Intro to Learning in SD -1

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1- Introduction to RecNN

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DRAFT, please do not circulate!

www.di.unipi.it/groups/ciml

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Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

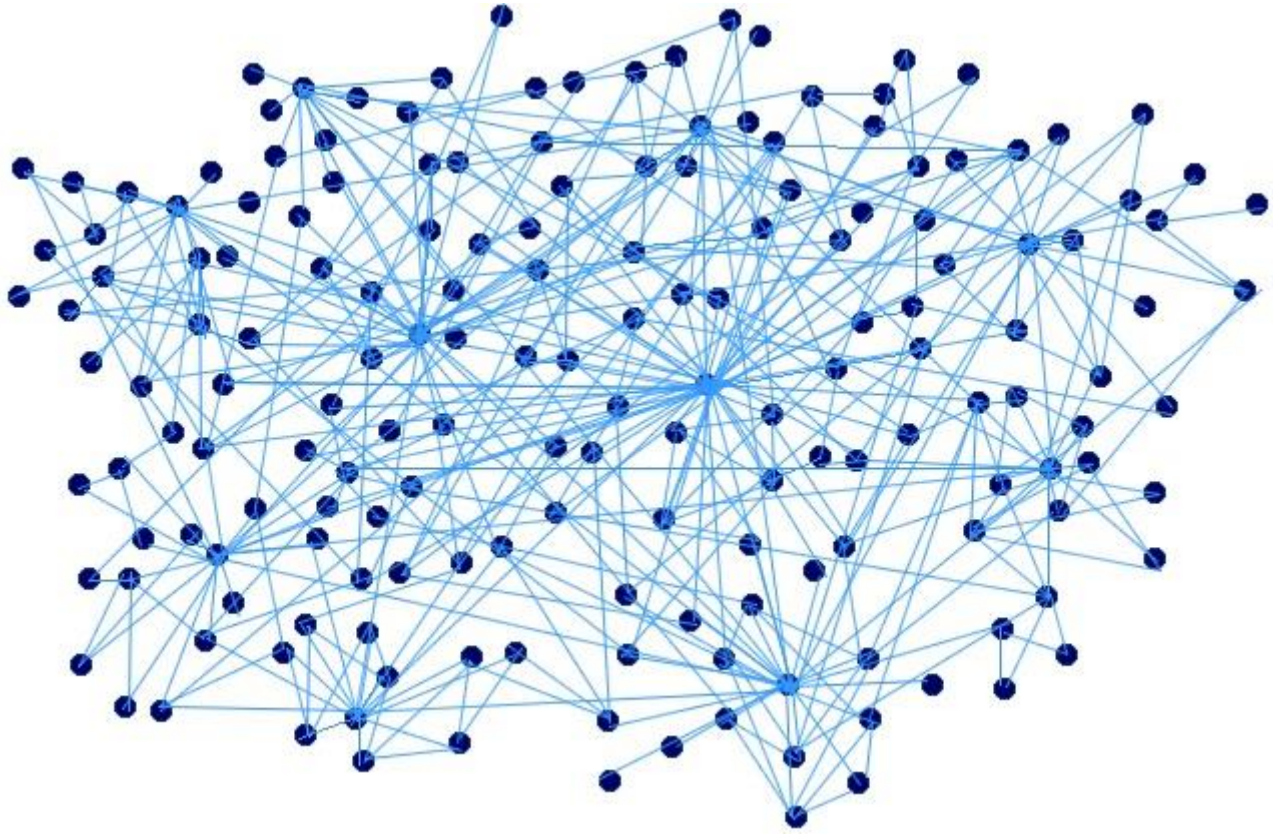
   Extensions of models for learning in structured domains

   - Motivation and examples (structured data)
   - The structured data (recursive)
   - Recursive models: RNN and RecNN
   - Recursive Cascade Correlation & other recursive approaches

2. Moving to DPAG and Graphs: the role of causality [Next Lecture (SD-2)]

An introductive aim for a research field in ML

Why structured data?



Because data have relationships

Introduction: Motivation of ML for SD

- Most of known ML methods are limited to the use of flat and fixed form of the data (vectors or sequences)

  fixed-length attribute-value vectors

- Central: *data representation*
- Graph: very useful abstraction for real data

- **Labeled graphs** = vector patterns + relationships
  - **natural**: for structured domain
  - **richness**
  - **efficiency**: repetitive nature inherent in the data

- **SD + ML =** adaptive processing of structured information

Introduction: Research Area

- **SD + ML =** adaptive processing of structured information
- **General Aim**: investigation of ML models for the adaptive processing of structured information: **sequences, trees, graphs/networks**
- Terminologies:
  - Structured domain learning/ Learning in Structured Domains
  - Graph Representation Learning, Learning with/for/on graphs
  - Relational Learning
  - Structures/Graphs Mining
    - Also sub-areas, e.g. Molecule Mining
  - Deep learning for graphs: (deep) NN for Graphs (NN4G/DNNG), NN on Graphs, Graph NN (GNN), Graph Convolutional Networks (GCN), RecGNN*, ConvGNN*, Graph Nets, Deep Graph Networks (DGN)**, …

* A Comprehensive Survey on Graph Neural Networks – TNNLS Jan. 2021

** A gentle introduction to deep learning for graphs – Neural Networks Sep. 2020

Increasing Attention in ML

- Dozens of new research papers in all the top-tier ML venues (literature is rapidly growing)

- And concrete real-world applications

Advancements from ML to SDL

Learning in Structured Domains (SD) in Pisa/CIML: Pioneering since the 90's the development of

- Theoretical analysis
- New approaches
- Applications

Especially on the basis of Recursive approaches.

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And for you?

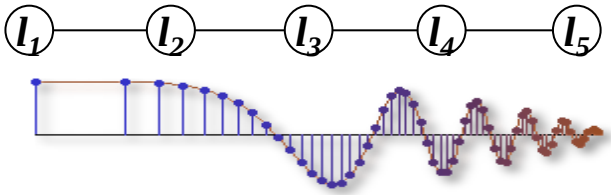
- To build and advanced background for
  - Analysis/development of innovative models
  - Applications in the are of interdisciplinary projects (@ ciml)
- Practical: **thesis are possible for the design of new models/applications for the extension of the input domains toward:**
  - Extension of the applicative domain
  - Adaptivity and accuracy
  - Efficiency

From flat to structured data

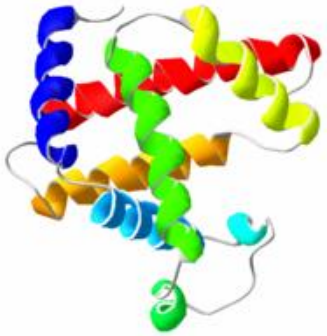
- **Flat: vectors** (as in most of the ML course)
- **Structured:** Sequences, trees, graphs, multi-relational data

stringa_in_italiano

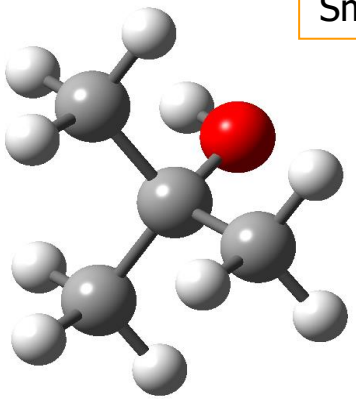
Strings



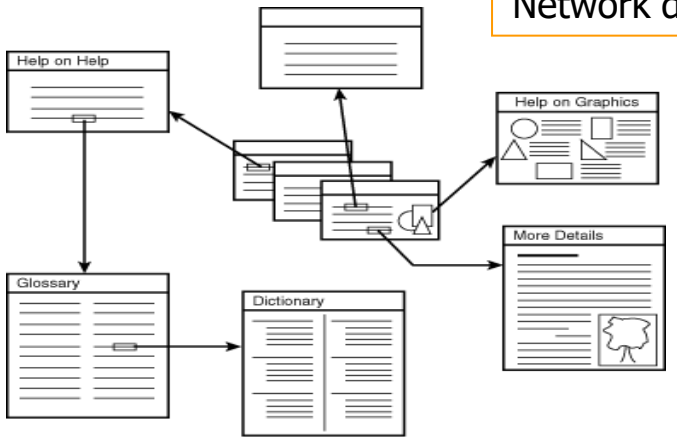
Series/
temporal stream



Proteins

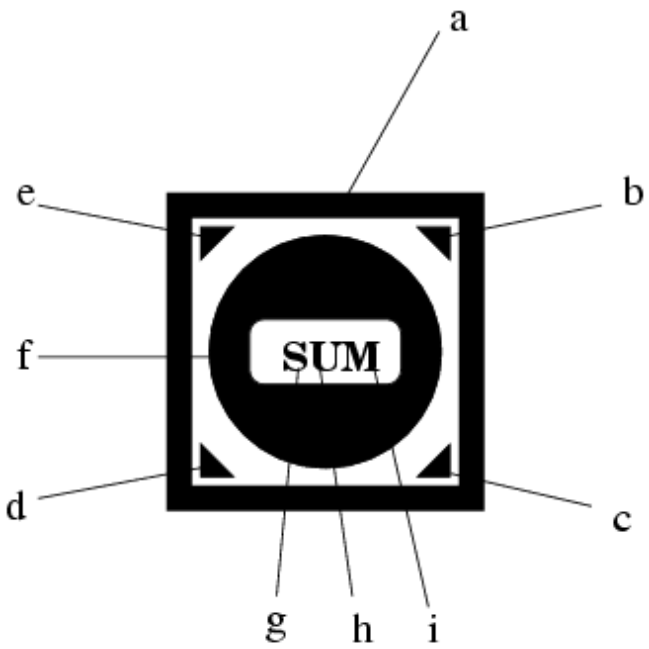


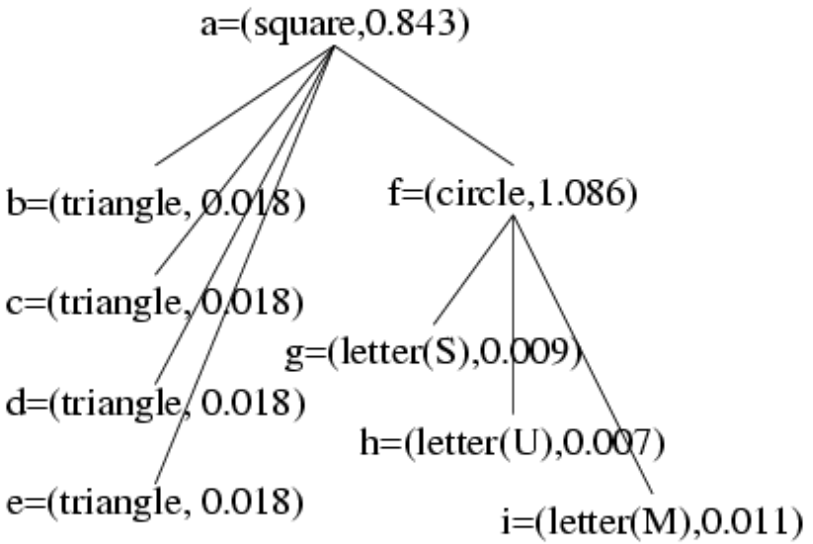
Small molecules

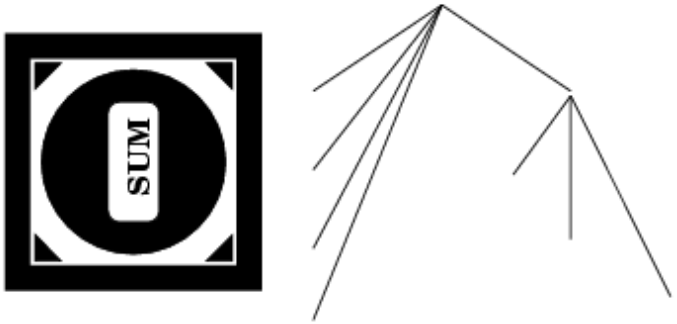


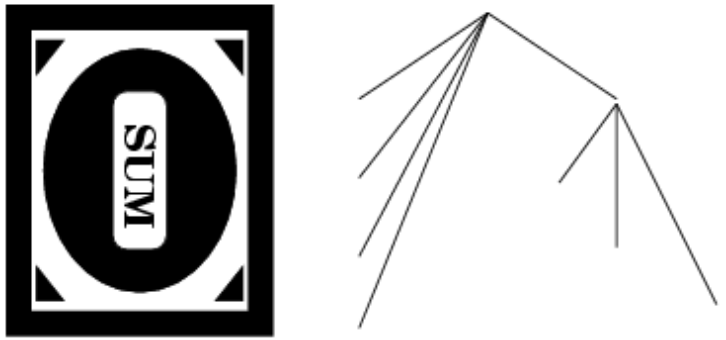
Network data

Example: logo recognition

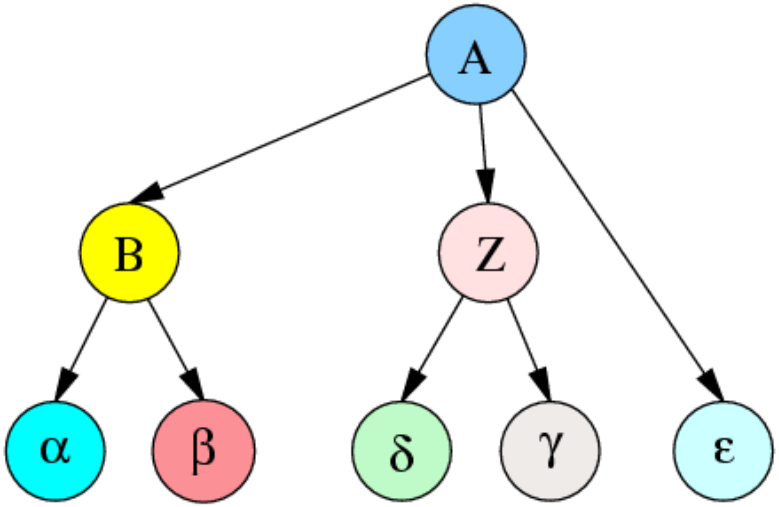




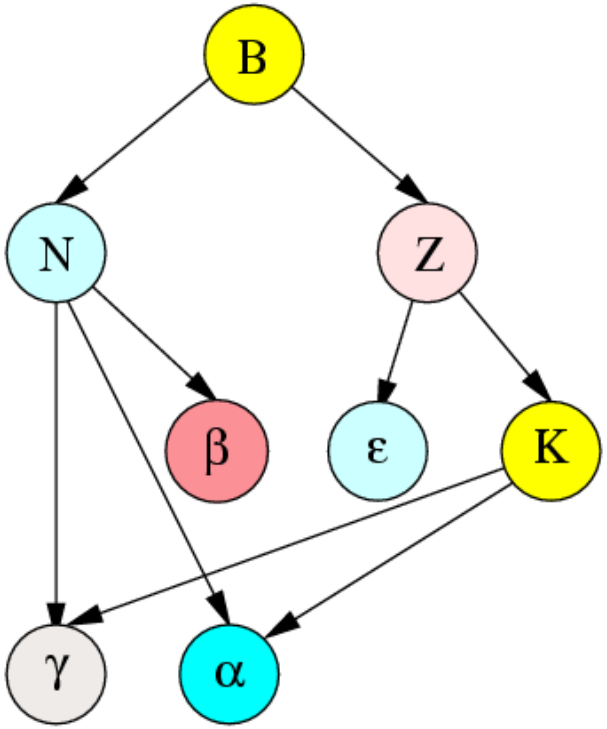




Example: Terms in 1st order logic

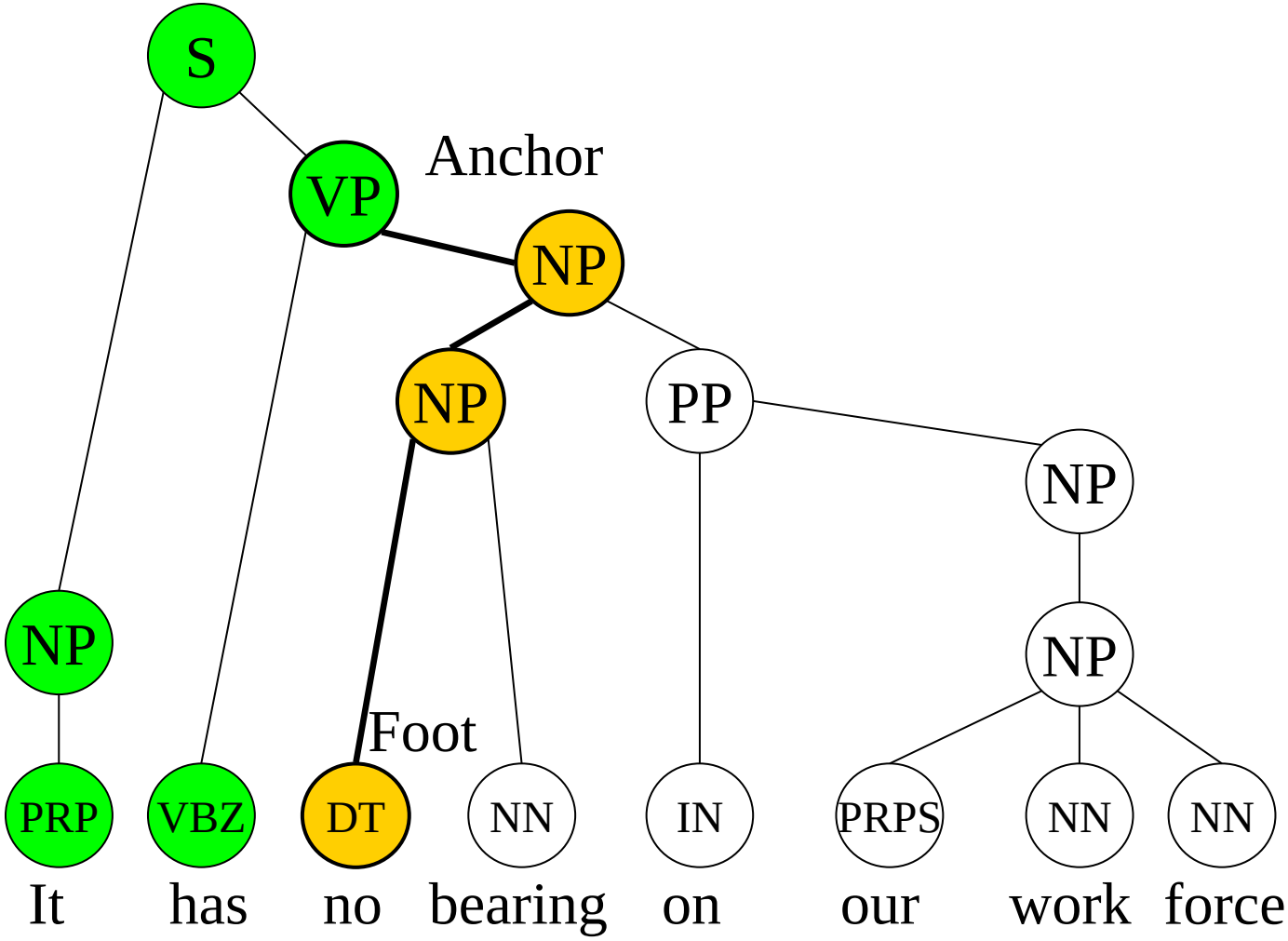


A(B(α,β),Z(γ,δ),ε)

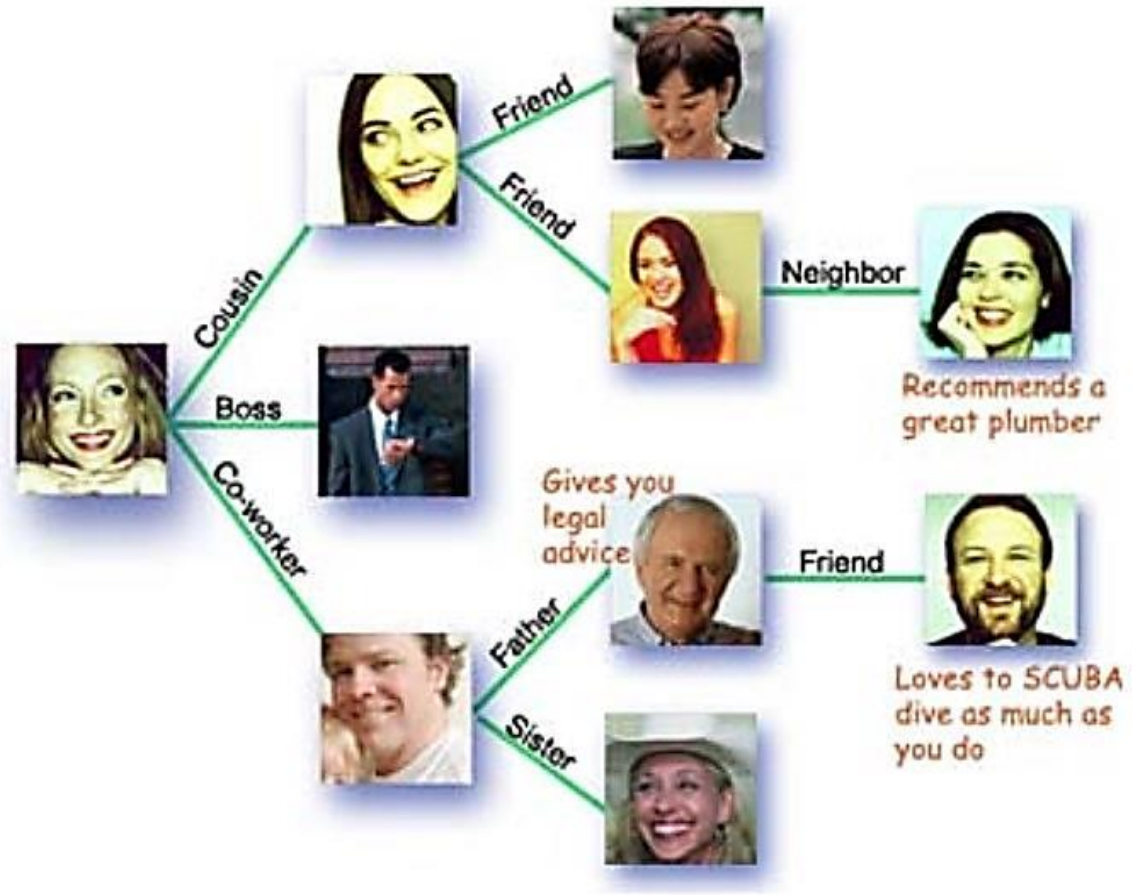


B(N(γ,α,β),Z(ε,K(γ,α)))

Example (trees): language parsing



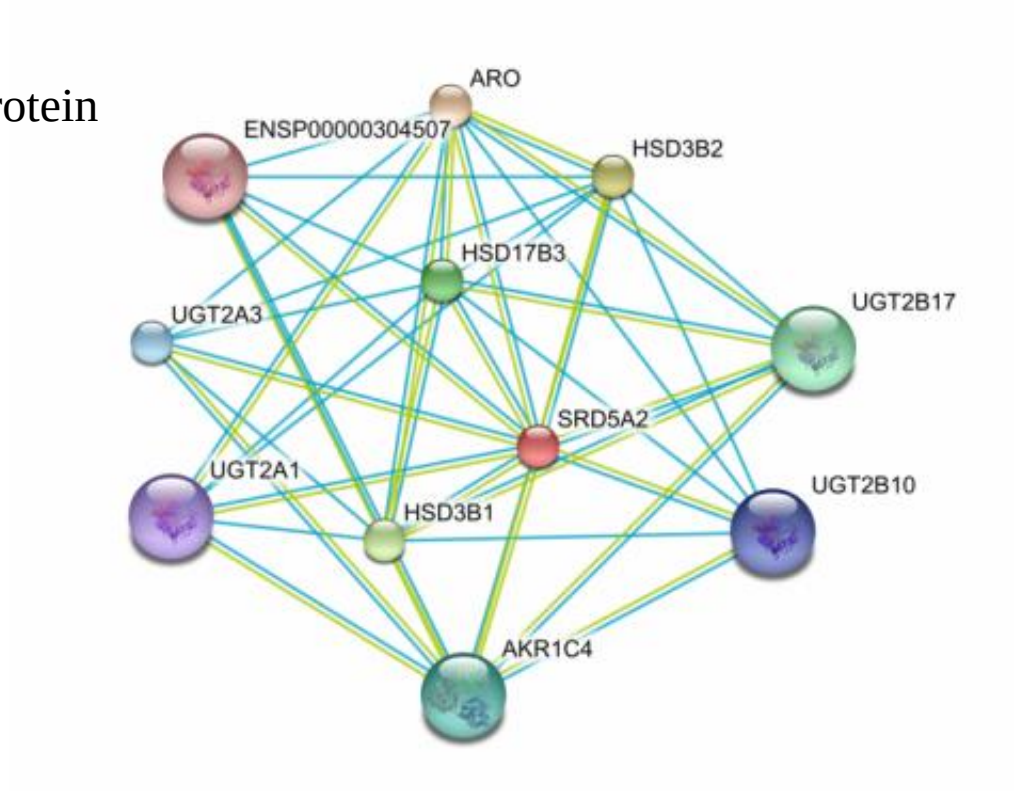
Example: Social networks



Example: Biological Networks

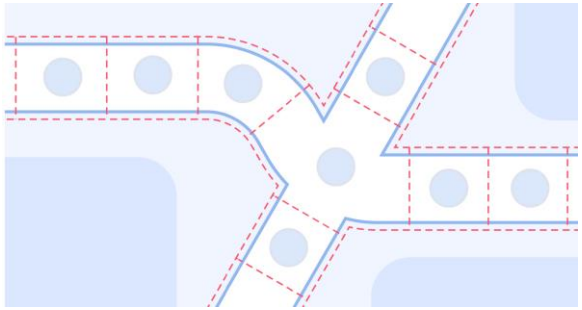
- Node for protein
- Link for **interaction** or similarity

Protein



Example: Google maps – traffic estimates

- DeepMind – Google Maps. Sept. 2020
- **Aim**: accurate traffic predictions and estimated times of arrival (ETAs)
- **Graphs**: networks of roads
  - Node: each route segment
  - Edges: between segments that are consecutive on the same road or connected throughh an intersection
- **Task**: predicts the travel time for each supersegment (multiple adjacent segments of road that share significant traffic volume - subgraphs)

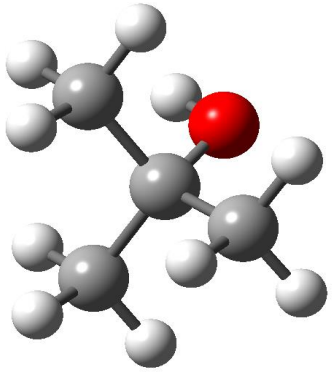


- **Results**: improve the accuracy of real time ETAs by up to 50% in places like Berlin, Jakarta, São Paulo, Sydney, Tokyo, and Washington D.C. by using Graph Neural Networks (indeed we will see *Convolutional NN for graphs*)

Traffic prediction with advanced Graph Neural Networks | DeepMind

Example (graphs): Molecules

- A fundamental problem in Chemistry: correlate chemical structure of molecules with their properties (e.g. physico-chemical properties, or biological activity of molecules) in order to be able to predict these properties for new molecules
  - Quantitative Structure-Property Relationship (QSPR)
  - Quantitative Structure-Activity Relationship (QSAR)



*Property/Activity = **T**(Structure)*

T

Property Value (regression)
Toxic (yes/no) (classification)

QSPR: Correlate chemical structure of molecules with their properties

Molecules are not vectors !

Molecules can be more naturally represented by varying size ***structures***

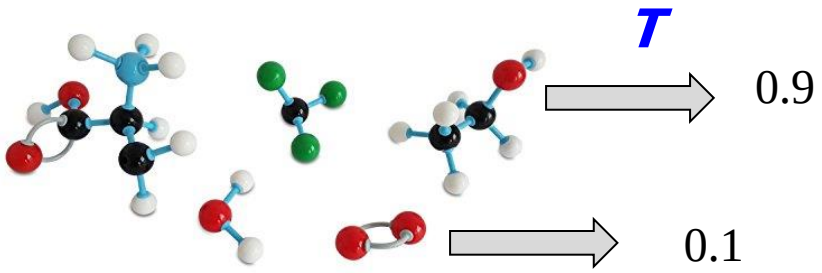
Can we predict directly from structures ?

Learn a transduction

- **Goal**: to learn a mapping between a structured information domain (SD) and a discrete or continuous space (*transduction **T***).

- Start with this problem: classify variable size graphs
  - For instance, classify different graphs starting from a training set of know couples as in the molecules example

- Given a set of examples ($graph_i$,$target_i$) (in the training set)
- Learn a hypothesis mapping *T(graph)*



Introduction: Learning Model for SD

- The problem: there has been no systematic way to extract features or metrics relations between examples for SD
  - We are looking to the automatic extraction of the salinet topological information directly from data
  - A representation learning instances (extended to SD)!

Our "mantra"
Instead of moving *data to models*
(e.g. Graphs into vectors or trees into sequences, with alignment problems, loose of information, etc.)
we move *models to data*

Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

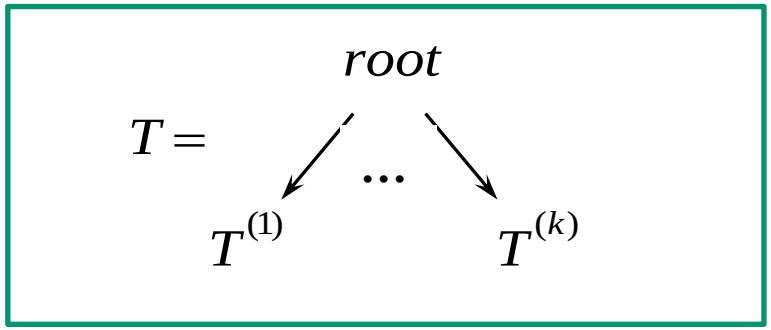
   Extensions of models for learning in structured domains

   - Motivation and examples (structured data)
   - **The structured data (recursive)**
   - Recursive models: RNN and RecNN
   - Recursive Cascade Correlation & other recursive approaches

2. Moving to DPAG and Graphs: the role of causality [Next Lecture (SD-2)]

K-ary Trees

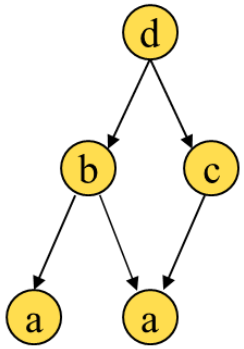
- ***k-ary trees*** (*trees* in the following) are rooted positional trees with finite out-degree k.
- Given a node v in the tree $T \in \boldsymbol{G}$:
  - The children of v are the node successors of v, each with a position $j=1,\ldots k$;
  - k is the maximum out-degree over G, i.e. the maximum number of children for each node;
  - $l(v)$ in is the input label associated with v, and $l_i(v)$ is the i-th element of the label;
  - The *subtree* $T^{(j)}$ is a tree rooted at the j-th children of v.



Structured Domains

- ***L***: set of attribute vectors $l(v)$
- *Structure G*: vertexes labels ***L*** + topology (*skeleton* of *G*)
- Sequences, Trees, DOAGs- DPAGs, graphs.

- We start considering sets of **DPAG**s (recursive structures), i.e.
- ***G*** as *labeled direct positional acyclic graphs* with:
  - *Super-source*: a vertex *s* such that every vertex can be reached by a direct path starting from *s.*
  - A total order (or the *position*) on the edges leaving from each vertex
  - *Bounded out-degree and in-degree* (the number of edges leaving and entering from a vertex *v*)



Data Domains *G*

- Include sub-classes:

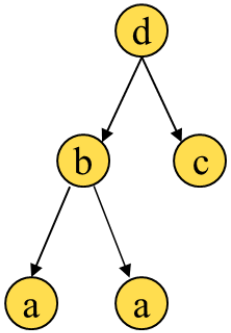
  DPAGs ⊃ DOAGs ⊃ k-ary trees ⊃ sequences ⊃ vectors.

- **DPAG**: supeclass of the **DOAG**s: besides ordering, a distinctive positive integer can be associated to each edge, allowing some position to be absent.

- **Trees**: labeled rooted order trees, or positional (*K-ary* trees).
  - Super-source: the root of the tree.
  - **Binary tree (K=2)**

  Mostly used in this lecture

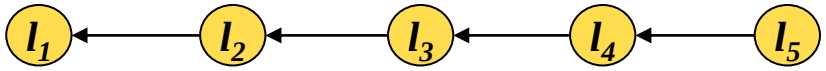
- Notations:
  - ch[*v*] set of successors of *v*
  - $ch_j[v]$ is the j-th child of the node *v*



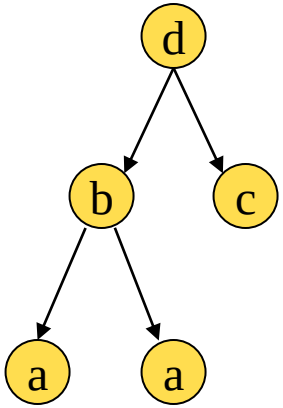
Structured Data: Examples

- Labeled Sequences, Trees, DOAGs- DPAGs, graphs

Single labeled vertex

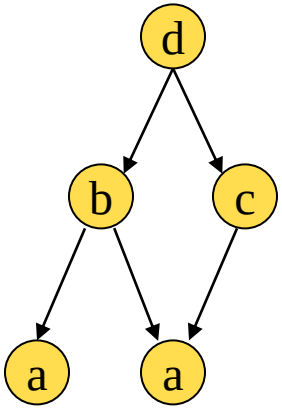


Sequence

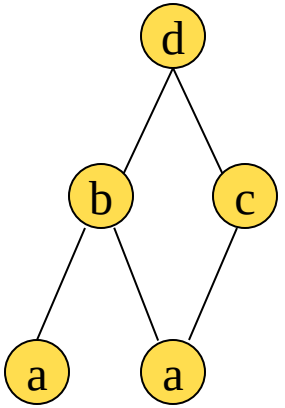


Rooted Tree

Supersource



DPAG



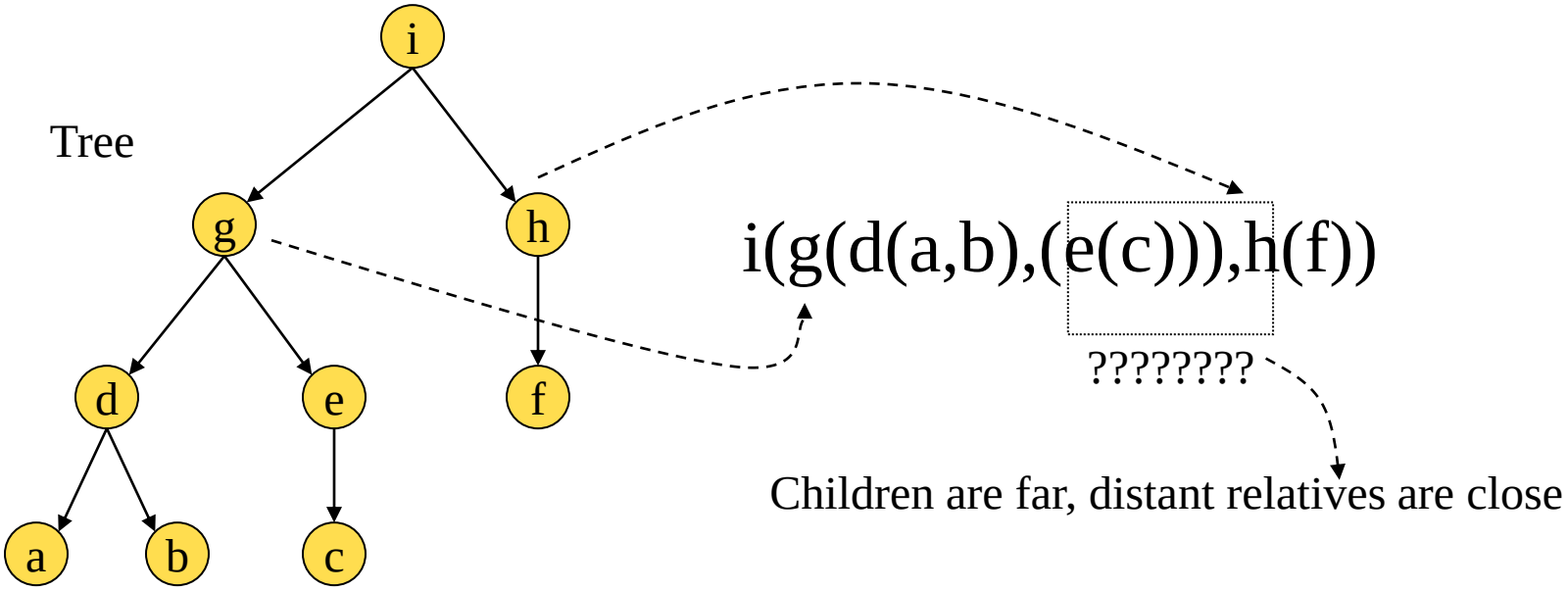
Graph (undirected)

DPAG: labeled direct positional acyclic graphs with *super-source*, bounded *in-degree* and *out-degree* (*k*).

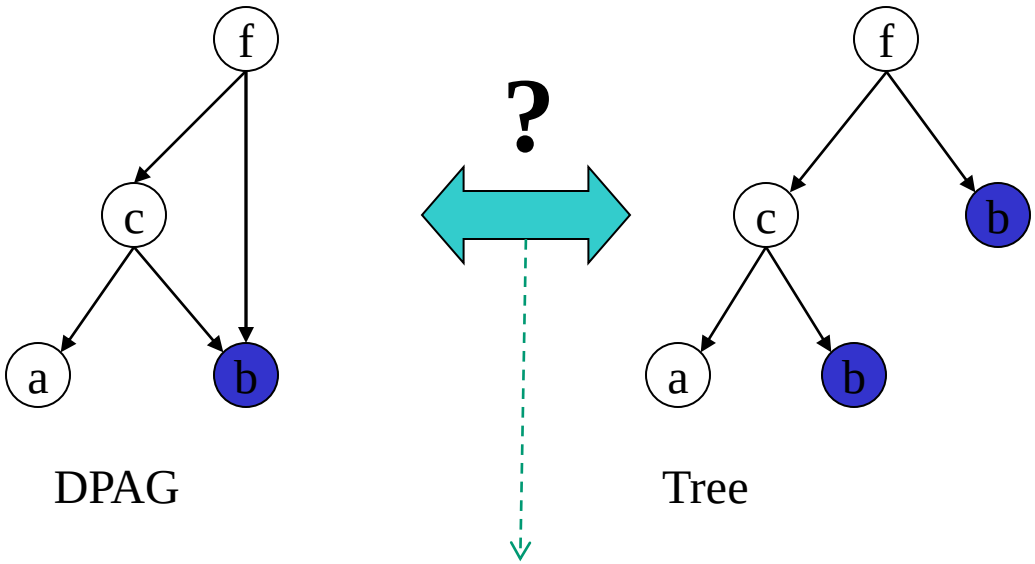
Structures: just use sequence ?

- Can we process structures like they are sequences?
- E.g. any tree can be converted into a sequence (no information loss) but:
  - Sequences may be long: number of vertices exponential w.r.t. height of tree

    (aka the paths are *log* of #nodes for the tree, so the dependencies are much shorter)
  - Dependencies are blurred out (arbitrary depending on the visit)



Trees and DPGAs



DPAG

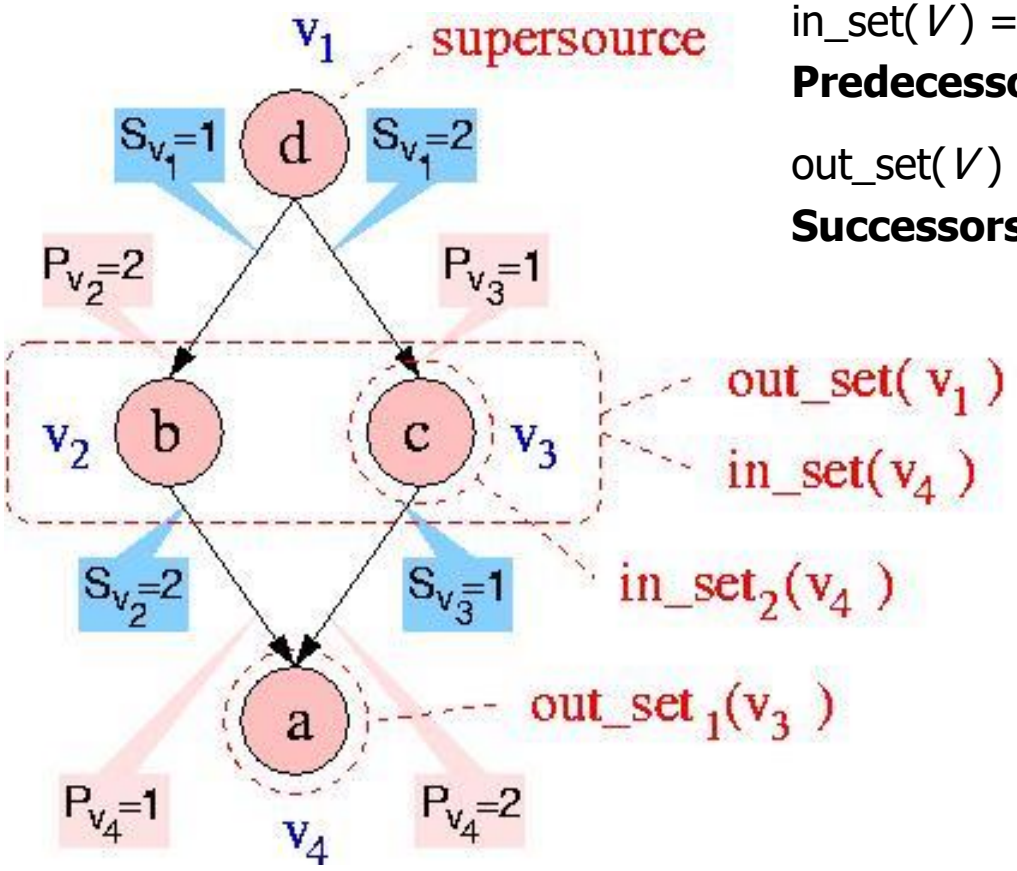
Tree

b: shared node

Exercise after the lecture SD-2

Positional versus Ordered (details)

- DPAG: for each vertex *v in vert(G)*, an injective function S_v: *edg(v)* → [*1,2,...,K*] is defined on the edges leaving from *v*



in_set(V) = {u | $v \in V$ and $u \rightarrow v$}
Predecessors

out_set(V) = {u | $v \in V$ and $v \rightarrow u$}
Successors

Models:
Restarting from the beginning:
Recurrent and Recursive models

Learning in Structured Domain
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1. Recurrent and Recursive Neural Networks

   Extensions of models for learning in structured domains

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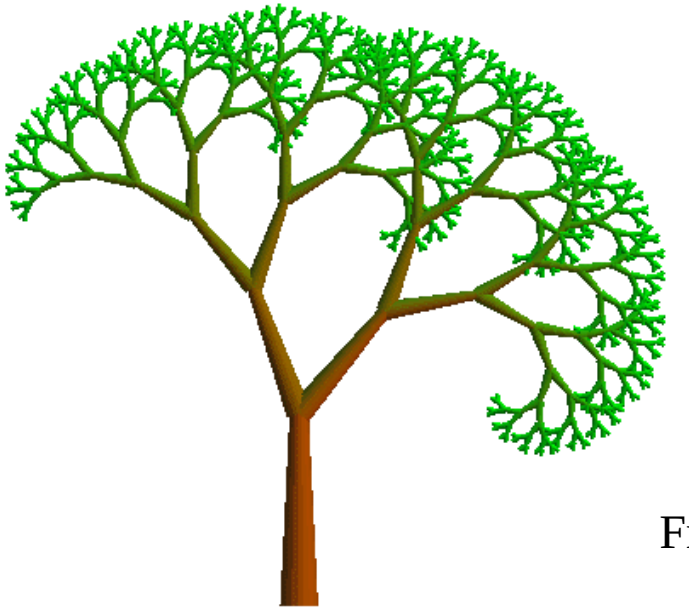
   - The structured data (recursive)
   - **Recursive models: RNN and RecNN**
   - Recursive Cascade Correlation & other recursive approaches

2. Moving to DPAG and Graphs: the role of causality [Next Lecture (SD-2)]

Preview: The RecNN idea

Recursive NN:

- **Recursive** and parametric realization of the transduction function
  - In other words: Node embedding by a neural state machine
- *Adaptive* by Neural Networks



We will see how RecNNs extend RNNs *matching* the *recursive* nature of trees (moving the model to the nature of the data)

Fractal tree: a recursive structure

Summary of the Neural Computing Approach

Domain	Neural Network
Static fixed-dim patterns (vectors, records, ...)	Feedforward
Dynamical patterns (temporal sequences, sequences ...)	**Recurrent**
Structured patterns (trees, DPAGs, ...)	**Recursive**

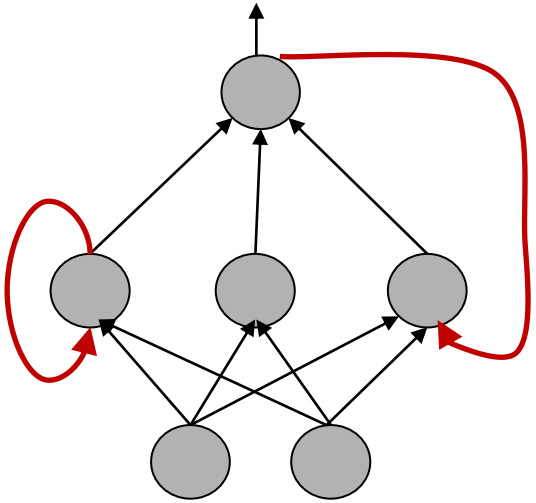
Feedforward versus Recurrent *(memento)*

- **Feedforward**: direction: input→ output
- **Recurrent** neural networks: A different category of architecture, based on the addition of *feedback loops* connections in the network topology,
  - The presence of **self-loop** connections provides the network with dynamical properties, letting a memory of the past computations in the model.
  - This allows us to extend the representation capability of the model to the processing of sequences (and structured data).

Recurrent neural networks:

- Introduced in the ML course
- They will be the subject

  (further developed) ISPR/CNS courses (see later).



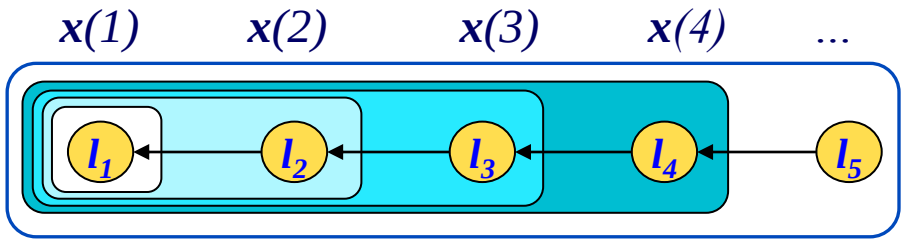
Recurrent Neural Networks (*resume*)

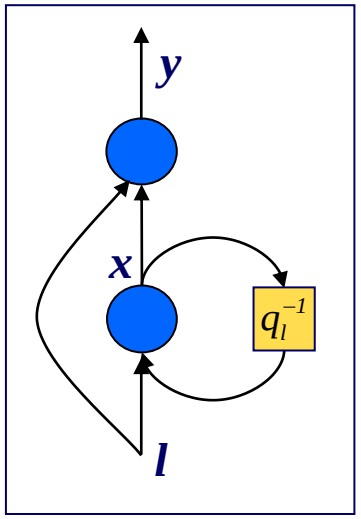
- Up to now:

Given $\boldsymbol{x(0) = 0}$

internal state

$$\begin{cases} \boldsymbol{x}(t) = \tau(\boldsymbol{x}(t-1), \boldsymbol{l}(t)) \\ \boldsymbol{y}(t) = g(\boldsymbol{x}(t), \boldsymbol{l}(t)) \end{cases}$$





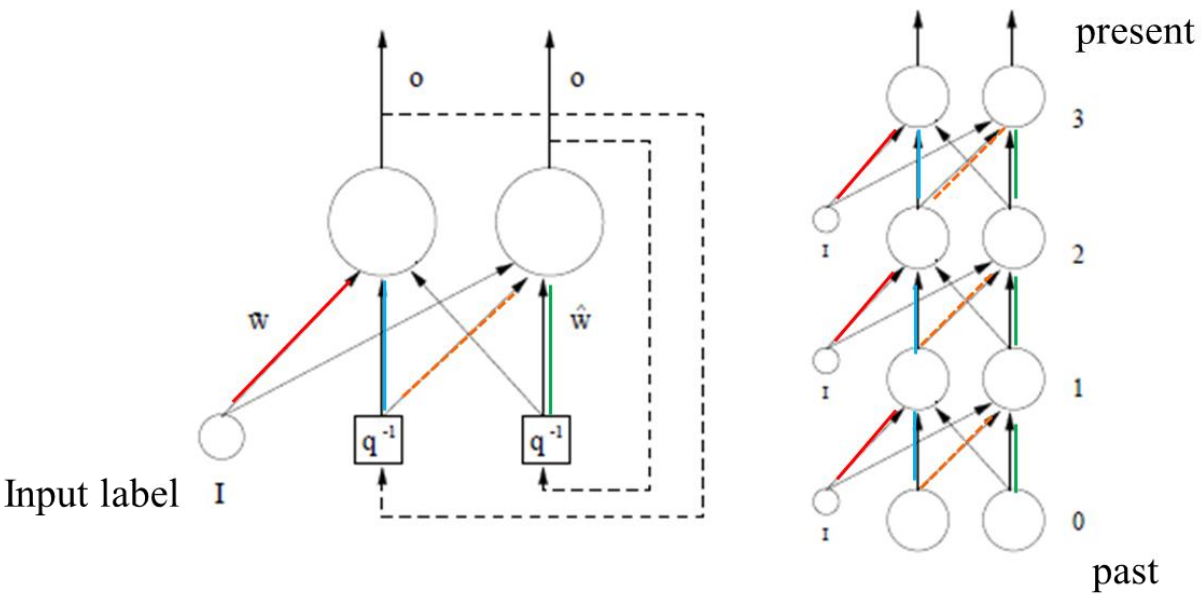
Graphical model

E.g. also **HMM**

- Tau is the *state transition (next-state)* function realized by a NN (say τ_{NN})

RNN training and properties (*resume*)

- BPTT/RTRL [see CNS course]
- Unfolding [see ML lecture RNN]:



Back-Prop Through Time: Backprop on this enrolled version

- Causality: A system is causal if the output at time t_0 (or vertex v) only depends on inputs at time $t<t_0$ (depends only on v and its descendants)
  - necessary and sufficient for *internal state*
- Stationarity: time invariance, state transition function τ is independent on node v (the same in any time)

Recursive Neural Networks (overview)

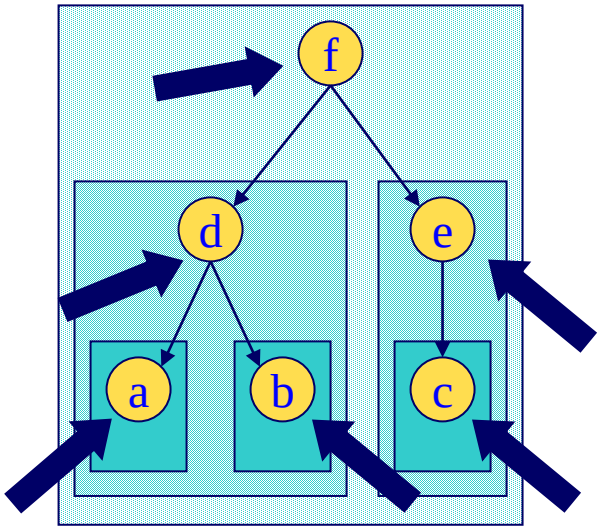
NEW

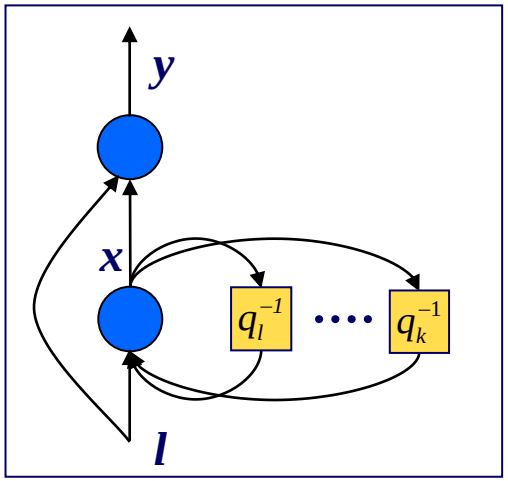
- Now:

$$\begin{cases} \boldsymbol{x}(v) = \tau(\boldsymbol{x}(\mathrm{ch}[v]), \boldsymbol{l}(v)) \\ \boldsymbol{y}(v) = g(\boldsymbol{x}(\mathrm{v}), \boldsymbol{l}(v)) \end{cases}$$

$$\boldsymbol{x}(\mathrm{ch}[v]) = \boldsymbol{x}(\mathrm{ch}_1[v]), \ldots, \boldsymbol{x}(\mathrm{ch}_k[v])$$

State transition system (for trees)





 # feedbacks = # children

Recursive Neural Networks (overview)

More precisely (with initial conditions)

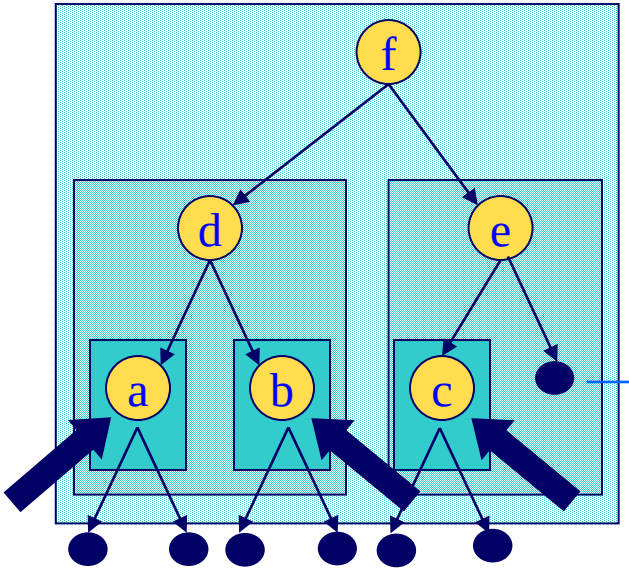
- Now:

Given $\boldsymbol{x}(nil) = 0$

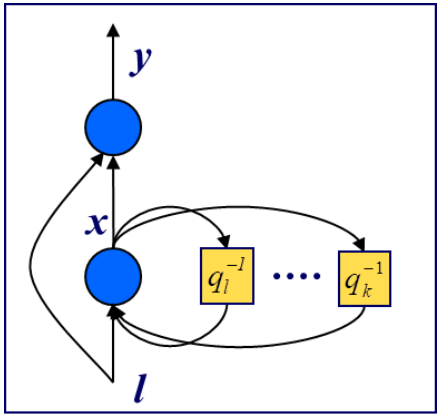
$$\begin{cases} \boldsymbol{x}(v) = \tau(\boldsymbol{x}(\mathrm{ch}[v]), \boldsymbol{l}(v)) \\ \boldsymbol{y}(v) = g(\boldsymbol{x}(\mathrm{v}), \boldsymbol{l}(v)) \end{cases}$$

$$\boldsymbol{x}(\mathrm{ch}[v]) = \boldsymbol{x}(\mathrm{ch}_1[v]), \ldots, \boldsymbol{x}(\mathrm{ch}_k[v])$$

State transition sytem



nil or $\boldsymbol{x}_0$
or empty node



 # feedbacks = # children

Generalized Shift Operators

- Standard shift operator (time):

$$q^{-1}\, S_t = S_{t-1}$$

- Generalized shift operators (structure):

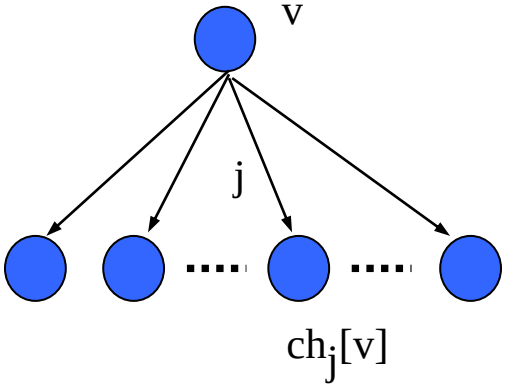
$$q_j^{-1}\, G_v = G_{ch_j[v]}$$

where $ch_j[v]$ is the j-th child of v

RecNN with q:

$$\begin{cases} \boldsymbol{x}(v) = \tau(\boldsymbol{l}(v), \boldsymbol{q}^{-1}\boldsymbol{x}(v)) \\ \boldsymbol{y}(v) = g(\boldsymbol{x}(\mathrm{v})) \end{cases}$$

$$\begin{cases} q_j^{-1} x_i(v) = x_0 & \text{if } \mathrm{ch}_j[v] = nil \\ q_j^{-1} x_i(v) = x_i(\mathrm{ch}_j[v])) & \text{otherwise} \end{cases}$$



Used to extend the states for children of vertexes of the tree

Learning in Structured Domain
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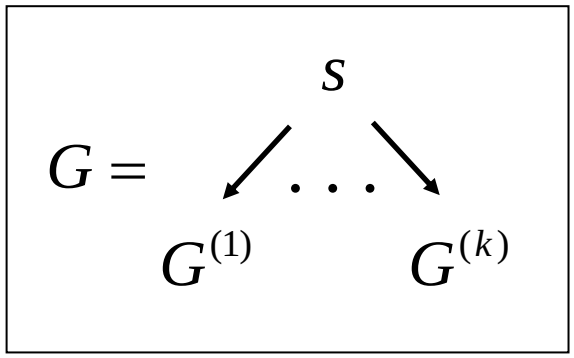
2. Moving to DPAG and Graphs: the role of causality
   [Next Lecture (SD-2)]

Recursive Processing (*a different point of view*)

Recursive definition of τ_E (*encoding function*)

Node/Graph embedding

$$\boldsymbol{x}(root) = \tau_E(G)$$



s can be either a *root* for a tree or a super-source for a DPAG

$G^{(j)}$ is a subgraph rooted in the children *j* of *s*.
s has a label $\boldsymbol{l}(s)=L_{root}$

$$\tau_E(G) = \begin{cases} \boldsymbol{0} & \text{if } G \text{ is empty} \\ \tau_{NN}(L_{root}, \tau_E(G^{(1)}),\ldots,\tau_E(G^{(k)})) \end{cases}$$

$\boldsymbol{\tau_E}$: systematic visit of $G \rightarrow$ it guides the application of τ (in the form of a NN τ_{NN}) to each node of tree (bottom-up).
Causality and *stationary* assumption.

Properties or RecNN (I)

Extension of *causality* and *stationarity* defined for RNN:

- **Causality:** the output for a vertex v only depends on v and its descendants (induced subgraphs)
  - Compositionality over the input structure!

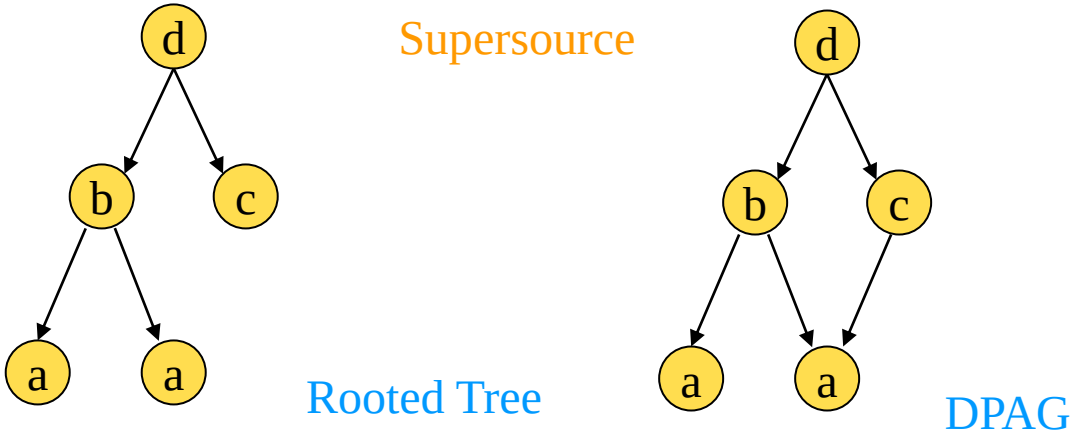
- **Stationarity**: state transition function τ_{NN} is independent on vertex v
  - Parsimony: we use the same NN for each vertex, regardless of the dimension of sequences (useful to process structures of variable size with a fixed size of the model)

Recurrent/recursive NN transductions admit a recursive state representation with such properties

- **Adaptivity** (NN. learn. Alg.) **+ Universal approximation** over the tree domain [Hammer 2005-2007]

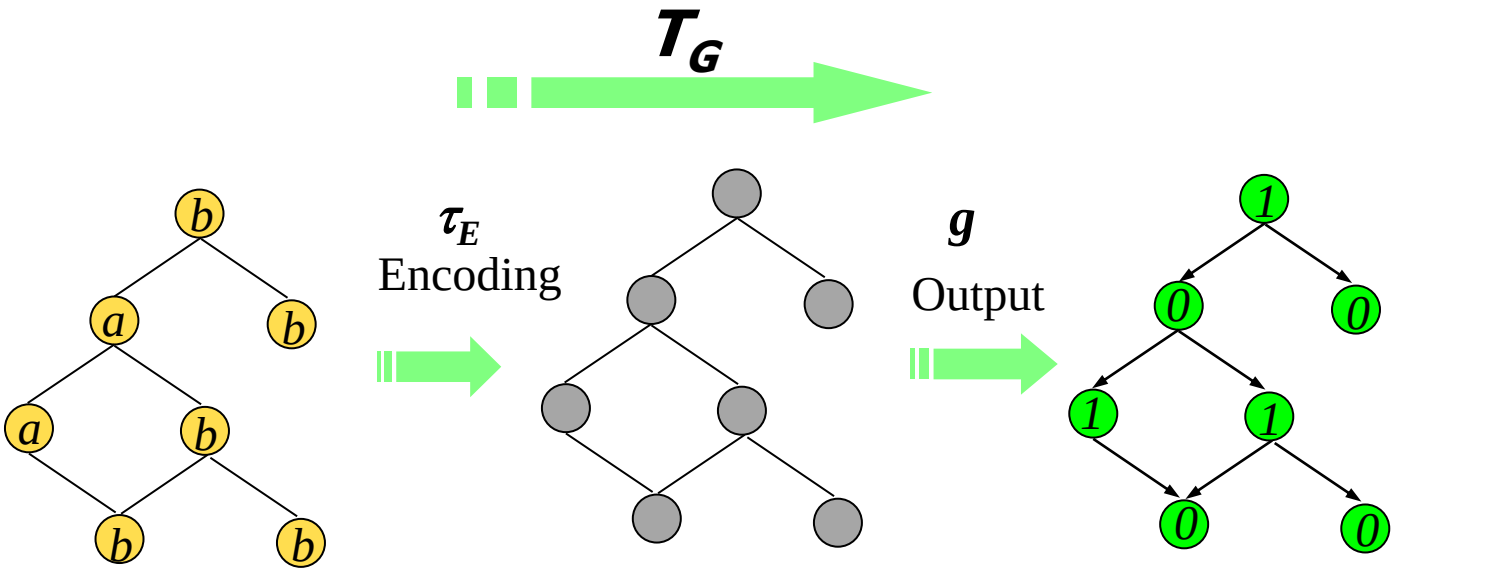
Property (II): Kind of graphs for RecNN

- RecNN can in principle treat both Trees and DOAGs/DPAGs
  - Whether it can discriminate completely also the DOAG/DPAGs will discussed later
  - But if there are no cycles the *recursive* model can visit the input DOAG/DAPG without special care



Properties (III): Transduction: graphical view

- $\boldsymbol{T_G}$ is *IO-isomorph* if G and $\boldsymbol{T_G}(G)$ have the same skeleton (graph after removing labels)



Input DPAG

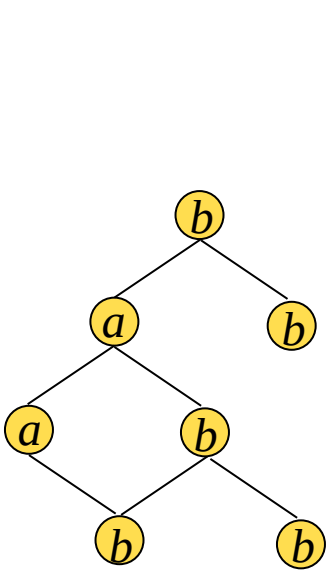
State space $x(G)$
internal rep./encoding
Node/Graph embedding

Output DPAG

Structure-to-Structure transductions

Properties (IV): Transduction: graphical view

- τ_G *Supersource* transductions



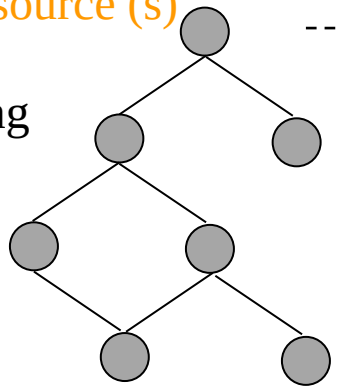
Input DPAG

τ_G

Supersource (s)

τ_E

Encoding



State space $x(G)$

internal rep./encoding

Node/Graph embedding

g

Output

$y(s)$

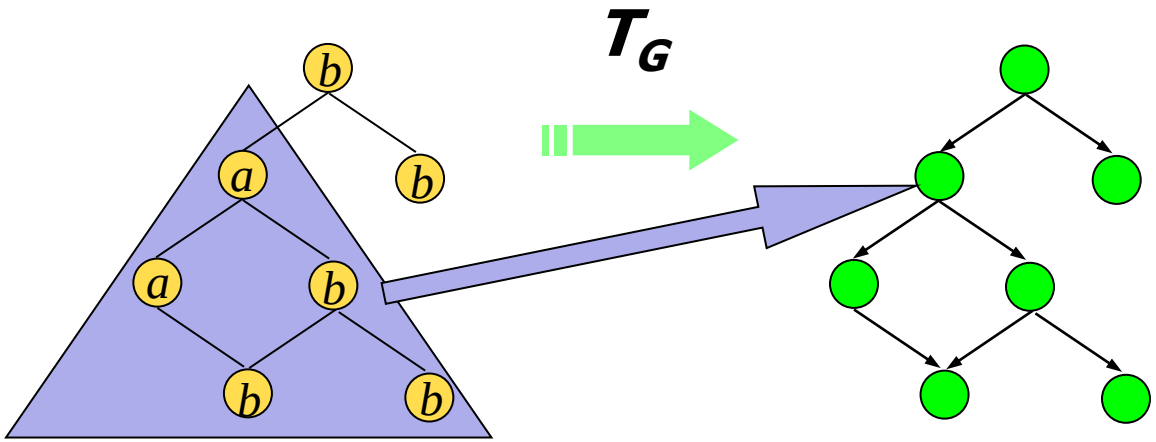
Scalar Value (regression/ classification)

Structure-to-Element

Or Supersource transductions

Properties (IV)

- IO-isomorph ***causal*** transduction
- **Causality:** the output for a vertex *v* only depends on *v* and its descendants (induced subgraphs)
  - Compositionality over the input structure!



Only the sub-structure is considered

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   [Next Lecture (SD-2)]

Unfolding and Enc. Network

- We will see (again) the RecNN data flow process with two points of view:

1. Unfolding by "Walking on structures" model (*stationarity*), according to *causal* assumption (inverse topological order*).
   - The model visits the structures

2. Building an Encoding network isomorph to the input structure (same skeleton, inverse arrows, again with *stationarity*) and *causal* assumption):
   - We build a different encoding network for each input structure

* see next slide

Topological Order

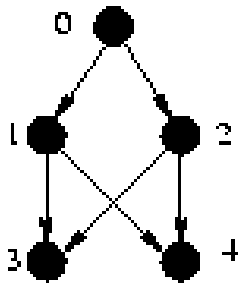
- A linear ordering of its nodes s.t. each node comes before all nodes to which it has edges. Every DAG has at least one topological sort, and may have many.

- A numbering of the *vertices* of a *directed acyclic graph* such that every *edge* from a vertex numbered i to a vertex numbered j satisfies i<j.

According to a Partial order

For RNN:

Inverse topological order

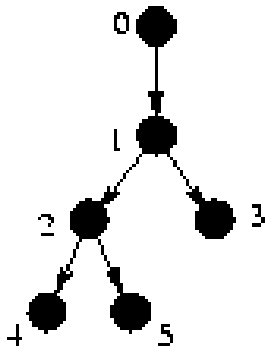


0,1,2,3,4

0,1,2,4,3

0,2,1,3,4

0,2,1,4,3



0,1,3,2,4,5

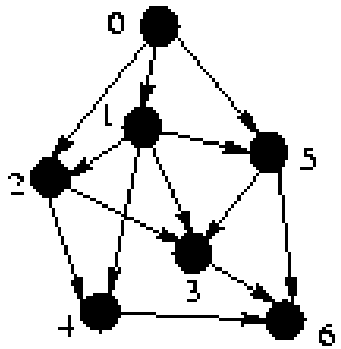
0,1,3,2,5,4

0,1,2,3,4,5

0,1,2,3,5,4

...

0,1,2,5,4,3



0,1,2,4,5,3,6

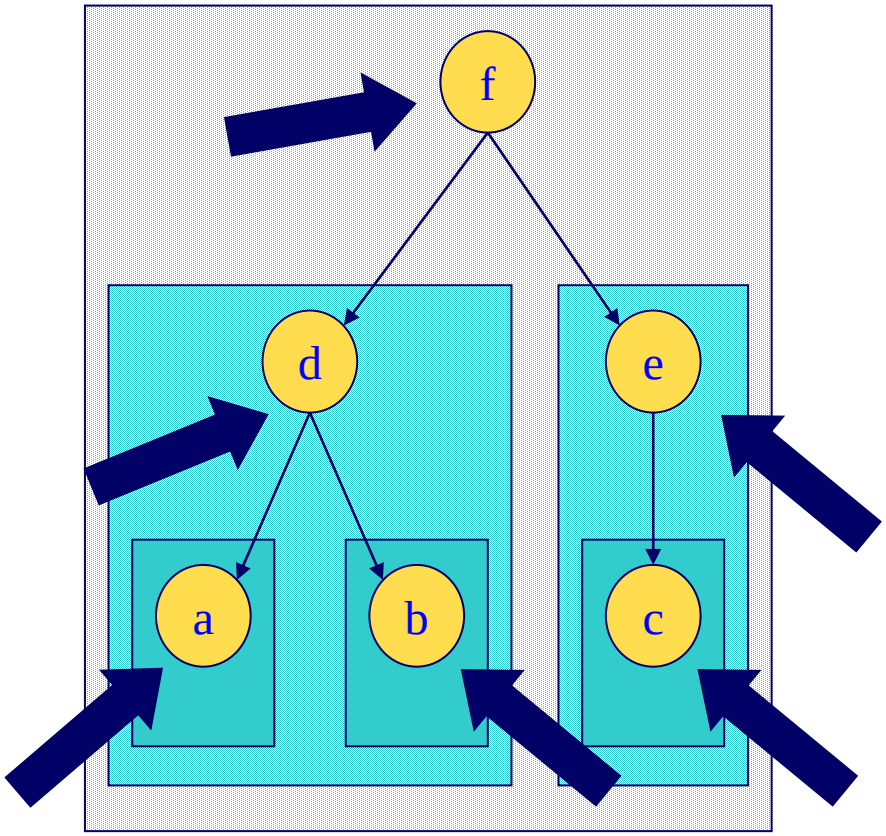
0,1,2,5,3,4,6

0,1,2,5,4,3,6

0,1,5,2,3,4,6

0,1,5,2,4,3,6

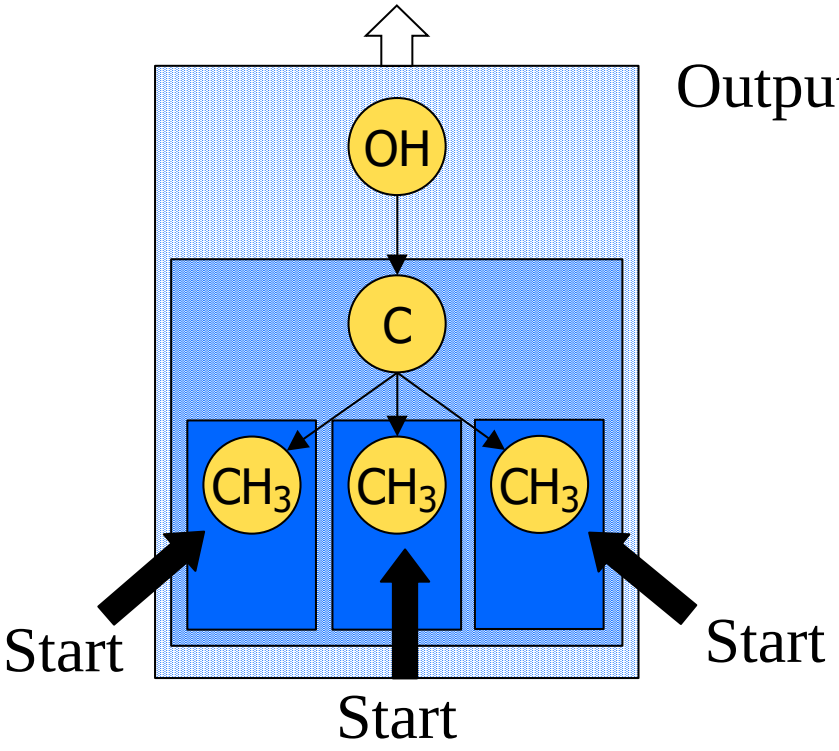
Unfolding & Encoding Process:
Unfolding view (1)



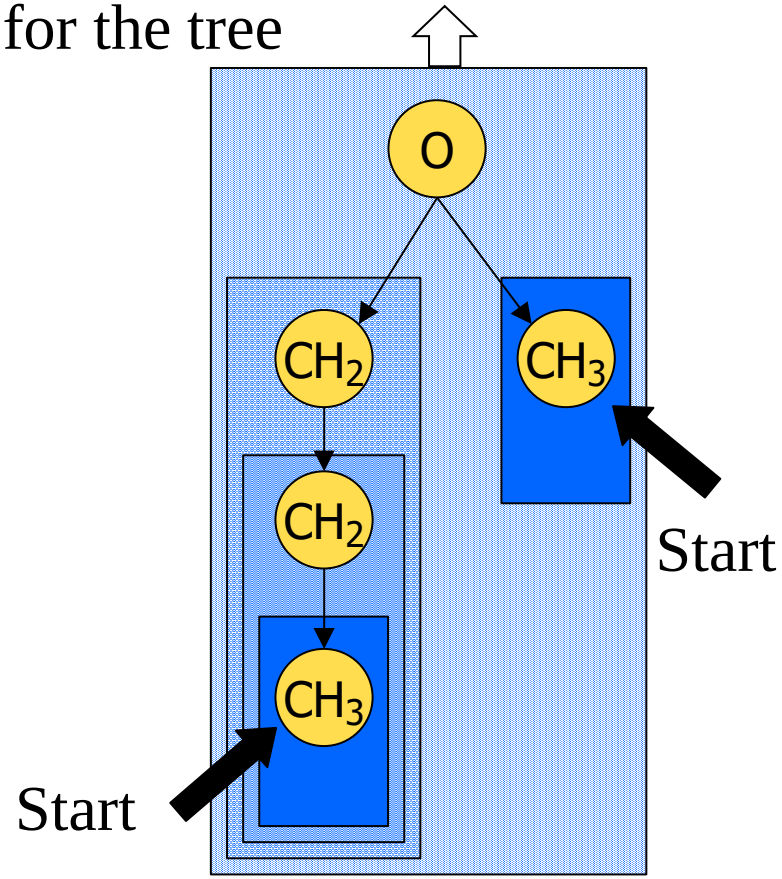
- Unfolding the encoding process trough structures
- Bottom-up process for visiting

- We will see later how to make it with τ_{NN} (and hence by NN) for each step: to build an *encoding network*

RecNN over different structures: unfolding 2



Output for the tree

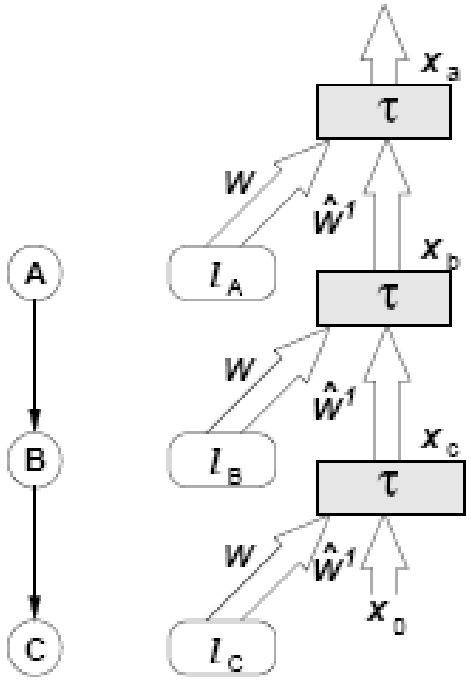


Examples on different trees for chemical compounds:

Unfolding through structures:

The same process applies to all the vertices of a tree and for all the trees in the data set

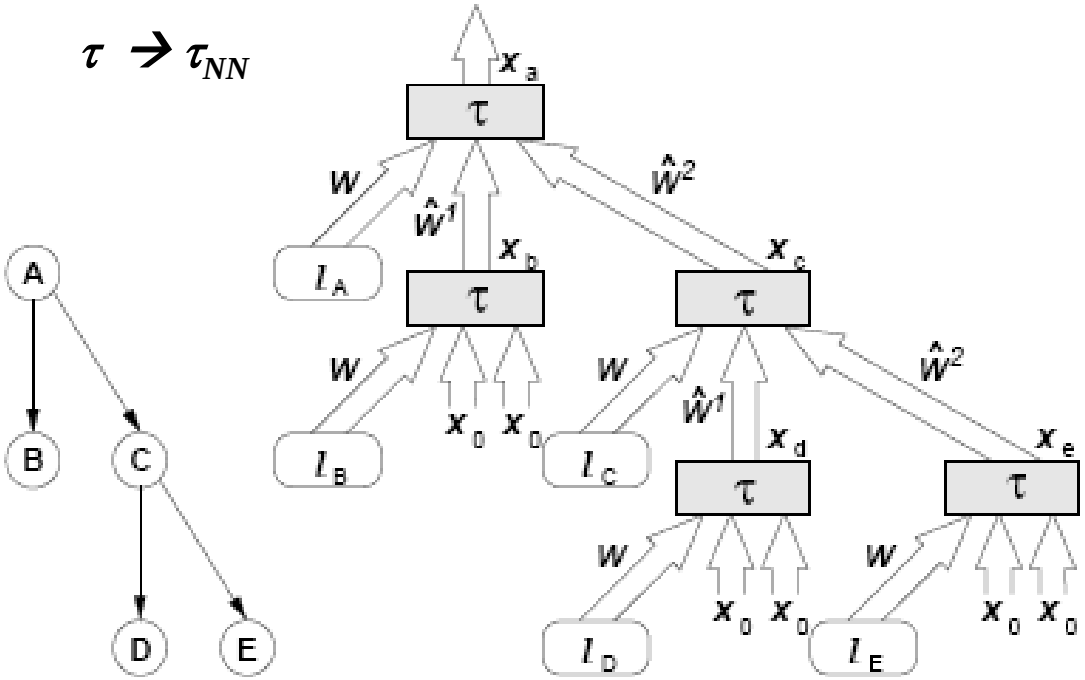
Unfolding (3) & Enc. Net. For Recurrent and Recursive NN
(or Recursive unfold. for two different structures)



Structured Data

Encoding Network

$\tau \rightarrow \tau_{NN}$



Structured Data

Encoding Network

- τ (τ_{NN}) for each step (with weight sharing): ***encoding network***
- Adaptive encoding via the free parameters of τ_{NN}

τ_{NN} (and **weight**) **sharing** : units are the same for the all the vertices of a tree and for all the trees in the data set!!!

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2. Moving to DPAG and Graphs: the role of causality
   [Next Lecture (SD-2)]

RecNN: going to details for the domains

- $\boldsymbol{X} = IR^m$ continuous (real values) state (code) space (encoded subgraph space)
- $\boldsymbol{L} = IR^n$ vertex label space
- $\boldsymbol{O} = IR^z$ or $\{0,1\}^z$
- $\tau =$ $\tau_{NN} : IR^n \times \underbrace{IR^m \times \ldots \times IR^m}_{k \text{ times}} \rightarrow \boxed{IR^m}$ Subgraph code
- g output function
- $x_0 = \mathbf{0}$

$$\boldsymbol{T_G}: \boldsymbol{G} \rightarrow \boldsymbol{O}$$

$$G \xrightarrow{\tau_E} \boxed{IR^m} \xrightarrow{g} IR \qquad \boldsymbol{T_G}$$

- τ and g realized by NN with free parameters **W**

RNN realize $g \circ \tau_E$

Realization of τ_{NN} (RecNN) unit

$$\tau_{NN} : IR^n \times \underbrace{IR^m \times \ldots \times IR^m}_{k \text{ times}} \rightarrow \boxed{IR^m}$$

Dim m

m x m

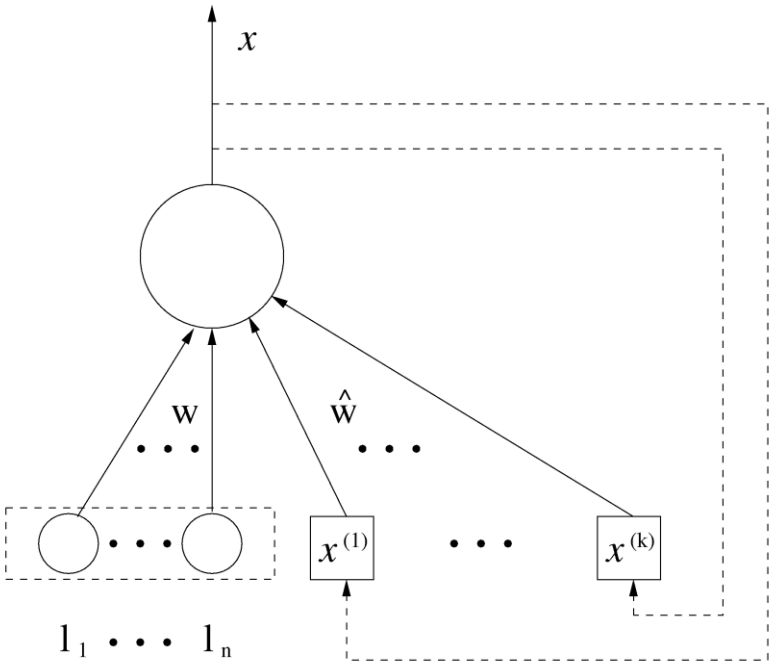
Subgraph code

$$\boldsymbol{x}(v) = \tau_{NN}(\boldsymbol{l}, \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(k)}) = \sigma(\boldsymbol{W}\boldsymbol{l} + \sum_{j=1}^{k} \hat{\boldsymbol{W}}_j \boldsymbol{x}^{(j)} + \theta)$$

where $\boldsymbol{x}^{(j)} = \boldsymbol{x}(\mathrm{ch}_j[v])$

# of children

Free parameters



1 recursive neuron

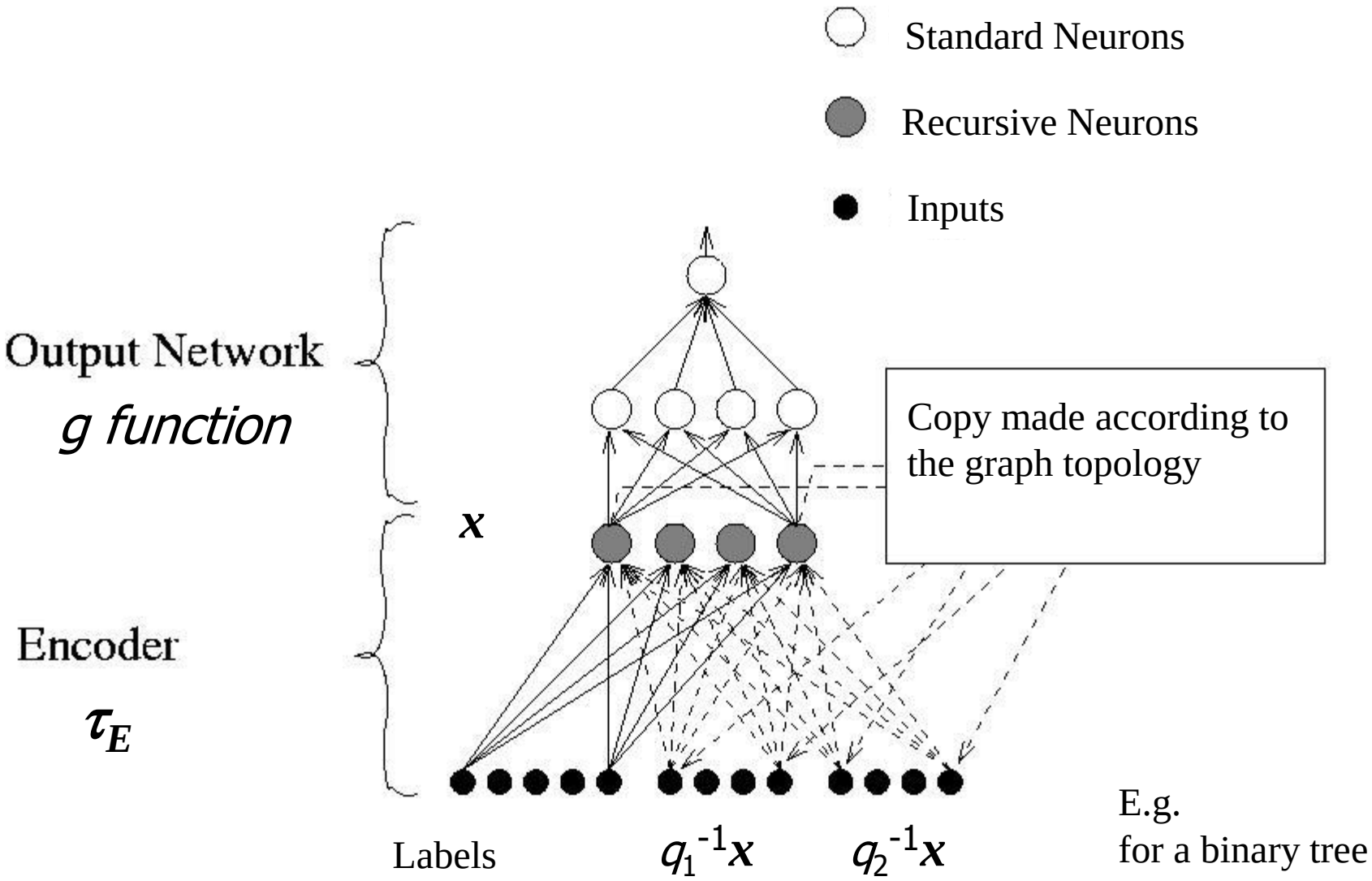
(τ_{NN} with $\underline{m=1}$)

Process a vertex

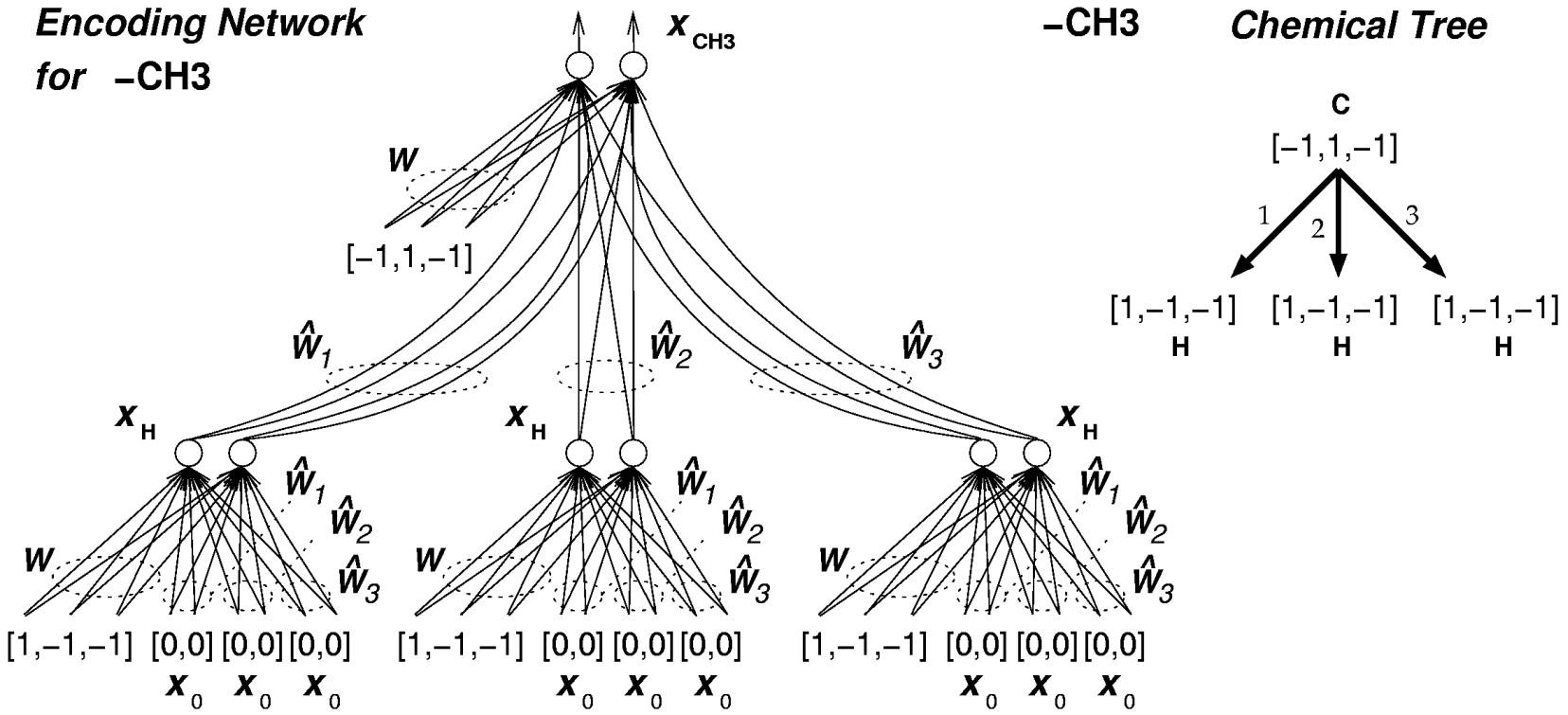
 # feedbacks = # children

(max *k*)

Fully-connected RecNN



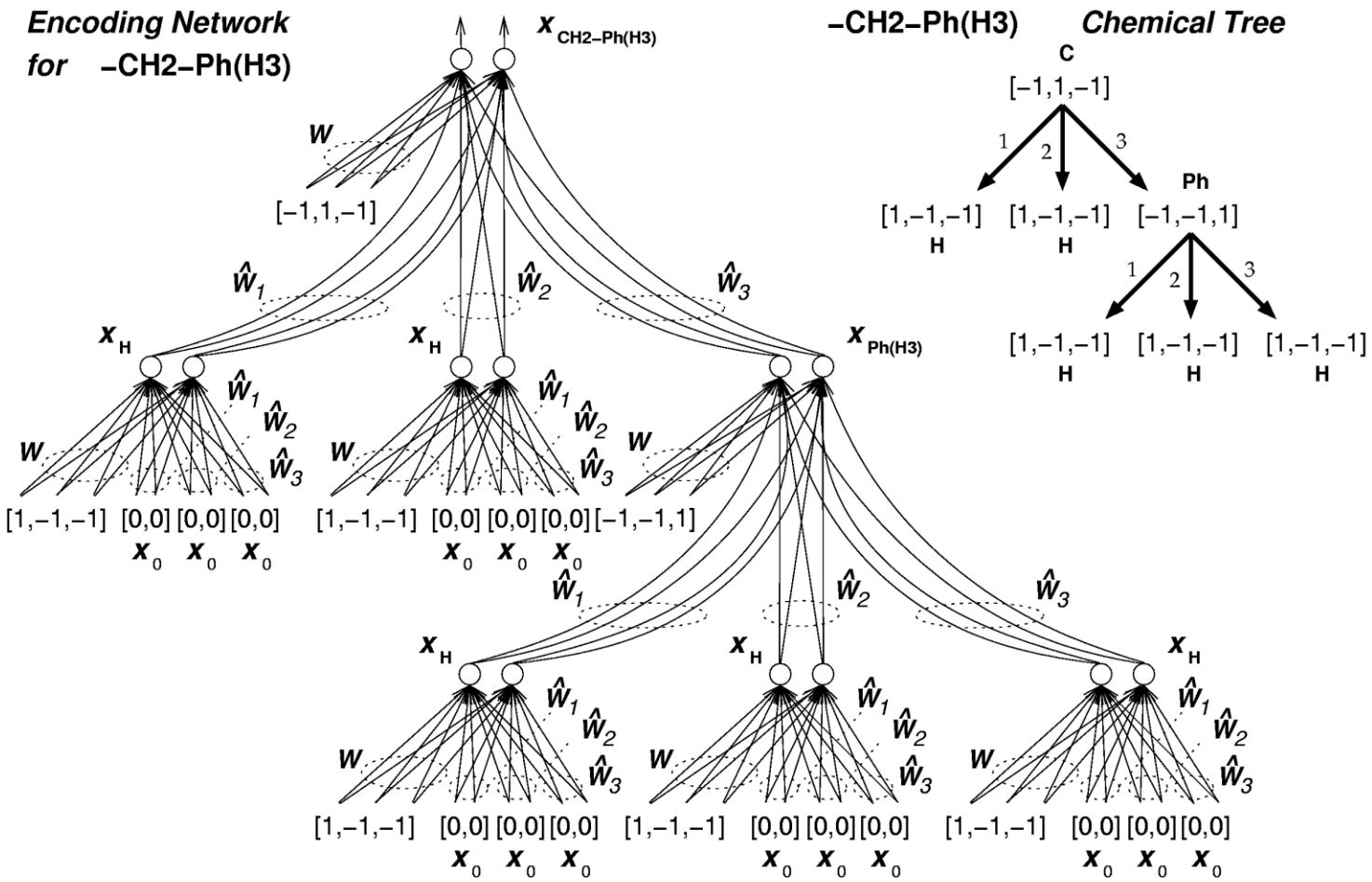
In details: Encoding Network with NN (I)



Start here !

Tau (and **weight**) **sharing** : units are the same for the all the vertices of a tree and for all the trees in the data set!!!

In details: Encoding Network with NN (II)



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   [Next Lecture (SD-2)]

RecNN applications

- Representing **hierarchical** information in many real-world domains
- Many examples:
  - Molecular Biology
  - Document (**XML**) Processing
  - **Natural Language Processing**
    - E.g. Stanford NLP group shown the effectives of RecNN applied to tree representation of language (and images) data and tasks.
    - Sentiment Tree Bank
    - Next slides

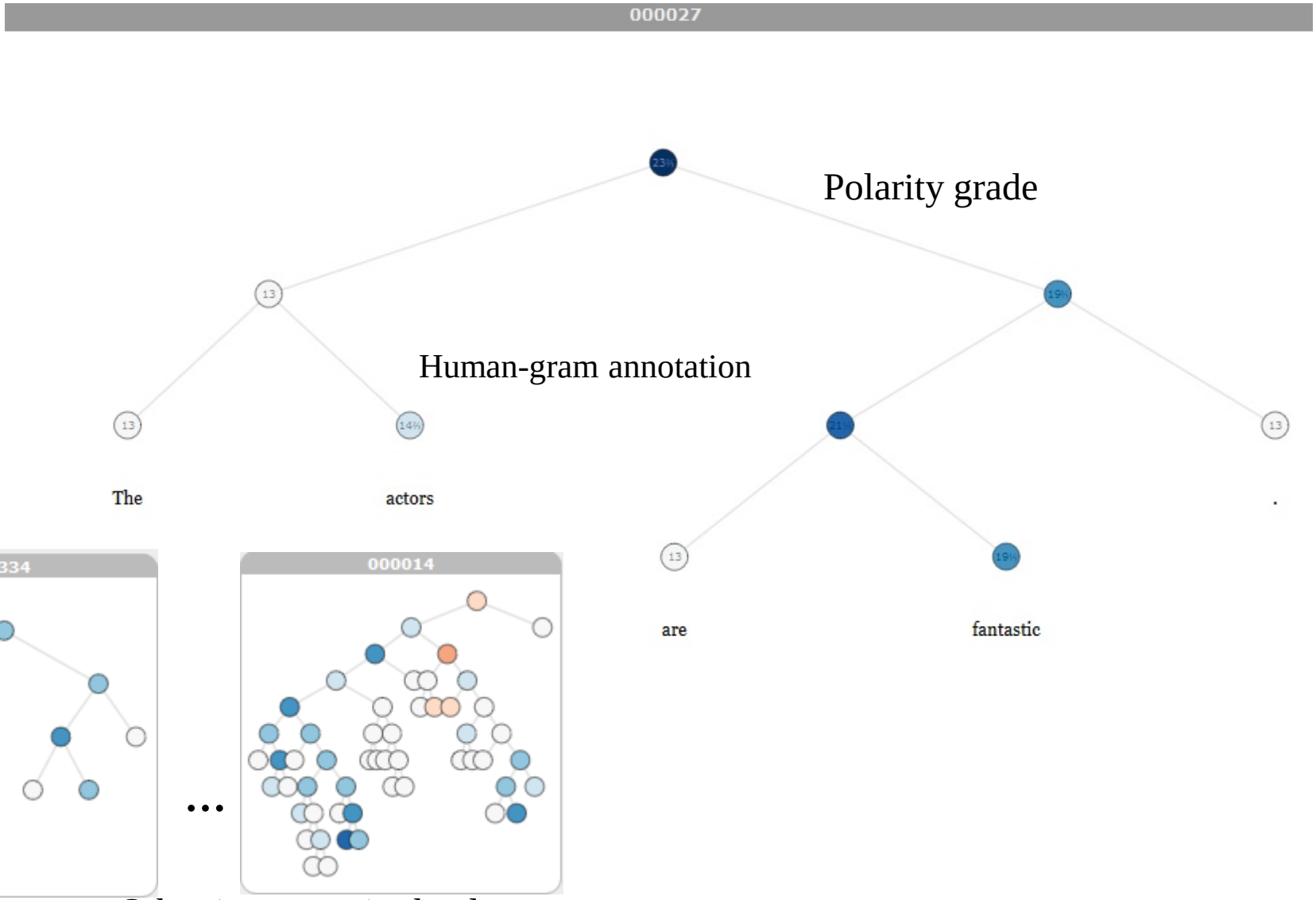
Recent Applications: Repetita (da ML): RecNN for NLP recent exploitment

- Currently wide successful application in NLP (e.g. by the Stanford NLP group)

- Shown the effectives of RecursiveNN applied to tree representation of language (and images) data and tasks. Started in 2011-13

- E.g. Sentiment Treebank (about movies)
  - Sentiment labels (movies reviews) for 215,154 phrases in the **parse trees** of **11,855** sentences
  - Recursive NN pushes the state of the art in single sentence positive/negative classification from 80% up to 85.4%.

Repetita (da ML): Examples



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   [Next Lecture (SD-2)]

RNN Learning Algorithms

- Backpropagation through structure: Extension of BPTT
  Goller & Küchler (1996)
  - Simple to understand using graphical formalism (backprop+weight sharing on the unfolded net) :
  - *The notation is adapted to the case of delta from the fathers*

- RTRL Sperduti & Starita (1997),

✓ Equations: See Cap 19 in

Kolen, Kremer , *A Field Guide to* ***Dynamical Recurrent Networks***.
IEEE press 2001

- RCC family based: next slides

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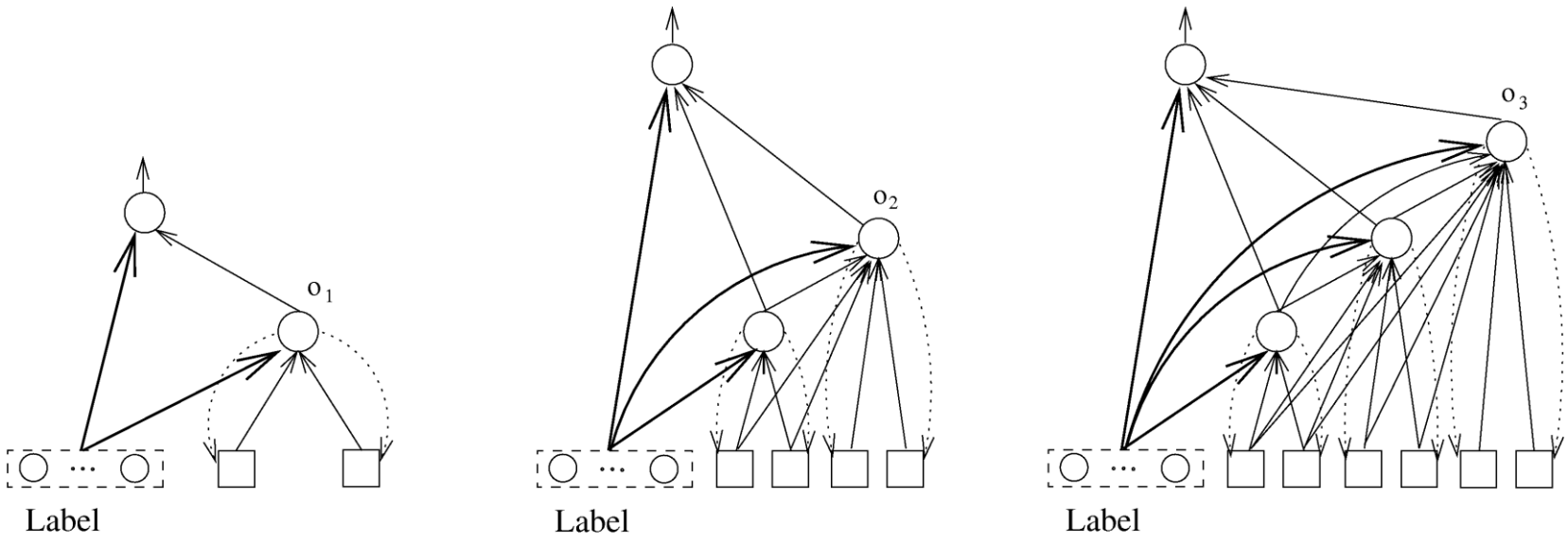
     - **RecCC**
     - **Panorama**

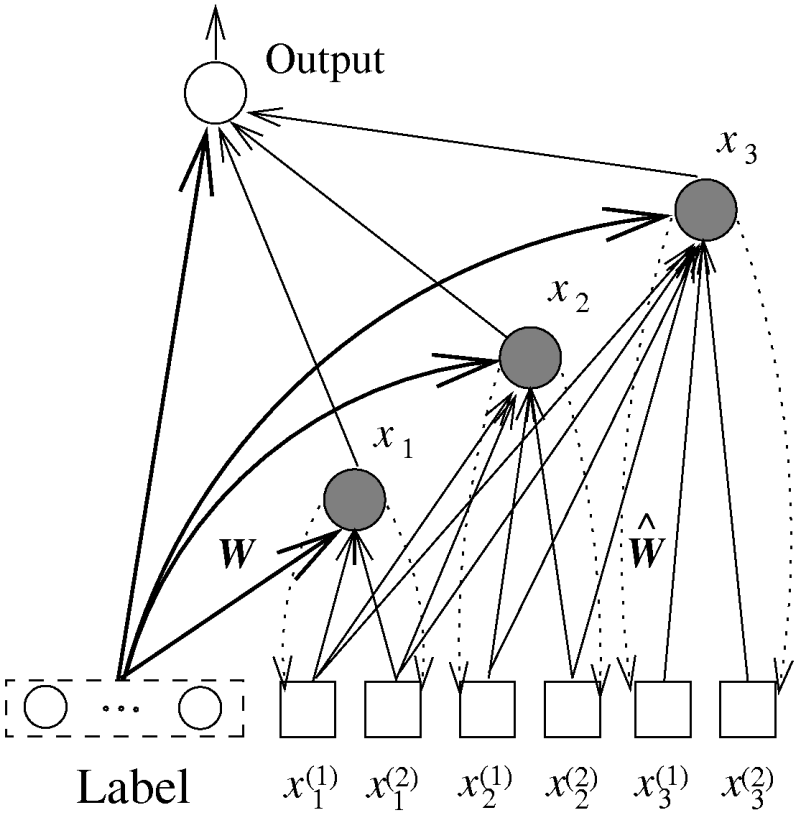
2. Moving to DPAG and Graphs: the role of causality [Next Lecture (SD-2)]

RCC (I)

- Architecture of Cascade Correlation for Structure (Recursive Cascade Correlation - RCC)
- RecNN with recursive units within a **constructive approach** $\Rightarrow$ *m* is automatically computed by the training algorithm.
- *A deep neural network!*



RCC (II)



Architecture of a RCC with 3 hidden units (**m=3**) and **k=2** .

Recursive hidden units (shadowed) generate the code of the input graph (function τ_E). The hidden units are added to the network during the training. The box elements are used to store the output of the hidden units, i.e. the code $x_i^{(j)}$ that represent the context according to the graph topology.

The output unit realize the function **g** and produce the final prediction value.

E.g. A.M. Bianucci, A. Micheli, A. Sperduti, A. Starita.
Application of Cascade Correlation Networks for Structures to Chemistry,
Applied Intelligence Journal. 12 (1/2): 117-146, 2000

RCC (III) Learning

Gradient descent: interleaving LMS (output) and maximization of correlation between new hidden units and residual error. Main difference with CC: calculation of the following derivatives by recurrent equations:

$$\frac{\partial x_h(v)}{\partial w_{hi}^j} = \frac{\partial \tau_h(\boldsymbol{l}, \boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(k)})}{\partial w_{hi}^j} = f'\left(l_i + \sum_{t=1}^{k} \hat{w}_{hh}^t \frac{\partial \boldsymbol{x}_h^{(t)}}{\partial w_{hi}^j} \right)$$

$$\frac{\partial x_h(v)}{\partial \hat{w}_{hi}^j} = \frac{\partial \tau_h(\boldsymbol{l}, \boldsymbol{x}^{(1)}, \cdots, \boldsymbol{x}^{(k)})}{\partial \hat{w}_{hi}^j} = f'\left(\boldsymbol{x}_i^{(j)} + \sum_{t=1}^{k} \hat{w}_{hh}^t \frac{\partial \boldsymbol{x}_h^{(t)}}{\partial \hat{w}_{hi}^j} \right)$$

where $\boldsymbol{x}^{(j)} = \boldsymbol{x}(\mathrm{ch}_j[v])$

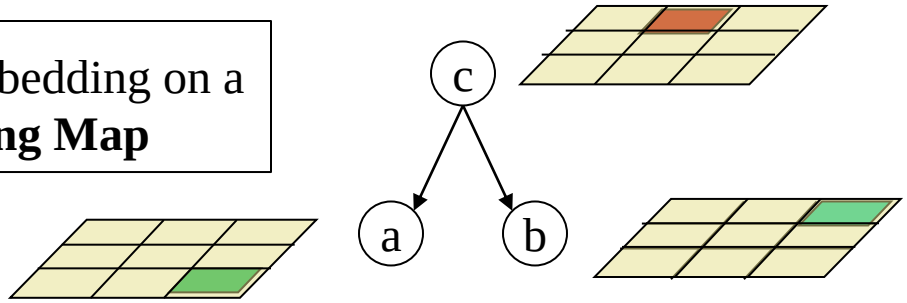
Note: simplification (of the sum on other units) due to the architecture difference with the RTRL for a fully connected RNN!
But compared to the recurrent case it *appears the summation on children!*

Unsupervised recursive models (2003-2005)

- Transfer *recursive* idea to unsupervised learning
- No prior metric/pre-processing (but still bias!)
- Evolution of the similarity measure through *recursive comparison* of sub-structures

- Iteratively compared via bottom-up encoding process

Recursive nodes embedding on a **Self-Organizing Map**



It uses e.g. the SOM coordinates for node embedding

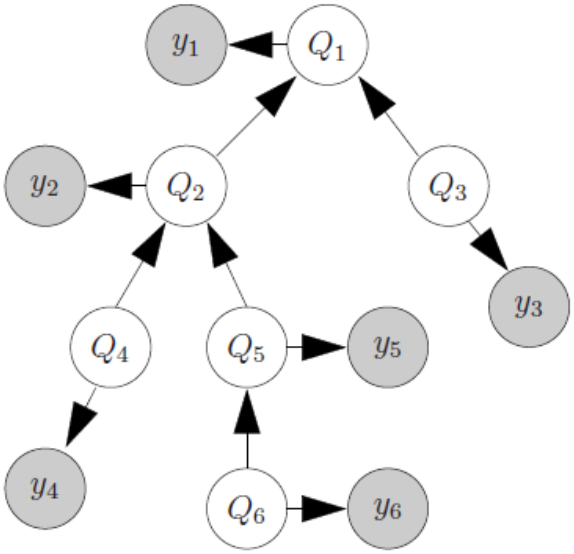
Node embedding

l	C_1	C_2

M. Hagenbuchner et al. IEEE TNN, 2003
B. Hammer et al. Neural Networks, 2005

Generative: HTMM (2012-2018)

- E.g Bottom-up Hidden Tree Markov Models extend HMM to trees exploiting the recursive approach

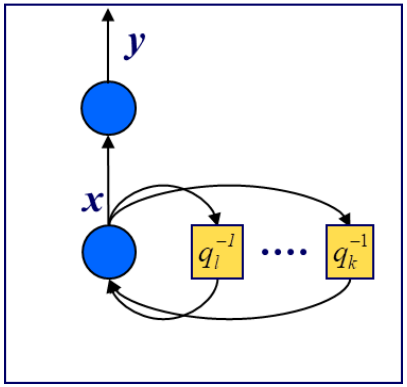


- Generative process from the leaves to the root
- Markov assumption (conditional dependence)
  $Qch1(u), \ldots, Qch_K(u) \rightarrow Qu$

Children to parent hidden state transition

$P(Qu \mid Qch1(u), \ldots, Qch_K(u))$

Where (from a different paper)
$\boldsymbol{Q_v} \leftrightarrow \boldsymbol{x(v)}$



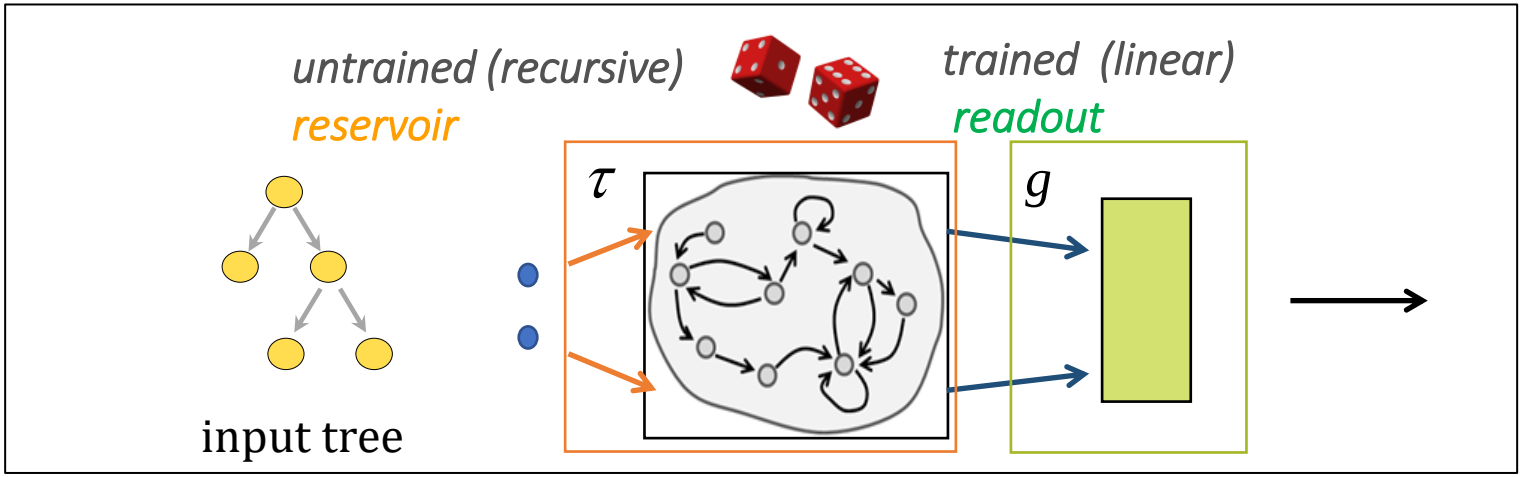
Bayesian network unfolding graphical model over the input trees; y: observed elements
Q: hidden states variables with discrete values

Issue: how decompose this joint state transition? (see ref.).

Bacciu, Micheli, Sperduti. IEEE TNNLS, 2012

Efficient: TreeESN (2010-13)

- Combine Reservoir Computing (un-trained layer of recurrent units with linear redout) and recursive modeling
  - Extend the applicability of the RC/ESN approach to tree structured data
  - Extremely efficient way of modeling RecNNs (randomized approaches)
  - Architectural and experimental performance baseline for trained RecNN models with often comptetive results.



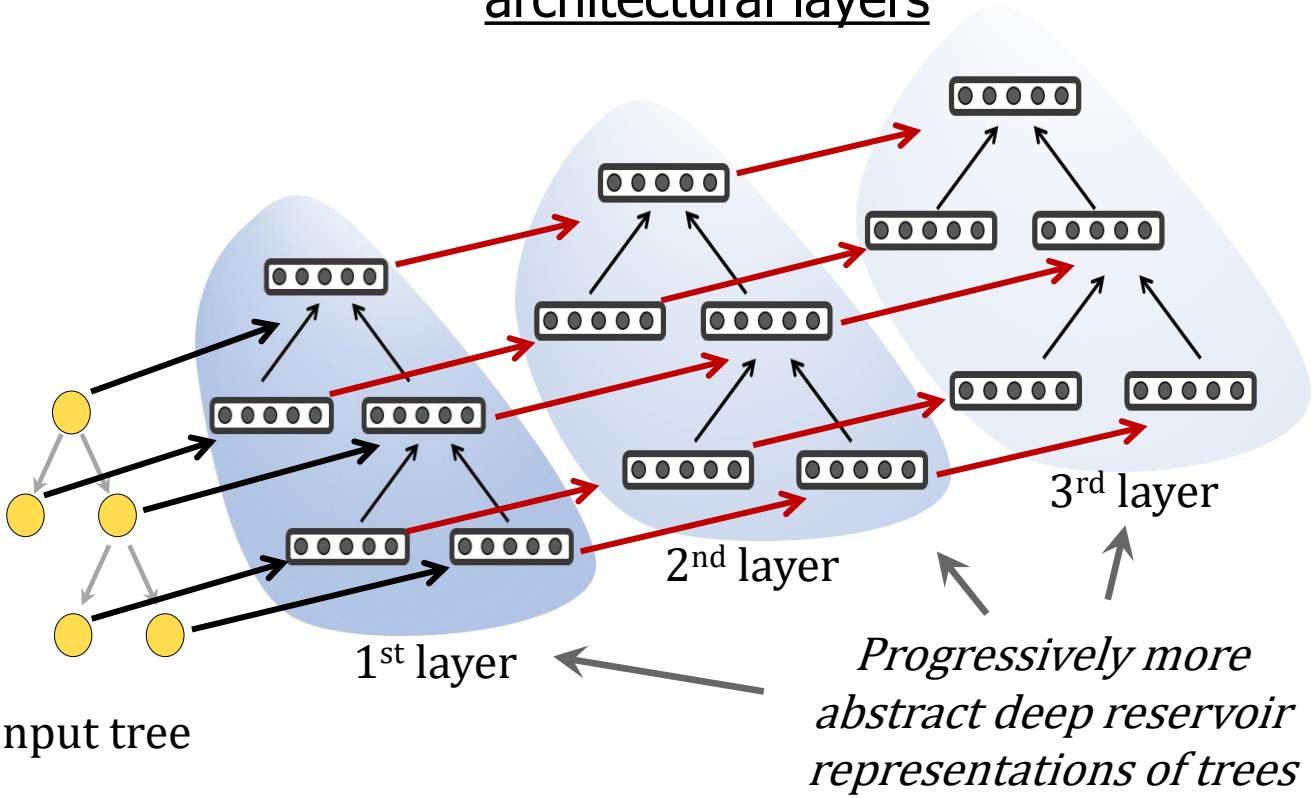
The recursive process of RecNN made by efficient RC approaches

C. Gallicchio, A. Micheli. Neurocomputing, 2013.

More in a NEXT LECTURE

Deep: Deep Tree ESN (2018)

Hierarchical abstraction **both** through the input structure and architectural layers



Pro:
1. Rec NN adv.s
2. Deep learning abstraction (even before training: arch. bias)
3. Extremely efficient

- Improve efficiency (giving same #units) by a factor = num. of layers
- Improve results

C.Gallicchio, A.Micheli IEEE IJCNN 2018
C.Gallicchio, A.Micheli Information Sciences 2019

Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

   Extensions of models for learning in structured domains

   - Motivation and examples (structured data)
   - The structured data (recursive)
   - Recursive models: RNN and RecNN
   - Recursive Cascade Correlation & other recursive approaches

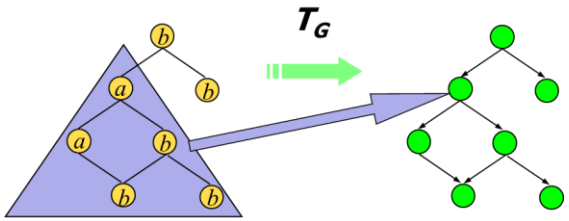
2. Moving to DPAG and Graphs: the role of causality [Next Lecture (SD-2)]

Toward next lecture

RecNN Analysis

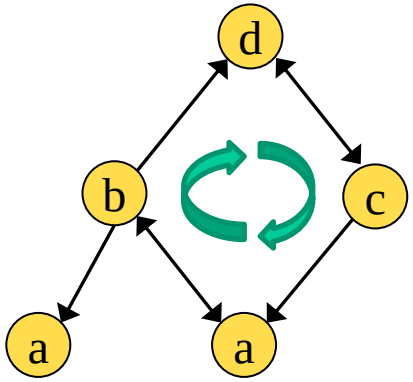
- RecNNs allow adaptive representation of SD
  - Handling of variability by causality and stationarity
  - **Adaptive** transduction: BPTS, RTRL, ...
- **Stationarity**:
  - efficacy solution to parsimony (reducing the number of parameters) without reducing expressive power (universal approximation theorem)

- **Causality:** affects the computational power !
  - RNN are only able to memorize past information (sub-sequences)
  - RecNN outputs depend only on sub-structures
  - The domain is restricted to sequences and trees due to causality
  - Toward partial relaxation (or **extension**) of the causality assumption



Graphs by NN?

- For Graphs by NN: see next lecture!
- Following a journey through the *causality* assumption!

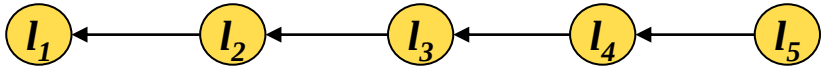


How to deal with cycles and causality?

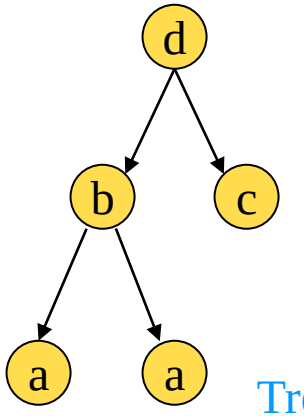
We will see:
Or by relaxing the causality assumption
Or by imposing constraints on the recursive processing

Summary of MODELS for SD (examples)

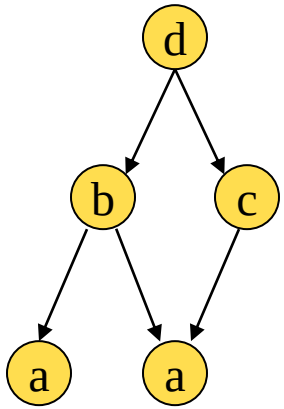
Standard ML models for flat data



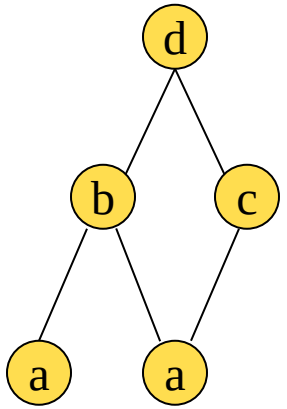
- Recurrent NN/ESN
- HMM
- Kernel for strings …



Tree:
- Recursive NN
- Tree ESN
- HTMM
- Tree Kernels
- …



DPAG:
- CRCC



- GNN/GraphESN
- NN4G, DGN, ..
- Graph Kernels
- SRL
- …

See references for models in the bibliography slides (later)

Bibliography: aims

Different parts in the following:

- Basic/Fundamentals
- To go ahead

  - Many topics can be subject of study and development
  - Many many works in literature (they arrive continuously)!
  - Many possible topics for demand and possible thesis

  - **More bibliography on demand:** micheli@di.unipi.it

Bibliografia (Basic, origins of RecNN)

RecNN

- A. Sperduti, A. Starita. *Supervised Neural Networks for the Classification of Structures*,IEEE Transactions on Neural Networks. Vol. 8, n. 3, pp. 714-735, 1997.

- P. Frasconi, M. Gori, and A. Sperduti, *A General Framework for Adaptive Processing of Data Structures*, IEEE Transactions on Neural Networks. Vol. 9, No. 5, pp. 768-786, 1998.

- A.M. Bianucci, A. Micheli, A. Sperduti, A. Starita. *Application of Cascade Correlation Networks for Structures to Chemistry*, Applied Intelligence Journal (Kluwer Academic Publishers), Special Issue on "Neural Networks and Structured Knowledge" Vol. 12 (1/2): 117-146, 2000.

- A. Micheli, A. Sperduti, A. Starita, A.M. Bianucci. *A Novel Approach to QSPR/QSAR Based on Neural Networks for Structures,* Chapter in Book : "Soft Computing Approaches in Chemistry", pp. 265-296, H. Cartwright, L. M. Sztandera, Eds., Springer-Verlag, Heidelberg, March 2003.

Bibliography: NN approaches-2

* UNSUPERVISED RecursiveNN

- B. Hammer, A. Micheli, M. Strickert, A. Sperduti.
  A General Framework for Unsupervised Processing of Structured Data,
  Neurocomputing (Elsevier Science) Volume 57, Pages 3-35, March 2004.
- B. Hammer, A. Micheli, A. Sperduti, M. Strickert.
  Recursive Self-organizing Network Models. Neural Networks, Elsevier Science. Volume 17, Issues 8-9, Pages 1061-1085, October-November 2004.

* TreeESN: efficient RecNN

- C. Gallicchio, A. Micheli.
  Tree Echo State Networks, Neurocomputing, volume 101, pag. 319-337, 2013.
- C. Gallicchio, A. Micheli.
  Deep Reservoir Neural Networks for Trees. Information Sciences 480, 174-193, 2019.

* HTMM: further developments (generative)

- D. Bacciu, A. Micheli and A. Sperduti.
  Compositional Generative Mapping for Tree-Structured Data - Part I: Bottom-Up Probabilistic Modeling of Trees, IEEE Transactions on Neural Networks and Learning Systems, vol. 23, no. 12, pp. 1987-2002, 2012

Bibliography: RecNN applications (example)

* NLP applications (that you can extend with recent instances, and relate them to the general RecNN framework present in this lecture and the basic RecNN bibliography references)

- R. Socher, C.C. Lin, C. Manning, A.Y. Ng,
  Parsing natural scenes and natural language with recursive neural networks,
  Proceedings of the 28th international conference on machine learning (ICML-11)
- R. Socher, A. Perelygin, J.Y. Wu, J. Chuang, C.D. Manning, A.Y. Ng, C.P. Potts,
  Recursive Deep Models for Semantic Compositionality Over a Sentiment Treebank
  Proceedings of the 2013 Conference on Empirical Methods in Natural Language Processing, pages 1631–1642, Seattle, Washington, USA, 18-21 October 2013

Bibliography: basic items for the next lecture

* RecNN for DPAGs : how to extend the domain (I)

- A. Micheli, D. Sona, A. Sperduti.
  Contextual Processing of Structured Data by Recursive Cascade Correlation. IEEE Transactions on Neural Networks. Vol. 15, n. 6, Pages 1396- 1410, November 2004.
- Hammer, A. Micheli, and A. Sperduti.
  Universal Approximation Capability of Cascade Correlation for Structures.
  Neural Computation. Vol. 17, No. 5, Pages 1109-1159, (C) 2005 MIT press.

* NN for GRAPH DATA: how to extend the domain (II)

- * A. Micheli. *Neural network for graphs: a contextual constructive approach*, IEEE Transactions on Neural Networks, volume 20 (3), pag. 498-511, doi: 10.1109/TNN.2008.2010350, 2009.

- F. Scarselli, M. Gori, A.C.Tsoi, M. Hagenbuchner, G. Monfardini. *The graph neural network model*, IEEE Transactions on Neural Networks, 20(1), pag. 61–80, 2009.
- C. Gallicchio, A. Micheli. *Graph Echo State Networks*, Proceedings of the International Joint Conference on Neural Networks (IJCNN), pages 1–8, 2010.

DRAFT, please do not circulate!

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