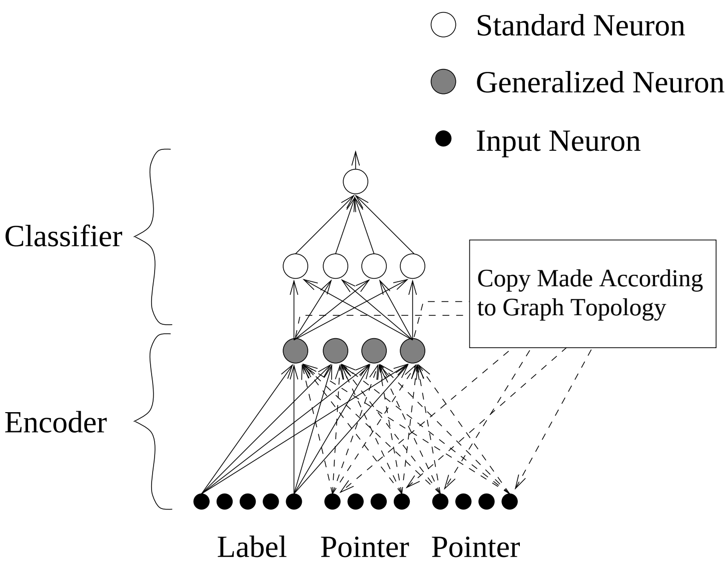
$+$

- Generalized Recursive Neurons

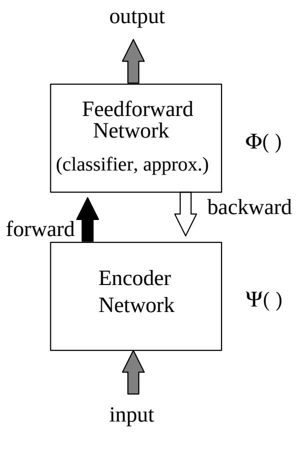
$\Downarrow$

- **NEURAL NETWORKS FOR STRUCTURES**

Back-Propagation Networks

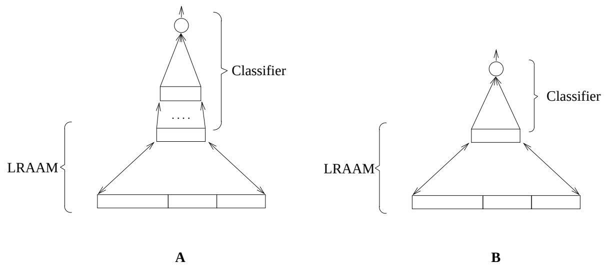


Back-Propagation Networks (cont.)



- DAGs → Back-Propagation Through Structure (see Goller)
- Cyclic Graphs → Extension of Recurrent Back-Propagation (Pineda)

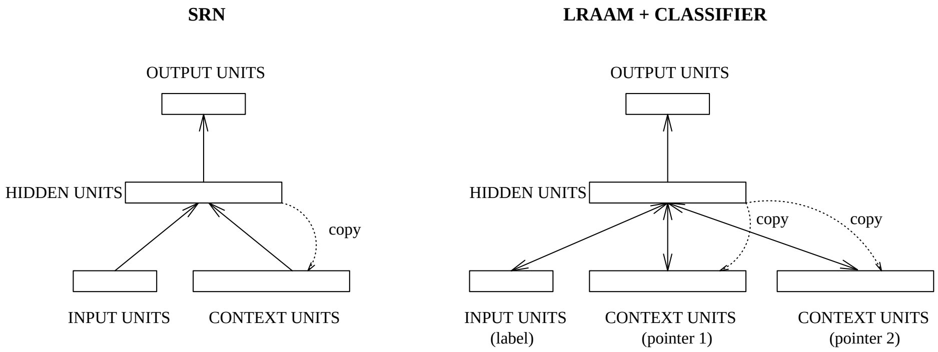
LRAAM-based Networks



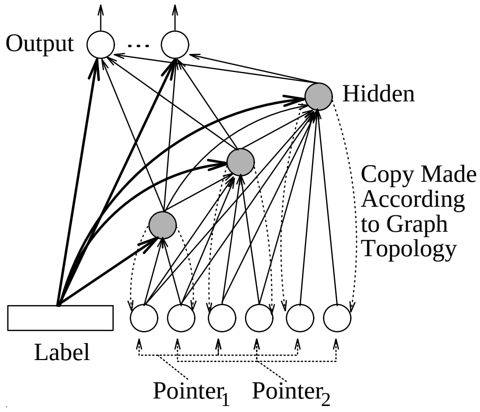
Several options for training networks **A** and **B** are available:

- different learning rates for the classifier and the LRAAM
- classifier training is not started until **x** percent of the training set has been correctly encoded and subsequently decoded by the LRAAM
- the error from the classifier is backpropagated across **y** levels of the structures encoded by the LRAAM

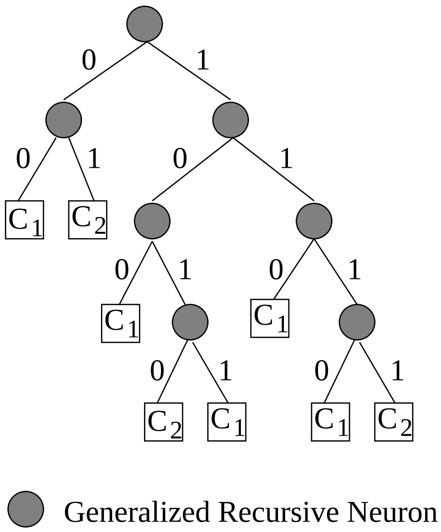
Elman-Style Networks



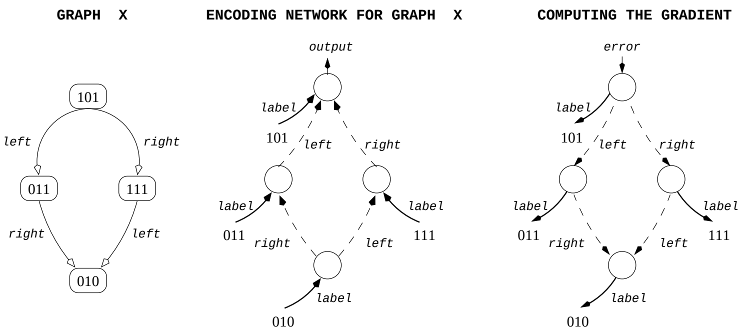
Cascade-Correlation



Neural Tree

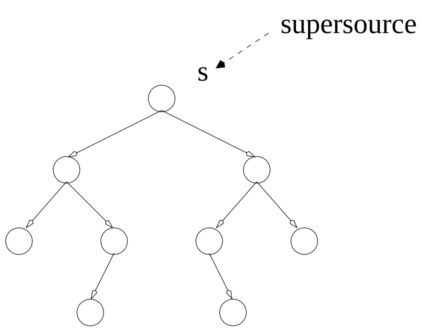


Computing the Gradient



Computing the Real-Time Gradient

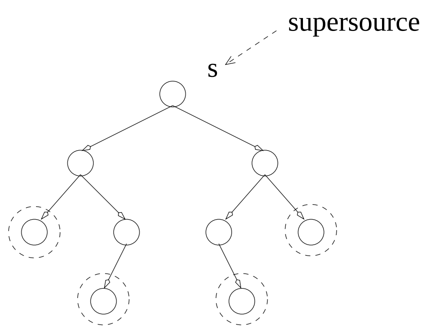
$$o(s) = f(W^t L(s) + \sum_{j=1}^{out\_degree(s)} \hat{w}_j o(out(s,j)))$$



Computing the Real-Time Gradient (cont.)

Consider v such that $out\_degree(v) = 0$, then

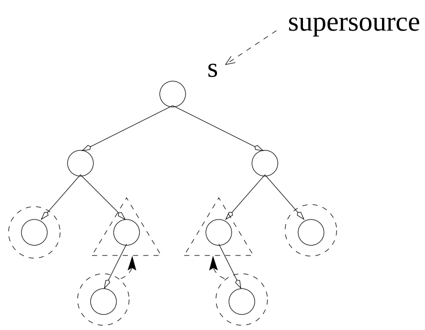
$$\frac{\partial o(v)}{\partial w_i} = f' L(v)_i \quad \frac{\partial o(v)}{\partial \hat{w}_j} = 0$$



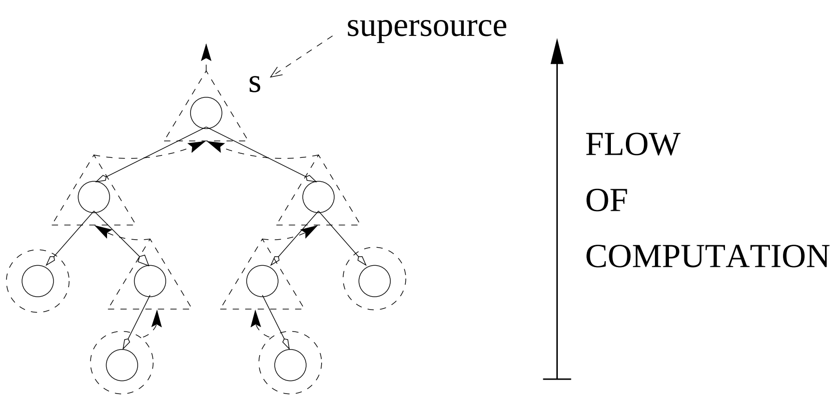
Computing the Real-Time Gradient (cont.)

$$\frac{\partial o(v)}{\partial w_i} = f'(L(v)_i + \sum_{k=1}^{out\_degree(v)} \hat{w}_k \frac{\partial o(out(v,k))}{\partial w_i})$$

$$\frac{\partial o(v)}{\partial \hat{w}_j} = f'(o(out(v,j)) + \sum_{k=1}^{out\_degree(v)} \hat{w}_k \frac{\partial o(out(v,k))}{\partial \hat{w}_j})$$



Computing the Real-Time Gradient (cont.)



Computational and Complexity Issues

- Tree Grammars and Tree Automata
- Computational Power of Some Models
- Complexity Issues
- Approximation

COMPUTATIONAL POWER

Recurrent Networks $\Longleftrightarrow$ *Finite State Automata*

Networks for Structures $\Longleftrightarrow$ Tree Automata

Tree Grammars in Expansive Form

$\Updownarrow$

Frontier-to-Root Tree Automata

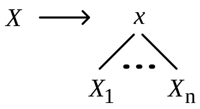
TREE GRAMMARS

TREE GRAMMAR $G_t = (V, r, P, S)$

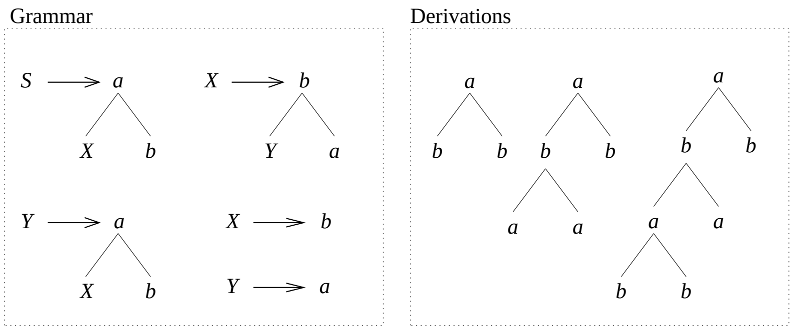
- $V = N \cup \Sigma$ is the grammar alphabet (nonterminals and terminals)
- (V, r) a ranked alphabet
- productions in P are of the form $T_i \rightarrow T_j$, where T_i and T_j are trees
- S in T_V is a finite set of starting trees
- T_V denotes the set of trees with nodes labeled by elements in V

TREE GRAMMARS (cont.)

TREE GRAMMARS in EXPANSIVE FORM

- all productions are of the form 

- example



TREE AUTOMATA (frontier-to-root)

TREE AUTOMATON $\mathcal{A}_t = (Q, F, \{f_a | a \text{ in } \Sigma\})$ (deterministic)

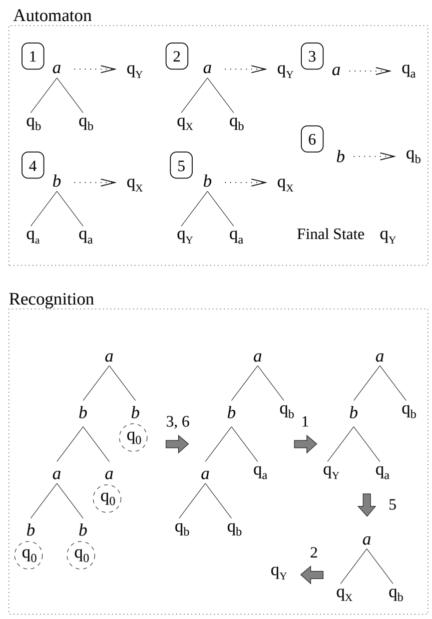
- Σ is a ranked alphabet
- Q is a finite set of states
- F is a set of final states, a subset of Q
- $\{f_a | a \text{ in } \Sigma\}$ is a set of transition functions $f_a : Q^m \to Q$ such that m is a rank of the symbol $a \in \Sigma$

TREE AUTOMATA (cont.)

RECOGNITION PROCESS (informal)

1. The frontier of the state tree is labeled q_0 (the status associated to nodes with $m = 0$, i.e, the leaves)
2. For any node in the input labeled l with rank m, the corresponding node of the state tree is labeled $f_l(q_1, \ldots, q_m)$, where $q_1, \ldots, q_m$ are the states labeling the offsprings of that state tree node
3. an input tree is accepted by $\mathcal{A}_t$ if the automaton can enter a final state upon encountering the root

EXAMPLE OF TREE AUTOMATON (FRA)



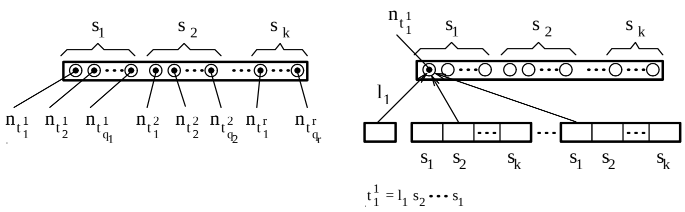
COMPUTATIONAL RESULTS

Theorem An Elman-style network can simulate any FRA.

Proof Schema

For *each* tuple $t_i^j \in V_{s_j}$, $i \in [1, \ldots, \#V_{s_j}]$, and for *each* state s_j, we introduce a unit $n_{t_i^j}$ at the hidden level

The units $n_{t_i^j}$ will represent the state s_j at the hidden level of the network



COMPUTATIONAL RESULTS (cont.)

Theorem A Cascade-Correlation network for structures (CCS) cannot simulate any FRA.

Proof Schema

CCS with $N_v = 1$ is equivalent to Recurrent Cascade - Correlation (RCC)

RCC cannot simulate any Finite State Machine (FSM) (Giles et al., 1995; Kremer, 1995; Kremer, 1996)

FSM is equivalent to FRA with relations having rank 1

Theorem A Neural Tree for structures cannot simulate any FRA.

COMPUTATIONAL RESULTS (cont.)

Theorem Any Neural Tree for structures can be implemented by a CCS.

Proof Schema

- A Neural Tree (NT) can be restructured as a layered network by following the rules below:

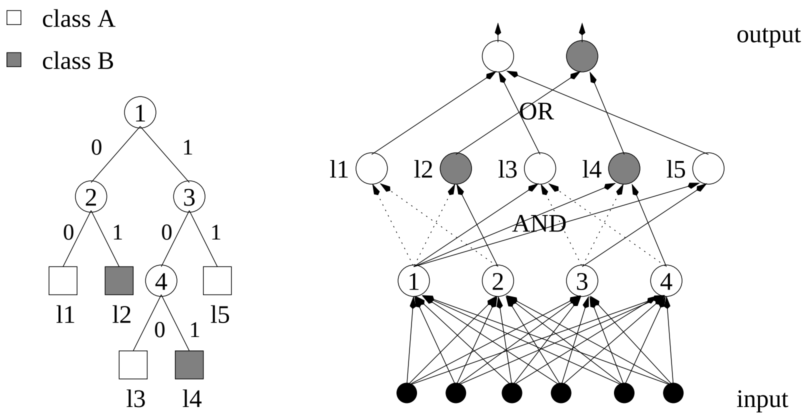
(R1) same units as the internal nodes of the NT

(R2) **and** of nodes which belong to the same path

(R3) **or** of paths

- Layered network implemented by a Cascade-Correlation network.

COMPUTATIONAL RESULTS (example)

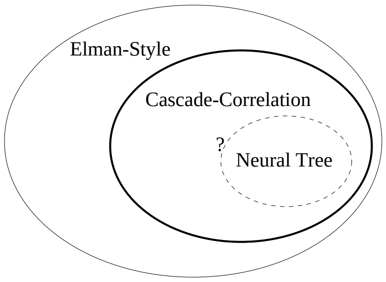


COMPUTATIONAL RESULTS (cont.)

Corollary A Neural Tree for **sequences** cannot simulate any Finite State Machine.

Corollary Any Neural Tree for **sequences** can be simulated by a Recurrent Cascade-Correlation network.

SUMMARY



COMPLEXITY

Question:

how many nodes are needed to implement an m-state FRA ?

- l input-output labels (alphabet) encoded in $\lceil \log l \rceil$ bits
- maximum rank N_v
- m different states encoded in $\lceil \log m \rceil$ bits
- transition (and output) function as a boolean logic function:

$$\Phi : \{0,1\}^{\log l + N_v \log m} \rightarrow \{0,1\}^{\log l + \log m}$$

COMPLEXITY RESULTS: four layers

Theorem[Four Layers Insertion]

A four layers recurrent neural network can implement FRAs with m states, l input-output labels, and maximum rank N_v, with a node complexity of $O(\sqrt{\frac{(\log l+\log m)lm^{N_v}}{\log l+N_v \log m}})$.

Proof

Follows from the lemma:

Lemma (Lupanov, 1972) Arbitrary boolean logic functions of the form $f:\{0,1\}^x \rightarrow \{0,1\}^y$ can be implemented in a four layer network of perceptrons with a node complexity of $O(\sqrt{y2^x/(x-\log y)})$.

COMPLEXITY RESULTS: three layers

Theorem[Three Layers Insertion]

A three layers recurrent neural network can implement FRAs with m states, l input-output labels, and maximum rank N_v, with:

- a node complexity of $O((\log l+\log m)\sqrt{lm^{N_v}})$
- a number of connections of $O((\log l+\log m)lm^{N_v})$.

Proof

Follows from a construction based on the telescopic lemma (Siu et. al. 1995)

Approximation

- S set of Σ-labeled trees
- $\bar{f} : S \rightarrow \Re^q$
- $\mathcal{F}$ set of functions implementable by a feed-forward NN for structures

Theorem (Hammer, 1996) For any $\epsilon > 0$ there exists a function $f^\epsilon \in \mathcal{F}$ such that $\forall s \in S,\ P(|f^\epsilon(s) - \bar{f}(s)| > \epsilon) < \epsilon$

NN Memory Models for Structures

Outline

- **PROBLEM 3**: Storing and Recalling Structures
- From LRAAM to the Content Access Network
- Stability Results for the Content Access Network
- One Step Beyond: Generalized Hopfield Model

LRAAM network

$$\mathbf{F}_E(\vec{x}) = \mathbf{F}(\mathbf{E}\vec{x} + \vec{\theta}_H) \equiv \vec{h},$$
$$\mathbf{F}_D(\vec{h}) = \mathbf{F}(\mathbf{D}\vec{h} + \vec{\theta}_O) \equiv \vec{o},$$

Encoding Matrix:

$$\mathbf{E} = [\mathbf{E}^{(l)}, \mathbf{E}^{(p_1)}, \ldots, \mathbf{E}^{(p_n)}]$$

Decoding Matrix:

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}^{(l)} \\ \mathbf{D}^{(p_1)} \\ \vdots \\ \mathbf{D}^{(p_n)} \end{bmatrix}$$

CA Network

The Content Access (CA) network:

$$\textbf{LRAAM network} \; + \; \vec{o} \equiv \vec{x}.$$

- discrete time asymmetric Hopfield network
- pattern in the LRAAM training set $\rightarrow$ fixed point of the CA network
- fixed points asymptotically stable $\rightarrow$ memories
- the structure of each pattern exploited to constrain the relaxation of the CA network

Constraints

- constraint c is defined as a couple $(id, \vec{k}^{(id)})$, where:
  - $id \in \{l, p_1, \ldots, p_n\}$ is the name of a field in the network
  - $\vec{k}^{(id)}$ is the *access key*
- during the relaxation of the CA network, the output of the field id is fixed to $\vec{k}^{(id)}$
- access procedure defined as a set C of constraints

Network Dynamics

given a set C of constraints

- $\mathbf{E}^C$ is the matrix obtained by removing from $\mathbf{E}$ the submatrices associated with fields whose names appear in C (the same for $\mathbf{D}^C$)
- $\vec{o}^{\,C}$ is the vector obtained by removing from $\vec{o}$ the subvectors associated with fields whose names appear in C (the same for $\vec{\theta}_O$)

Dynamics:

$$\mathbf{F}_{E^C}(\vec{o}^{\,C}(t)) = \mathbf{F}(\mathbf{E}^C \vec{o}^{\,C}(t) + \vec{\theta}_H + \vec{\theta}^{\,C}_{key}) \equiv \vec{h}(t)$$

$$\mathbf{F}_{D^C}(\vec{h}(t)) = \mathbf{F}(D^C \vec{h}(t) + \vec{\theta}^{\,C}_O) \equiv \vec{o}^{\,C}(t+1)$$

$$\vec{\theta}^{\,C}_{key} = \sum_{(id, \vec{k}^{(id)}) \in C} \mathbf{E}^{(id)} \vec{k}^{(id)}$$

Access by Content

Access procedure on the CA network:

1. choosing one or more fields in the input layer according to the access key(s)
2. clamping the output of these units to the information known, i.e., the access key(s)
3. randomly setting the output of the remaining units in the network
4. letting the unclamped units in the network to relax into a stable state.

Validation of a Fixed Point

A validation test of the reached stable state can be performed:

1. by unfreezing the clamped units in the input layer
2. if the stable state is no longer stable the result of the procedure is considered to be **wrong** and another run is performed
3. otherwise the stable state is considered a **success**

Stability

pointer transformations:

$$\mathbf{F}^{(p_j)}(\vec{d}\,) = \mathbf{F}(\mathbf{D}^{(p_j)}\vec{d} + \vec{\theta}_O^{(p_j)}), \quad j = 1, \ldots, n,$$

label decoding function:

$$\mathbf{F}^{(l)}(\vec{d}\,) = \mathbf{F}(\mathbf{D}^{(l)}\vec{d} + \vec{\theta}_O^{(l)})$$

- $\mathbf{J}^{(p_j)}(\vec{d}\,) = \mathbf{\Lambda}(\vec{net}^{(p_j)})\mathbf{D}^{(p_j)}$ is the Jacobian matrix of $\mathbf{F}^{(p_j)}(\vec{d}\,)$
- $\vec{net}^{(p_j)} = \mathbf{D}^{(p_j)}\vec{d} + \theta_O^{(p_j)}$
- $\mathbf{\Lambda}(\vec{net}^{(p_j)}) \in \Re^{N_H \times N_H}$ is the diagonal matrix whose ith diagonal element is $f'(\vec{net}_i^{(p_j)})$
- $(\vec{d}_H, \vec{d}_O^{\,C})$ fixed point of the **CA** network under the set of constraints C

Stability: Sufficient Conditions

Theorem A fixed point is asymptotically stable if at least one of the following two conditions is verified:

Condition at layer H

$$\sum_{k=1}^{N_H} |b_{ik}| < 1, \qquad i = 1, \ldots, N_H$$

where b_{ik} is the element (i,k) of $\mathbf{B}^{(H,C)} = \mathbf{J}^{(E^C)}(\vec{d}_O^{\,C})\mathbf{J}^{(D^C)}(\vec{d}_H)$;

Condition at layer O

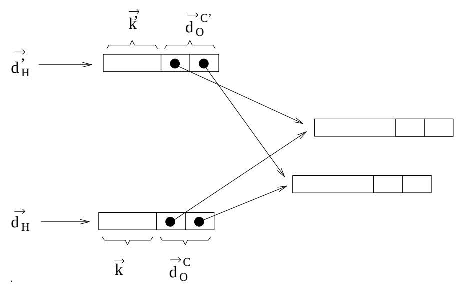
$$\sum_{k=1}^{N_O^C} |b_{ik}| < 1, \qquad i = 1, \ldots, N_O^C$$

where b_{ik} is the element (i,k) of $\mathbf{B}^{(O,C)} = \mathbf{J}^{(D^C)}(\vec{d}_H)\mathbf{J}^{(E^C)}(\vec{d}_O^{\,C})$.

Stability: Sufficient Conditions (cont.)

There are other theorems defining sufficient conditions for:

- Preservation of asymptotical stability of a fixed point when adding a constraint to C
- Extension of asymptotical stability to related components, e.g.:

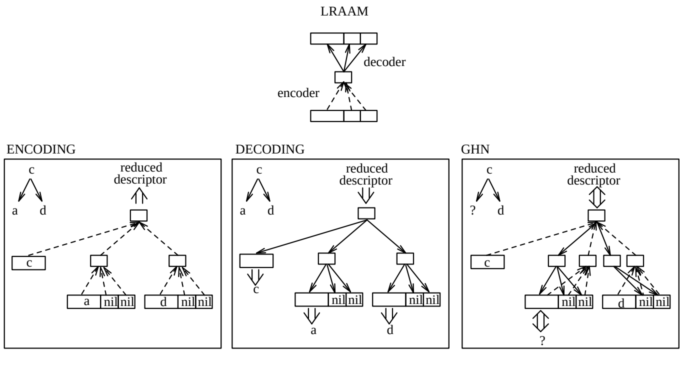


- Other cases

ACCESS by PARTIAL STRUCTURE

Question: how can we modify the model to cope with **access by partial structure** ?

Answer: by combining the encoding and decoding procedures

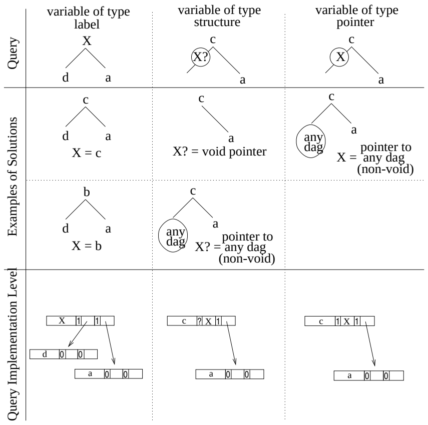


Generalized Hopfield Network

Query (def.)

QUERY: Tree with

- constants and variables of type: label, pointer, and structure
- partially defined labels, and pointers



Network Generation

Question: how do we construct the GHN from the query ?

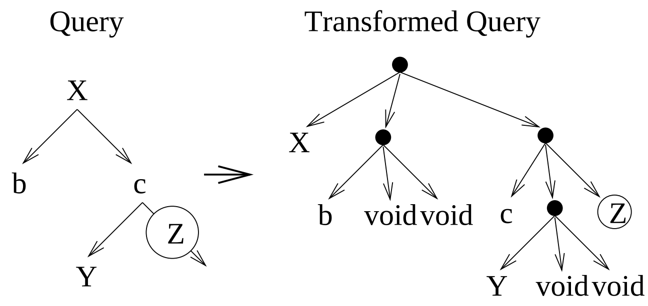
(t1) Query → Transformed Query

(t2) Transformed Query → Query Graph

(t3) Query Graph → Query Network

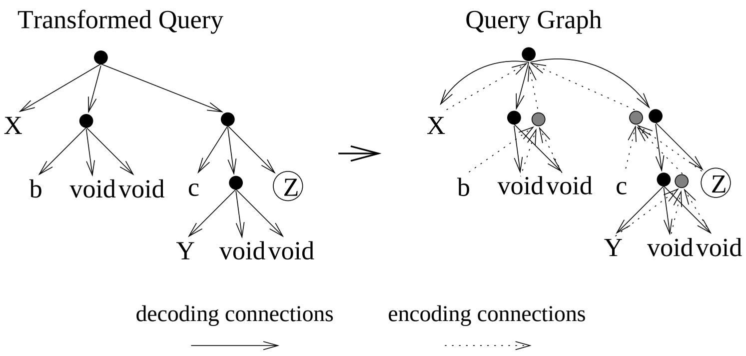
Query → Transformed Query

- the Query tree is transformed in a tree with:
  - unlabeled internal nodes
  - labeled leaves which correspond to nodes of the original query
- variable and void pointers are explicitely represented by leaves



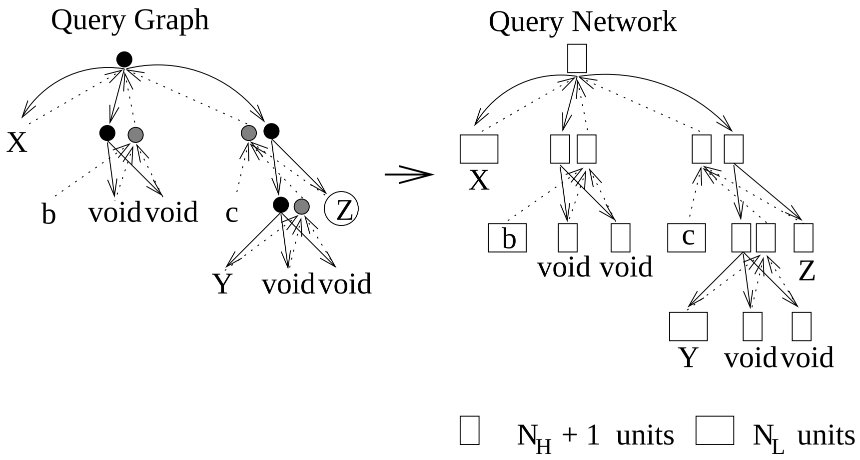
Transformed Query → Query Graph

- the Query Graph defines the general structure of the network implementing the query
- the Query Graph is obtained from the Transformed Query by duplicating internal nodes



Query Graph → Query Network

- the Query Network is build from the Query Graph using the weights of the LRAAM as bulding blocks.



Multiple Solutions

- Uniform Random Search

  uniformly distributed random pointers for the top layer

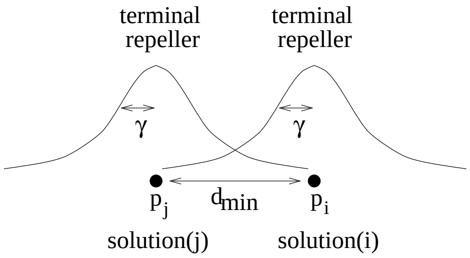
- Terminal Repellers

  introduction of Terminal Repellers (Zak, 89) at the top layer

$$\dot{x}_i^{(top)} + x_i^{(top)} = \sum_{j=1}^{N_O} E_{ij} f(x_j^{IN(top)}) +$$

$$\alpha \sum_{k=0}^{M} (x_i^{(top)} - p_i^{(s^k)})^{1/3} e^{-\gamma(\sum_{i=1}^{N_H} (x_i^{(top)} - p_i^{(s^k)})^2)}$$

How to Set γ ?



$$\gamma = -\frac{log(\epsilon)}{d_{min}^2}$$

$$d_{min} = \min_{ij} \quad \{d_{ij} | d_{ij} = \|p^{(i)} - p^{(j)}\|, \text{ and } p^{(i)},\ p^{(j)} \text{ are in the training set}\}$$

How to Set α ?

Problem:

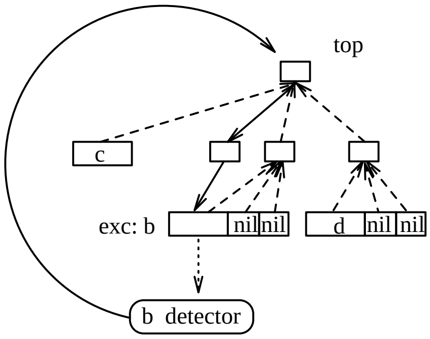
Terminal repellers can introduce cycles

Solution:

Decay equation for α

$$\dot{\alpha} = -\frac{1}{\tau}\alpha$$

Exceptions



Repeller

$$\alpha(x_i^{(top)} - x*_i^{(top)})^{1/3} e^{-\gamma(\sum_{i=1}^{N_H}(x_i^{(top)} - x*_i^{(top)})^2)}$$

Research Directions

Soft Computing BISC [1]

integration of fuzzy logic, neural networks, and probabilistic reasoning

Neurocontrol [2]

dynamic optimization of complex systems based on neural networks

Intelligent Agents

largely independent systems performing actions on behalf of the user

Autonomous Systems

self-contained systems acting in a real environment

[1] *B*erkeley *I*nitiative in *S*oft *C*omputing, [Zadeh, 1990]

[2] [Werbos, 1992]

Knowledge Fusion

integration of knowledge and information available in different modes (linguistic, visual, aural, etc.)

Artificial Life

development of complex systems based on evolutionary concepts

Data Mining

extraction of useful knowledge from huge amounts of data

Adaptive User Interfaces

systems learns preferences of the user

Conclusions

neural networks and structured knowledge

fundamental research

formal models to deal with validation and verification of complex systems
methods for the integration of different computation paradigms
representation methods for various types of knowledge
connections to cognitive phenomena

tools

development tools and environment for the efficient implementation of hybrid systems

applications

real-world applications to gain experience

Outlook

neural networks and structured knowledge

capabilities

more powerful systems through combinations of techniques

challenges

new, exciting research problems

promising applications

increasing importance

as successful applications and experience build up

visibility

might increase (see above)

might decrease because hybrid becomes the norm

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