Intro to Learning in SD -2

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2- Neural Networks for Graphs

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DRAFT, please do not circulate!

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Dipartimento di Informatica
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Computational Intelligence & Machine Learning Group

Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

Extensions of models for supervised and unsupervised learning in structured domains

- 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

- Recap SD1
- Causality for Recurrent and Recursive models &
- Contextual approaches (BRCC/CRCC and DPAGs)
- Neural Networks for graphs

By a journey through the causality assumption!

Recup SD-1: Adaptive processing of SD

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- The problem: there has been no systematic way to extract features or metrics relations between examples for SD

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

- **Recursive** and parametric realization of the transduction function
- *Adaptive* by Neural Networks: RecNN
  - Pro: RecNN adapts the model to the hierarchal data
  - Cons: Causality issue (*): it affects the computational power of RecNN and the class of graphs ! → new models!

The scenario, terms (and trends)

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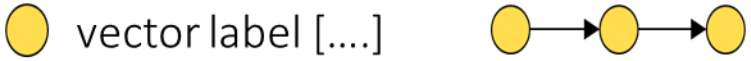
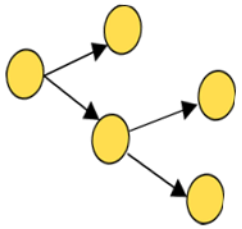
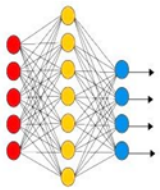
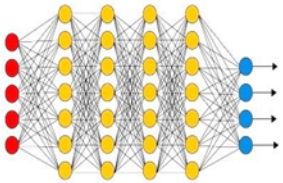
Input Domain		
Flat (vectors) (e.g. F.F.NN)	**Sequences** (RNN)	**Structures** (trees/graphs)





Layering	
Shallow	**Deep**





Multi-level input rep. abstraction

Focus

"Deep and wide" approaches

Our graphs (in the following)

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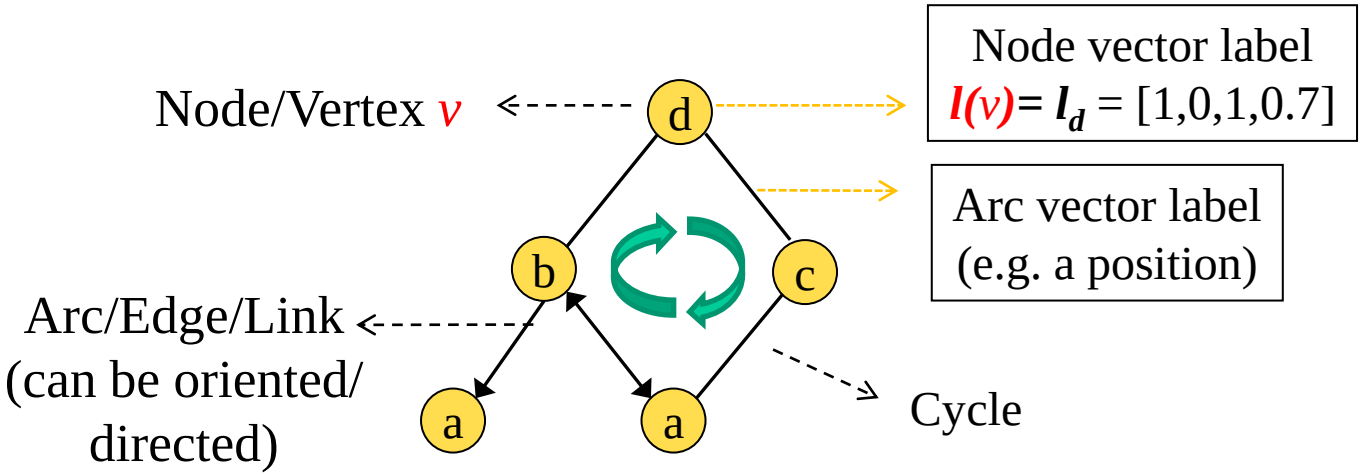
Labeled graphs g



Graph Representations

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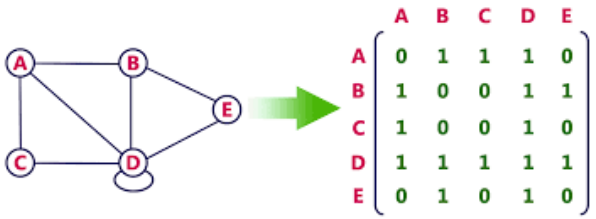
The problem: there has been no systematic way (of general validity for any task) to extract features or metrics relations between examples for SD

- **Features based** representations are incomplete (or strongly task-dependent, e.g. topological indexes)
- **Adjacent/incident matrix** representations (or other fixed-sizes representations). Issues:
  - Over-dim./incomplete (wasteful by padding/lose inf.)
  - Alignment among different graphs
  - Topological order (make difficult the generalization)



- ML issues for the high proportion between combinatorial number of possible data examples and available data

- "The ability to treat the proper **inherent nature of the input data** is the key feature for a successful application of the machine learning methodologies."

Learning Models for SD

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- 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*

- What we mean for *adaptive* processing of SD:

  extraction of the topological information directly from data/ *structure representation learning*

  - $\mathcal{H}$ has to be able to represent (hierarchic) relationships
  - **adaptive** measure of similarity on structures + apt **learning rule**
  - efficient handling of structure variability

Learning in Structured Domain Plan in 2 lectures

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By a journey through the causality assumption! *

CRCC: introduction

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- Analysis of the **causality** assumption for Recurrent and Recursive neural computing models
- Partial relaxation (or **extension**) of the causality assumption
- First approach to deal with contextual information in SD by Recursive models

Causal Systems

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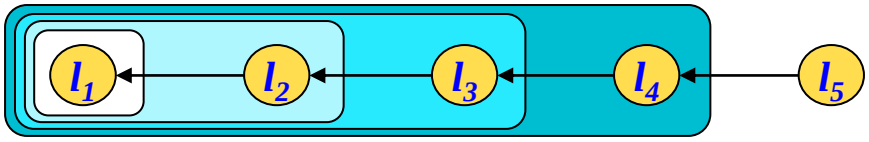
- Recurrent NN models are based on the **Causality** assumption, i.e. RNN are only able to memorize past information

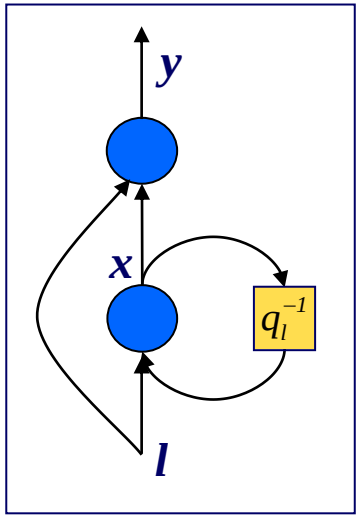
A system is causal if the output at time t_0 only depends on inputs at time $t \leq t_0$

necessary and sufficient for

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

Shift operator q^{-1}

Causal Systems in Structured Domain (RecNN)

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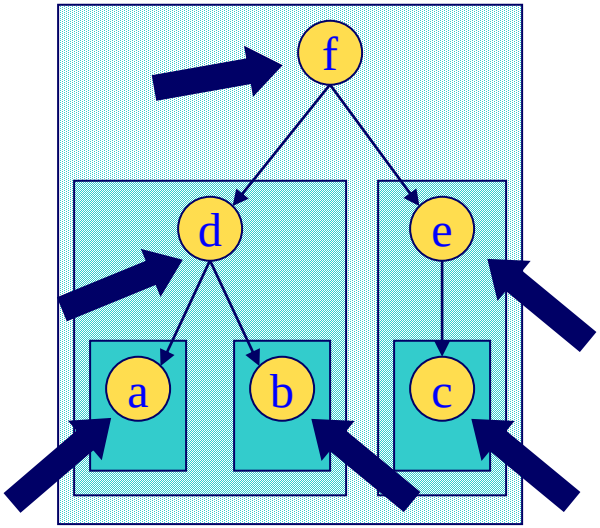
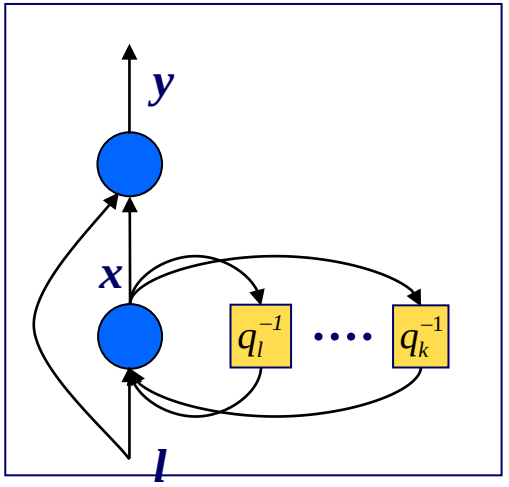
- The causality concept can be generalized to structured data transductions as follows

A system is causal if its output for a node v only depends on v and its descendants



Unfolding the encoding process through structure



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

Drawbacks of Causal Systems for sequence domain

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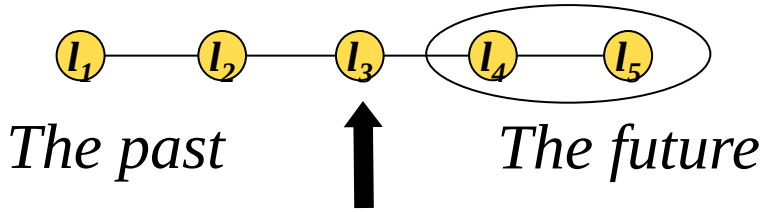
- Several prediction tasks involving **sequences** require past and "future" information (*on known sequences*)
  - DNA and Protein analysis / Language understanding / ...



Causality hampers to consider the right part

- Contextual information for **structured** domains: whenever the meaning of a sub-structure depends on the context in which it is found
  - some classes of transductions **cannot** be computed by causal models (also some causal transduction !!!)
  - extension of the class of graphs
  - *Properties in flat domains cannot be trivially "exported" in SD!*

Overcome the Causality Assumption

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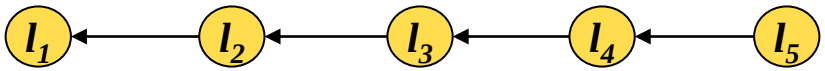
The Sequence Domain

- Standard Approaches
- BRCC



Bi-causal System

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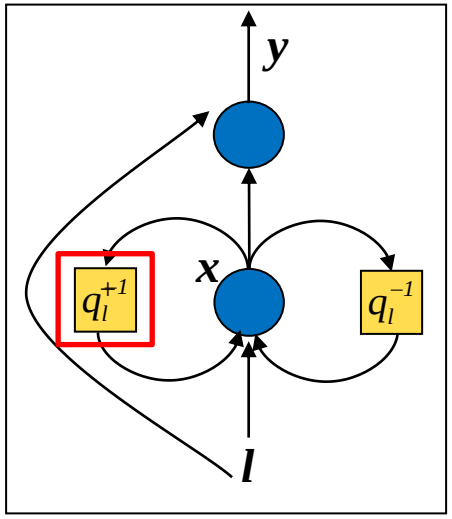
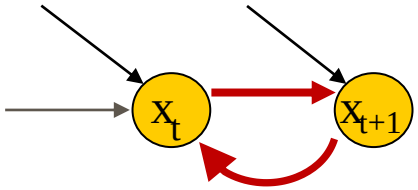
- A possible bi-causal model can be



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

Unfolding
with cylces



- However this is not easily implementable
  - Cycles: State equations and enc. net. become dynamical systems due to mutual dependencies
  - Different solutions are available (e.g. bidirectional approaches for RNN using a different state for left-to-right o right-to-left encoding)

Bi-directional Approaches

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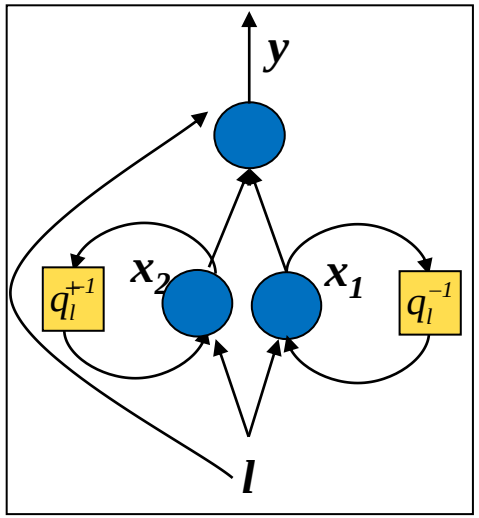
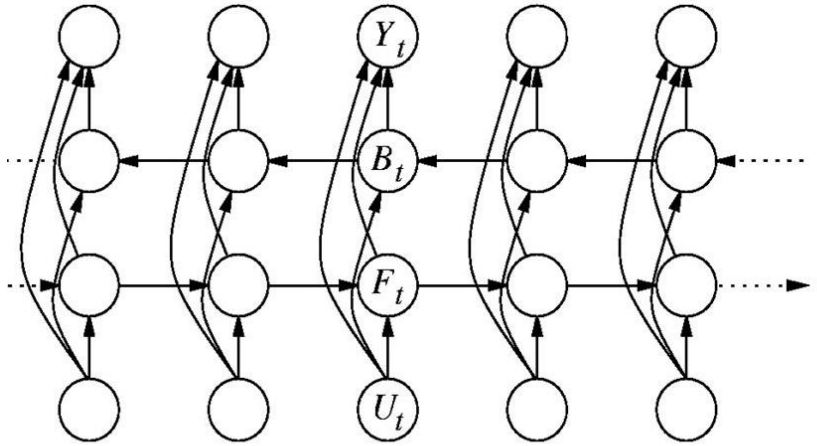
- A bi-directional approach has been proposed e.g. by Baldi et al. (1999) for Bioinformatics applications and nowadays popular in NLP etc., factorizing the internal state as:



$$\boldsymbol{x}(t) \equiv \begin{bmatrix} \boldsymbol{x}_1(t) \\ \boldsymbol{x}_2(t) \end{bmatrix} = \begin{bmatrix} \tau_1(\boldsymbol{x}_1(t-1), \boldsymbol{l}(t)) \\ \tau_2(\boldsymbol{x}_2(t+1), \boldsymbol{l}(t)) \end{bmatrix}$$

Typically

$$\boldsymbol{x}_1(t) = B_t$$
$$\boldsymbol{x}_2(t) = F_t$$



Output layer

B_t for Backward

F_t for Forward

Input layer

Bidirectional Recurrent NN (BRNN)

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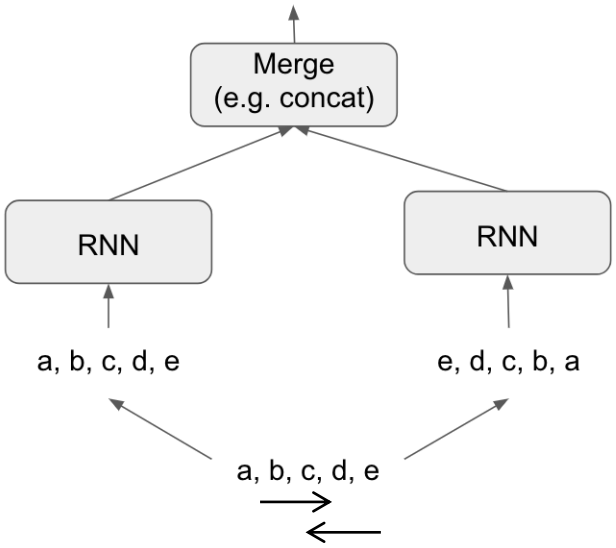
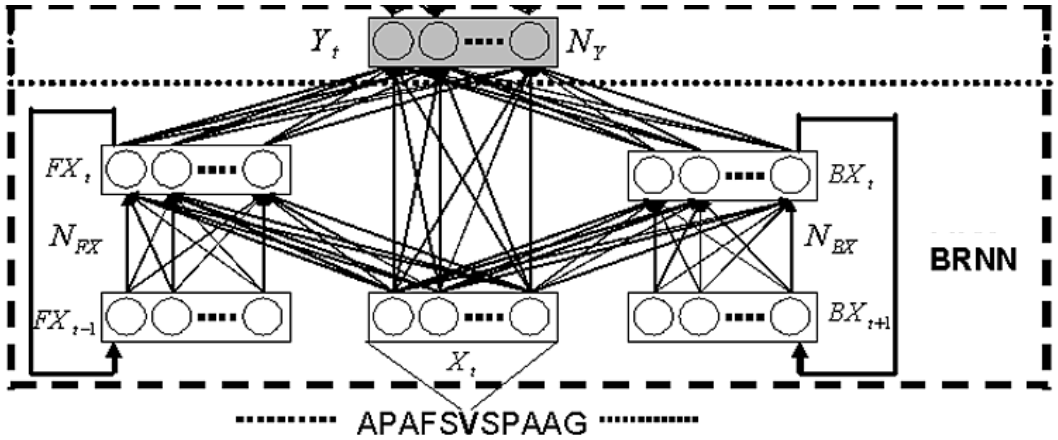
- Bi-directional Recurrent NN composed by a committee of three sub-networks, see these examples:
  - With the network size to be decided in advance
  - *Not easily extendible to structures*





A different idea by RCC Architecture

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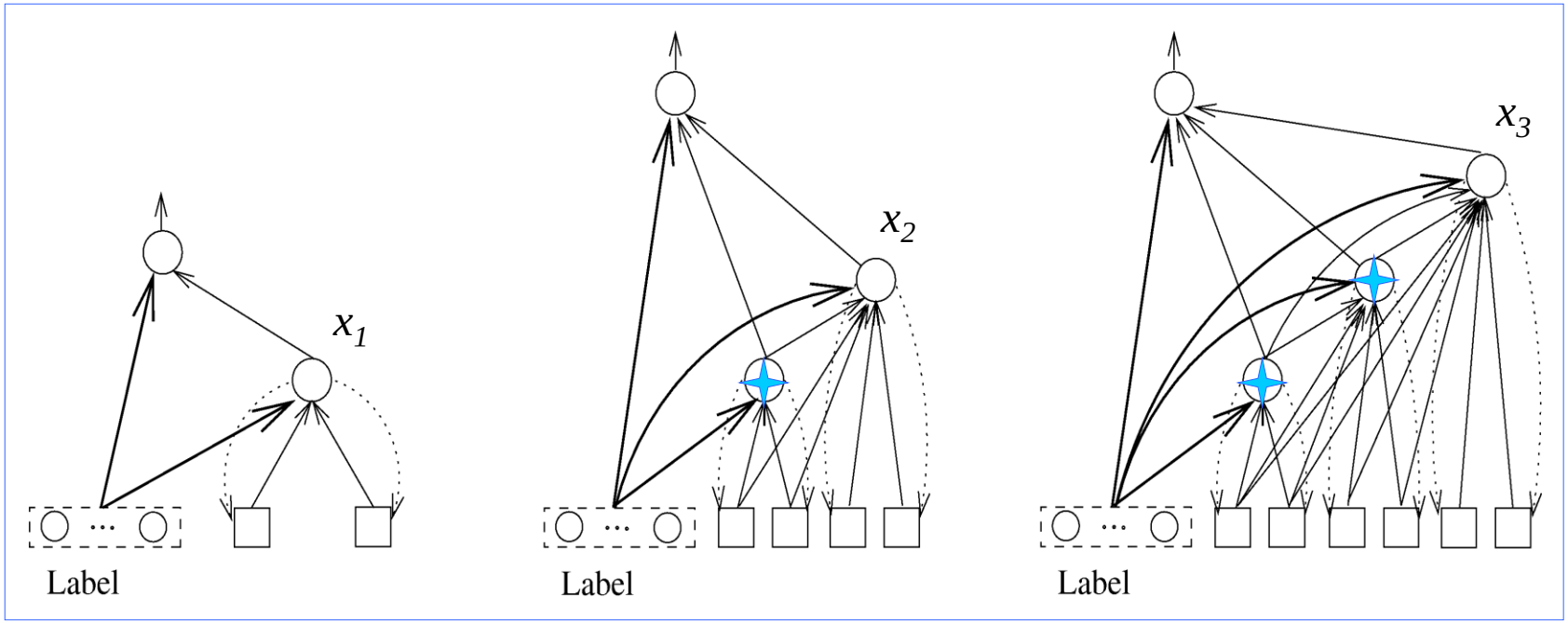
By a Recursive Cascade Correlation we can realize the recurrent/recursive network by a **constructive approach**:
The hidden units are added to the network, and frozen, during the training



BRCC/CRCC* Approach

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- We proposed an instance of Bi-Causality (BRCC) suitable for implementation with Recurrent Cascade Correlation
- Each time a unit is frozen, the portion of its (memorized) state encodes knowledge of the **whole** sequence

$$x_1(t) = \tau_1(x_1(t-1), \mathbf{I}(t))$$
$$x_2(t) = \tau_2(x_2(t-1), x_1(t-1), x_1(t+1), \mathbf{I}(t))$$
$$\vdots \qquad \vdots \qquad \vdots$$
$$x_m(t) = \tau_m(x_i(t-1), x_{m-1}(t-1), x_{m-1}(t+1), \ldots, x_1(t-1), x_1(t+1), \mathbf{I}(t))$$

unit m — frozen unit m-1 — ····· — frozen unit 1

* CRCC = Contextual RecCC (extended to structures)

Bi-Causal Recurrent Cascade Correlation

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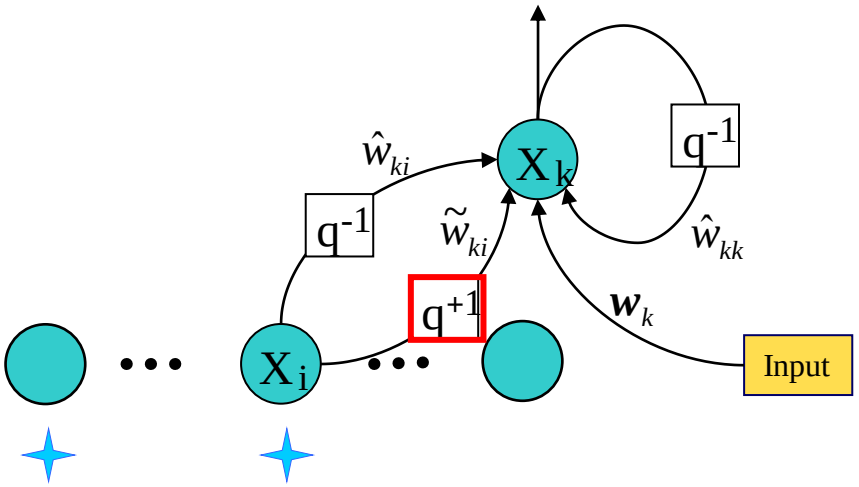
- Assuming stationary transitions the output of the *k*-th hidden unit of a BRCC can be computed as:

$$x_k(t) = f\left(\sum_{i=1}^{n} w_{ki} I_i(t) + \sum_{i=1}^{k} \hat{w}_{ki} x_i(t-1) + \sum_{i=1}^{k-1} \tilde{w}_{ki} x_i(t+1)\right)$$



Graphical Model

Example: CRCC on a sequence

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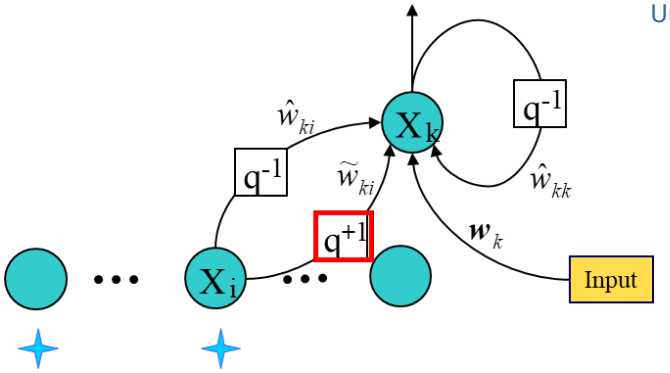
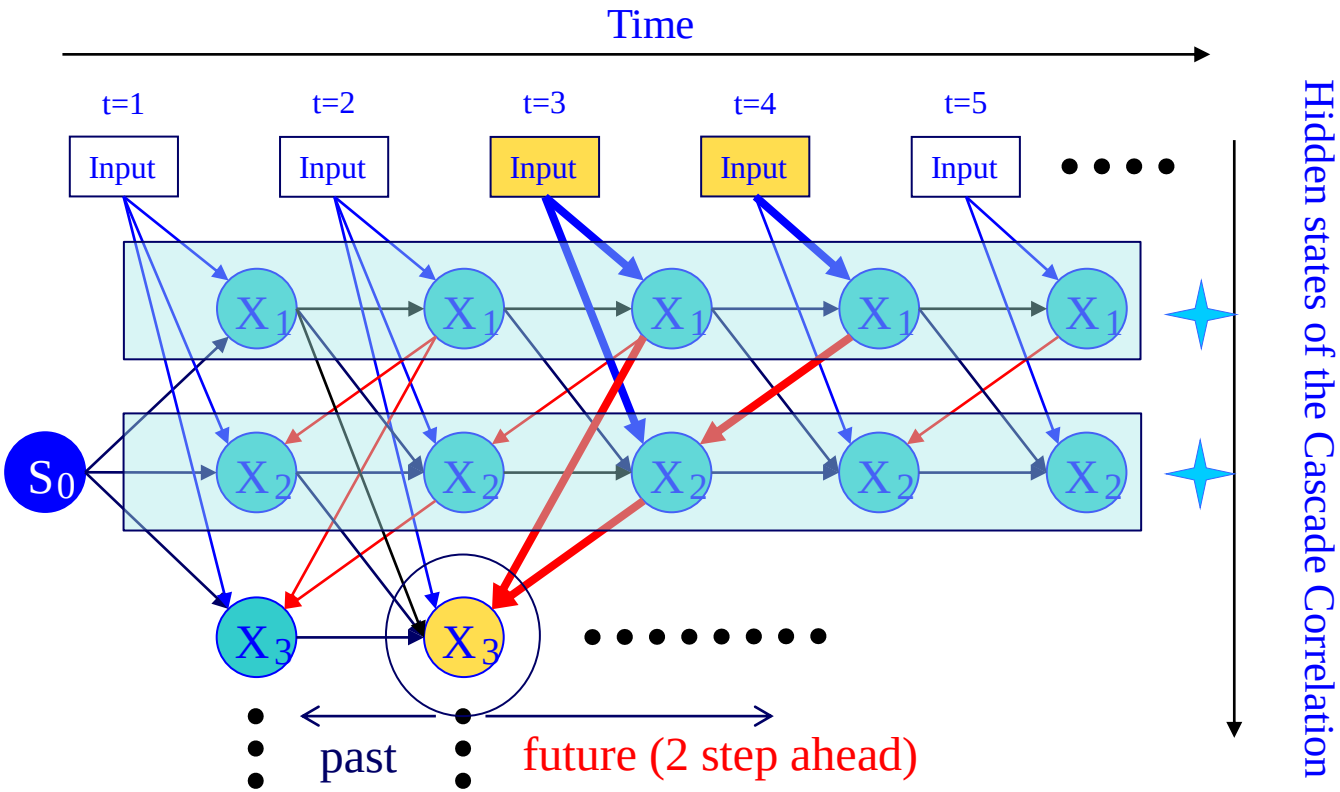
We can gain information on the "future" proportionally to the number of hidden units





Overcome the Causality Assumption for SD: CRCC

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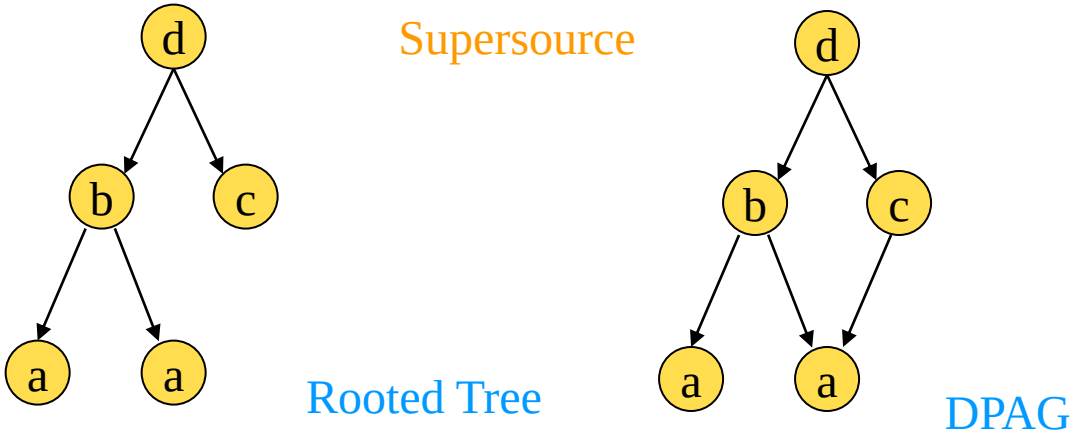
The Structure Domain

- CRCC: Cascade **Recursive** Cascade Correlation: Moving to trees and DPAGs
- Examples of Results



Contextual Target Functions

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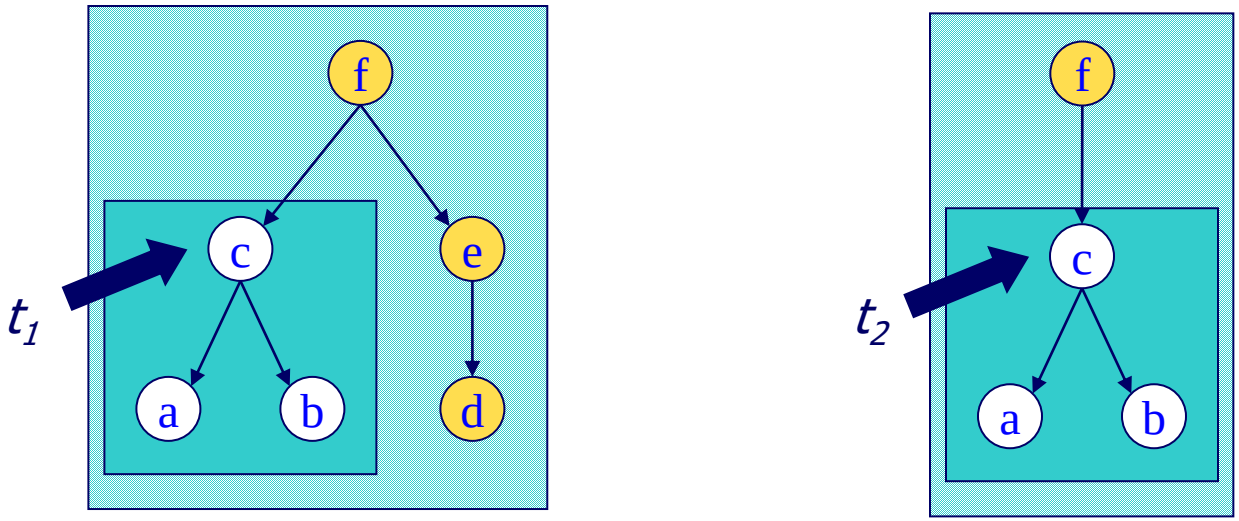
Relevance of contextual processing (I)

contextual IO-isomorphic transductions
(*where causal models fail*)



$$\text{Target}(t_1) \neq \text{Target}(t_2)$$
$$\text{out}_{\text{RecNN}}(t_1) = \text{out}_{\text{RecNN}}(t_2)$$
$$\boldsymbol{C}(x_k(c_1)) \neq \boldsymbol{C}(x_k(c_2))$$

Example on the PCA Code Plot

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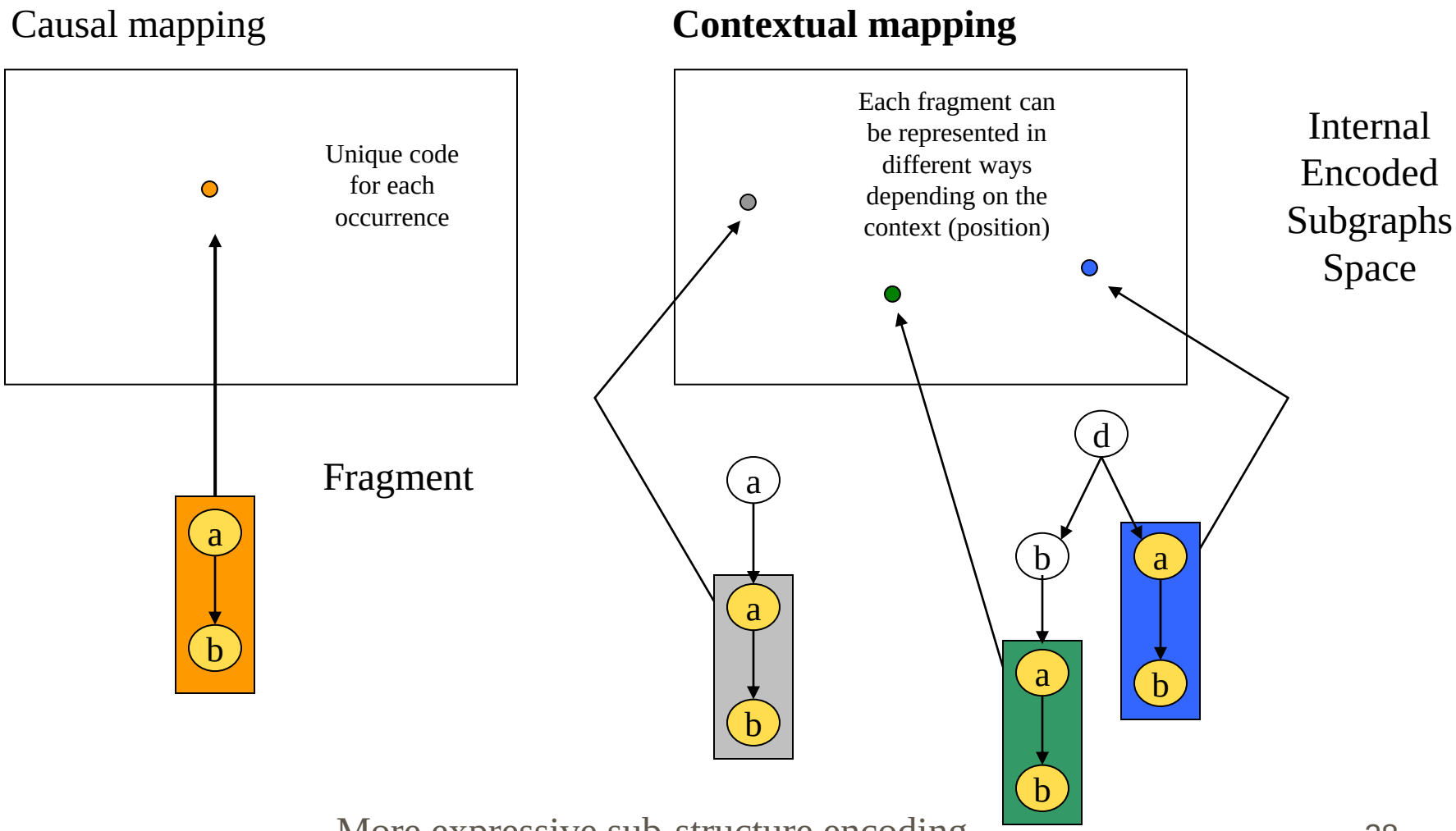

More expressive sub-structure encoding

DPAG representation: a counter-example

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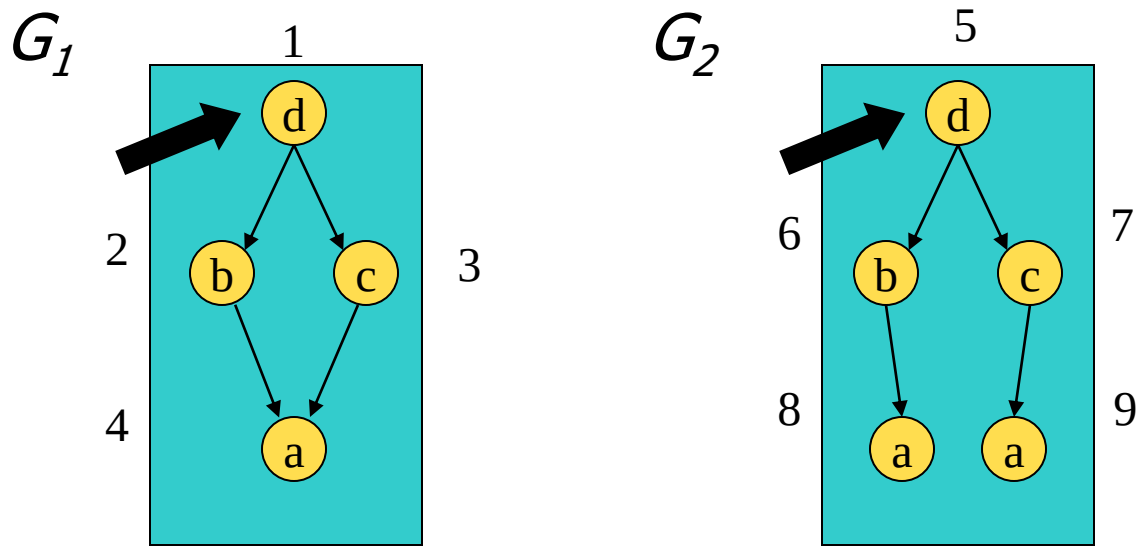
Relevance of contextual processing (II)

- Two different DPAG necessarily mapped into the same output by RecNN (*supersource* causal transductions) (*i.e. causal models fail*)



- CRCC **can** distinguish G_1/G_2 *(context for node "a" is different)*, RecNN **cannot** *(b and c see the same state values)*

DPAGs are not trees !

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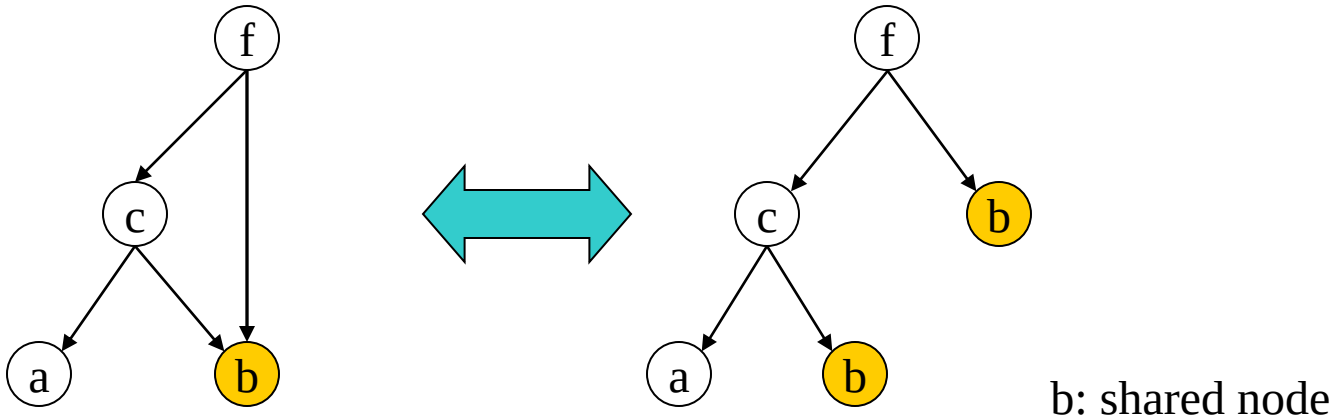
Relevance of contextual processing (III)

- Causual models allow to rewrite a DPAG as an equivalent tree



- CRCC distinguish them !
- *We (really) extended the domain from trees to DPAGs* !

The CRCC Contextual Approach

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- Each time a unit is frozen, the portion of its (memorized) state encodes knowledge of "the whole" structure

$$x_1(v) = \tau_1(x_1(\mathrm{ch}[v]), \boldsymbol{l}(v))$$
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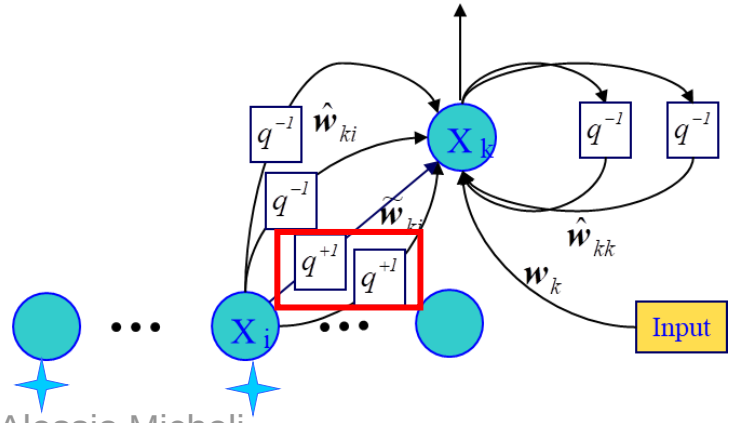
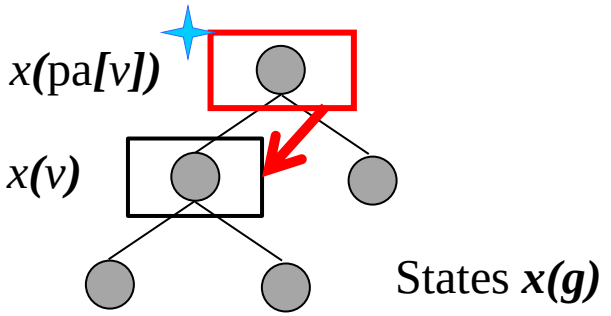
$$\vdots \qquad \vdots \qquad \vdots$$
$$x_m(v) = \tau_m(x_m(\mathrm{ch}[v]), x_{m-1}(\mathrm{ch}[v]), x_{m-1}(\mathrm{pa}[v]), \ldots, x_1(\mathrm{ch}[v]), x_1(\mathrm{pa}[v]), \boldsymbol{l}(v))$$

unit m — frozen unit m-1 — ····· — frozen unit 1

pa[v]: set of parents of v





Micheli et al. IEEE TNN, 2004

Example: *C(•) for* DPAGs

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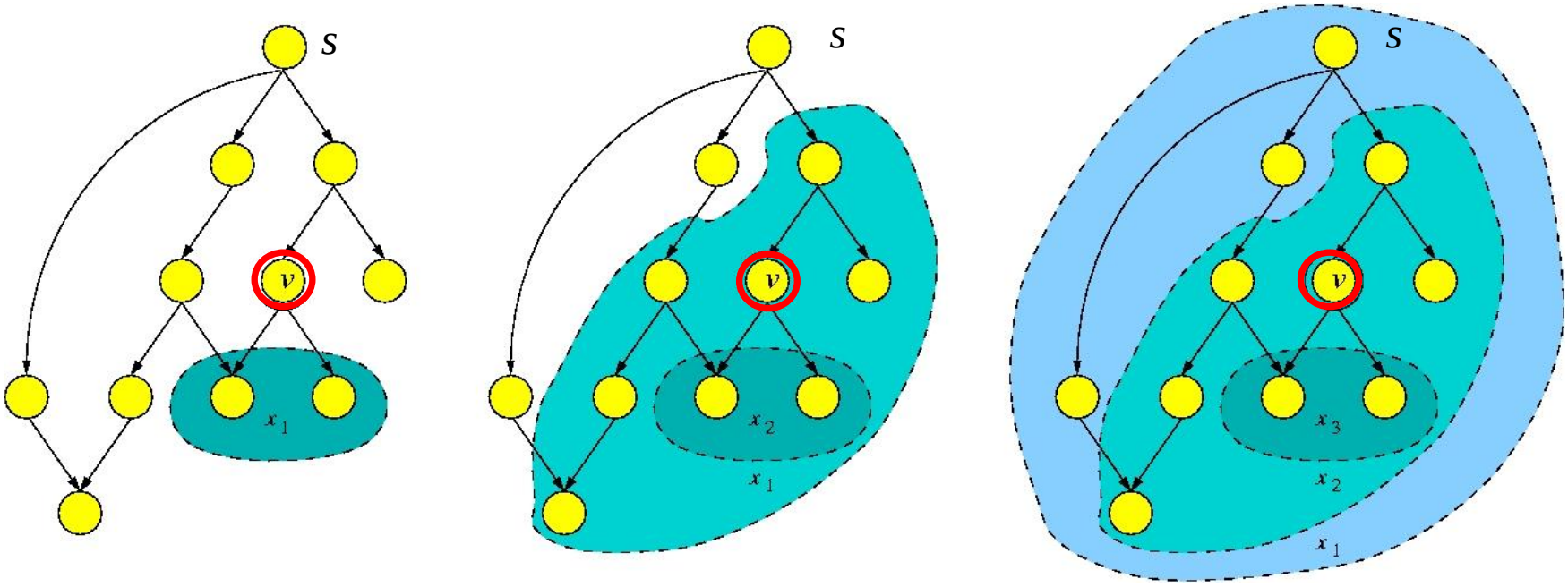

$C(x_1(v))$ $C(x_2(v))$ $C(x_3(v))$

The context grows (via in_set) including all sub-DPAG met along the (inverse) path $v \rightarrow s$ *and* $\downarrow v \rightarrow s$

Theory

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- Theoretical results have introduced to characterize the *computational power* of CRCC (class of computable functions/transductions vs causal models)

- Solving the examples before:
  - extension to *contextual* IO-isomorphic transductions,
  - e.g. *Target(v)=f (whole structure)*: future dependencies.
  - extension to the class of supersource (causal) transductions involving DPAGs that cannot be computed by causal models
  - while supporting all the function computable by RCC
  - And also:

- Formal compact expression of the "context window"
- Proof of computational power of CRCC (**abstracting from neural realization**)

Micheli et al. IEEE TNN, 2004

Example: $C(\bullet)$ for Sequences

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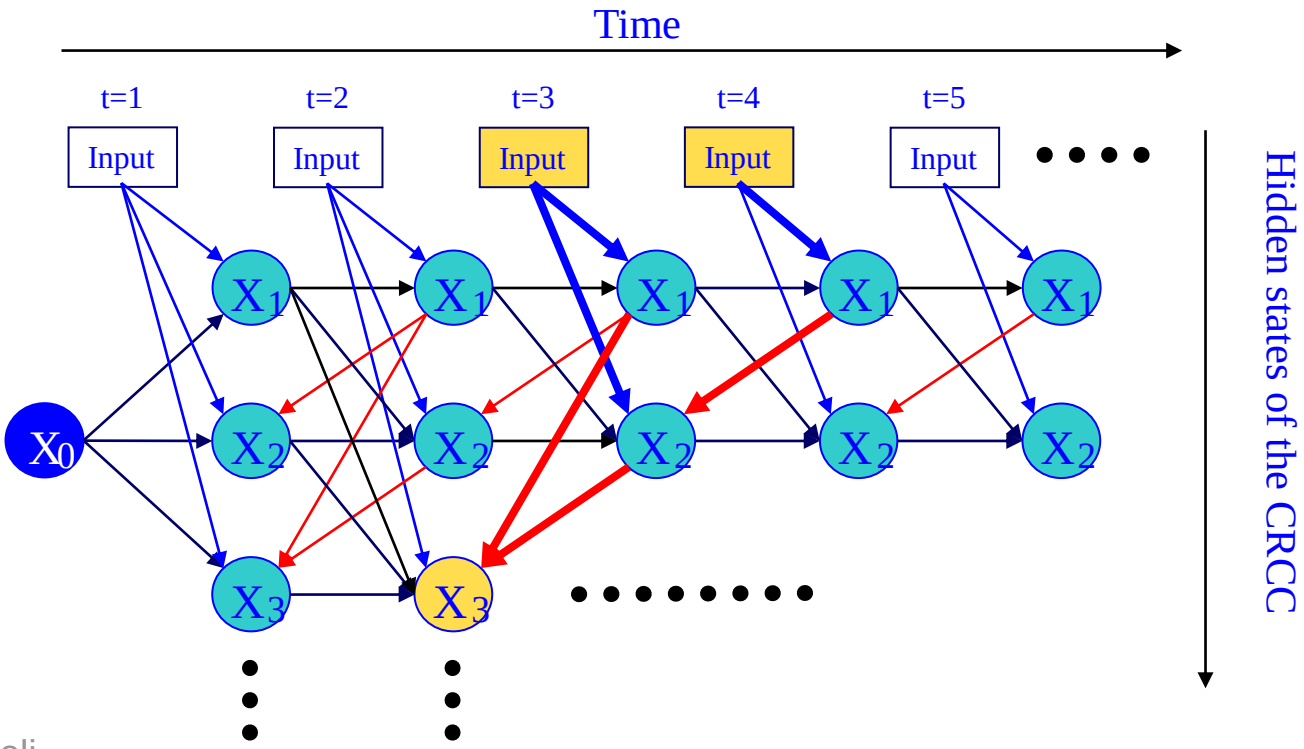
THEORY

$$C(x_k(v)) = \bigcup_{i=1}^{k-1} x_i.\downarrow v_{t+k-i} \cup x_k.\downarrow v_{t-1}$$

It is possible to formalize the **context** giving formal expression of state functional dependencies

Example here for sequences.



Context Scope:
Properties relating *h* and *C*

- **Proposition 1.** Given a DPAG G with supersource s, for any vertex v such that $dist(s,v)=d$, the contexts $C(x_h(v))$ with $h>d$ involve all the vertecies of G.

- **Proposition 2.** Given a DPAG G with supersource s, there exists a finite number h such that for each vertex v the context $C(x_h(v))$ involves all the vertecies of the graph. In particular, any

$$h > max_v\ dist(s,v)$$

satisfies the proposition.

SEE LATER

Universal Approximation

- B. Hammer, A. Micheli , A. Sperduti. **Universal Approximation Capability of Cascade Correlation for Structures** *Neural Computation* **17, 1109–1159** (2005)

- RecCC can approximate every measurable functions form sequences and trees to real values (in spite of their restricted recurrent architecture) for finite sets.

- **CRCC: Universal approximation capability extended to classes of labeled DPAGs**

f approximated up to any desired degree of accuracy
(up to inputs of arbitrary small probability)

$$P(x \in DPAG : \left| f(x) - CRCC(x) \right| > \delta) < \varepsilon$$

Hammer et al. Neural Computation, 2004

Context in a CRCC Application

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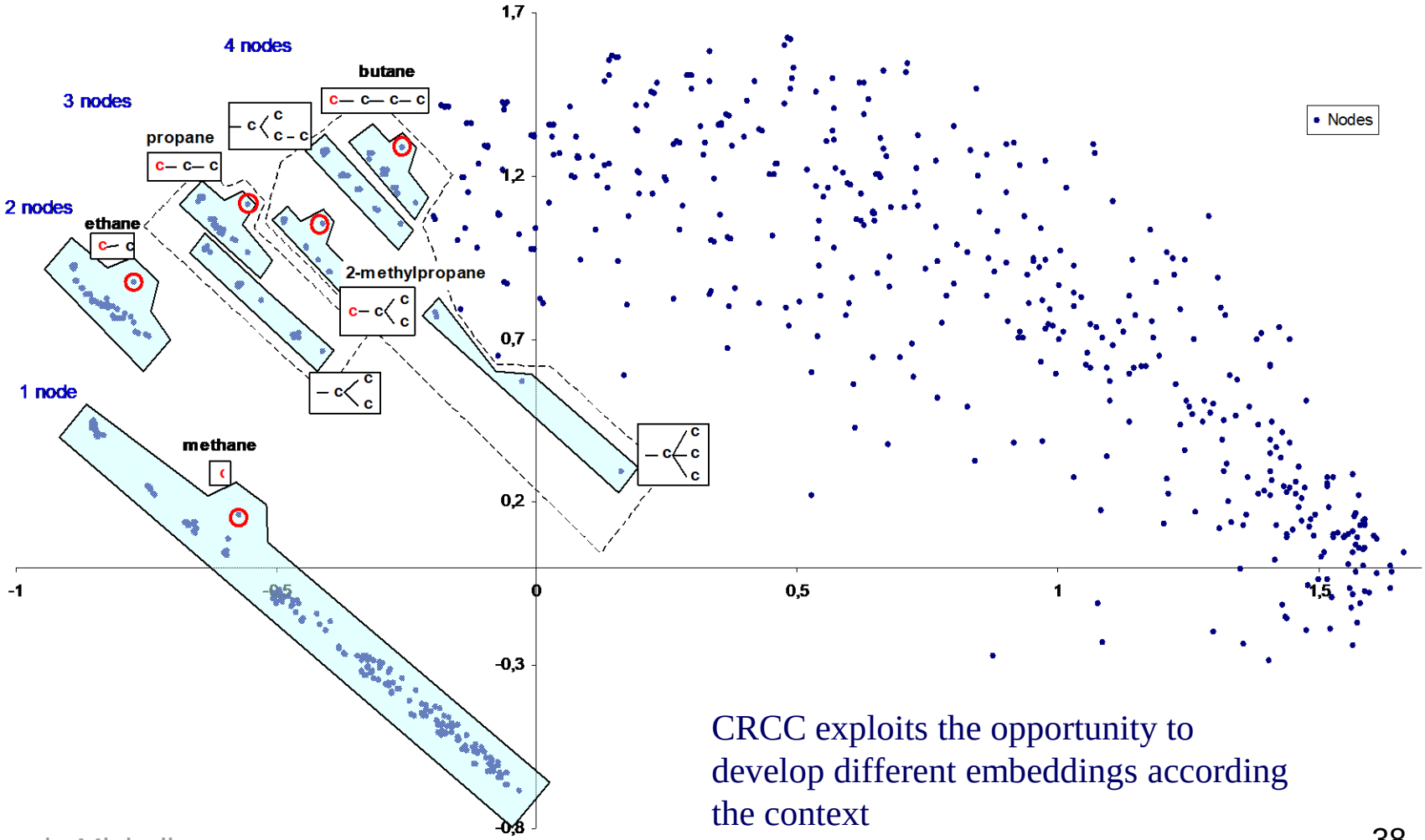
PCA of the represenation of the sub-structures developed by CRCC for a chemical regression task



CRCC exploits the opportunity to develop different embeddings according the context

CRCC Conclusions

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- Show advantages of including "context" (including parents)
  - Extension of the computation capability
  - Extension of the classes of data to DPAGs
  - Expressive encoding of substructures
  - Performance where causality assumption is unknown

- However, CRCC still requires topological order and supersource, still recursive dynamics: DPAGs/DAGs

- … New approaches : by retaining and extending context, removing **causality**/recursion ?
  - Yes, ***Move to graphs!***

Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

Extensions of models for supervised and unsupervised learning in structured domains

- 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

- Recap SD1
- Causality for Recurrent and Recursive models &
- Contextual approaches (BRCC/CRCC and DPAGs)
- Neural Networks for graphs

By a journey through the causality assumption!

Graphs by NN: Cycles

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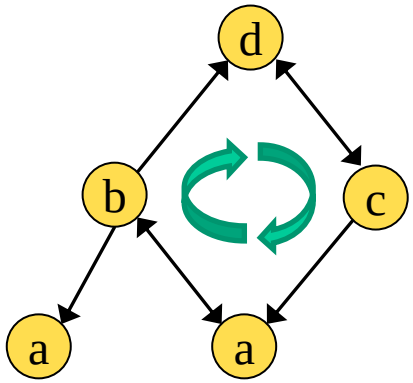
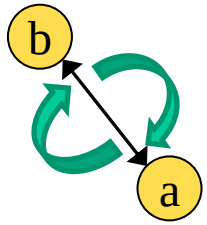
Causality assumption in RecNN introduce issues in processing cycles (due to the mutual dependencies among state values)

Cyclic graph





Occuring also for undirected edges!

How to deal with cycles and causality?

Main approaches for graphs by NN

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Different classes of approaches:

1. **Rewriting the graph**:
   - Atomic representation of cycles: e.g. functional groups in chemistry
   - To trees/DAGs (e.g. SMILES representation in chemistry)

2. **RecNN** by explicitly treating the cyclic dynamics by contractive constraints (GNN, GraphESN) [1,2]

3. **Layering**: contextual non-recursive approaches (NN4G [3] /Conv. NN for graphs [4]) → **Deep NN for graphs**

1. Scarselli, Gori, Tsoi, Hagenbuchner, Monfardini. IEEE TNN, 2009.
2. Gallicchio, Micheli. IJCNN, 2010.
3. Micheli. IEEE TNN, 2009.

2. GNN/GraphESN (2009-2010)

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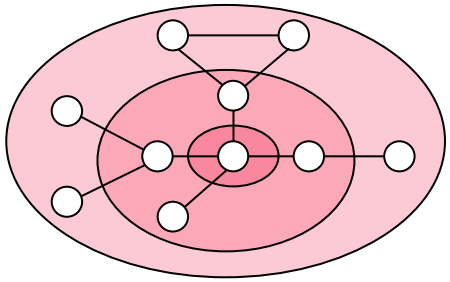
- In GraphESN and GNN the equation are similar to RecNN
- Cycles are allowed (in state computation), the state is computed iterating the state transition function until convergence
- Stability of the recursive encoding process is guaranteed by resorting to contractive state dynamics (Banach theorem for fixed point)
  - In *GNN* imposing constrains in the loss function (alternating learning and convergence)
  - In *GraphESN* the condition is inherited by contractivity of the reservoir dynamics (see ESP conditions): *very efficient!*



GraphESN state transitions

$$\mathbf{x}(v) = tanh(\mathbf{W}_{in}\mathbf{u}(v) + \sum_{v' \in \mathcal{N}(v)} \hat{\mathbf{W}}\mathbf{x}(v'))$$

Context evolution, with the iteration, of the state for the vertex in the center
(not just local, by *diffusion on graph*)

- Scarselli, et al. IEEE TNN, 2009
- Gallicchio, Micheli. IJCNN, 2010.

Also extended to GRU (Li et al. 2015)

2. GraphESN details (I)

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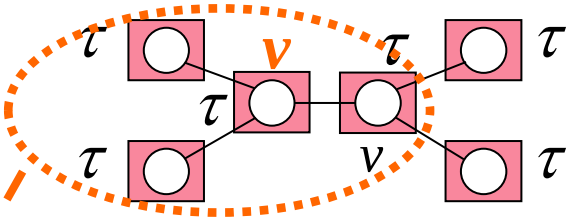
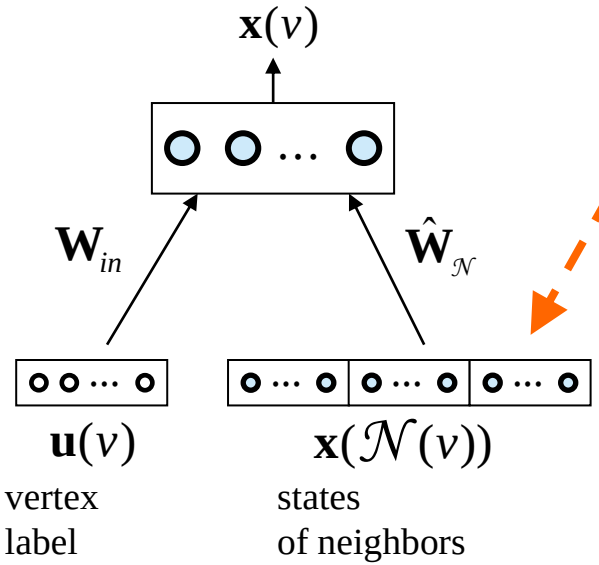
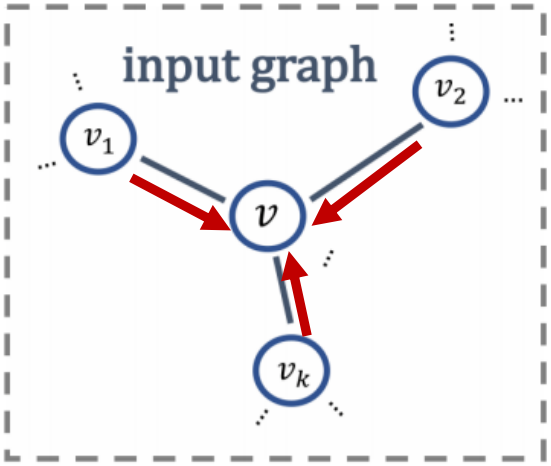
Iterative (t) computation of the local encoding

$$\mathbf{x}_t(v) = \tau(\mathbf{u}(v), \mathbf{x}_{t-1}(\mathcal{N}(v)))$$



Reservoir (τ)





$$\mathbf{x}_t(v) = \tanh(\mathbf{W}_{in}\mathbf{u}(v) + \hat{\mathbf{W}}_{\mathcal{N}}\mathbf{x}_{t-1}(\mathcal{N}(v)))$$

A state value is computed <u>for every vertex</u> of each **g**

State transition eq. (reservoir units): convergence to a fixed point

2. GNN/GraphESN

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Pro/Cons:

+ Extend the domain of RecNN to general graphs
+ Theoretical approximation capability and VC dimension have been proved
- [GNN] elongate training time with the convergence (double mutual iteration)
- Constraints of the weight values → bias to contractive transduction
+ GraphESN dose not require training time of the recursive part → efficient!
+ A deep (multi recurrent layers) version has been developed (see the references)

3. Layering

Contextual Multi-Layered approaches for graphs

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Layering basic idea:

- the mutual dependencies are managed (architecturally) through different layers (i.e. by a *deep* architecture)
  - Instead of iterating at the same layer, each vertex can take the context of the other vertices computed in the previous layers, accessing progressively to the entire graph/network
  - And each vertex take information from all the others, including the mutual influences: **Collective inferencing**

- **NN4G** since 2005-2009 : a pioneer approach following the RecNN/ CRCC line (completely *relaxing the recursive causality assumption*)
  - In the following
- **CNN for graphs** since 2015: moving the idea for 2D processing (images) to graph processing through many layer

NN4G: Motivations

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- Is it possible to find more general and simpler solutions removing *causality* without introducing cycles dependencies in the states definition **?**

NN4G : Neural Network for Graphs

- Two main ingredients:
  1) constructive (feedforwad) neural network approach
  2) Local and contextual information of each vertex of a graph

But recursive causality is removed

- Micheli, Sestito. WIRN 2005
- Micheli. IEEE TNN, 2009.

1) Constructive Approach

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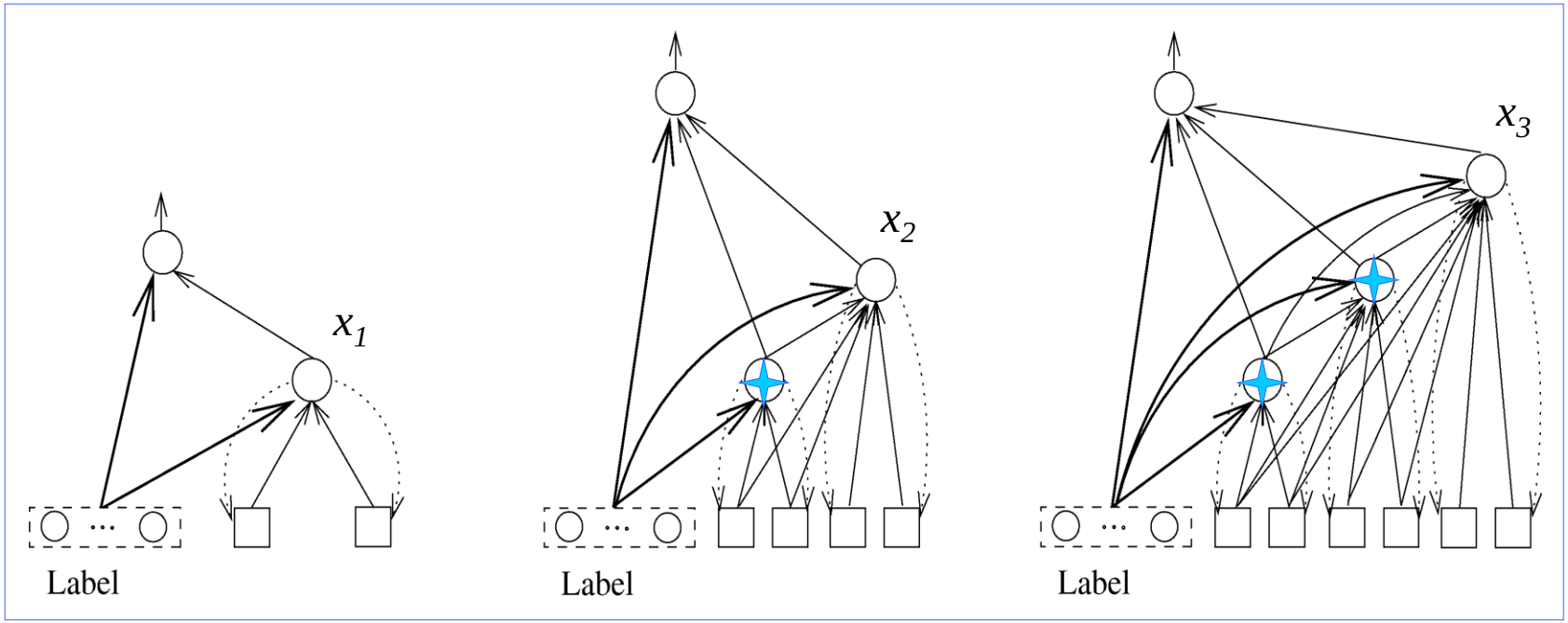
Cascade Correlation (*RecCC* in the picture):

The hidden units are progressively added to the network during training, and frozen after insertion



2) Local Context and Structured Domain

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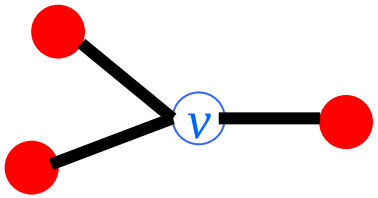
- We assume a fairly general class of labeled graphs $g \in \mathcal{G}$
- $Vert(g)$: set of vertexes of g; $l(v)$: label of v
- $edg(v)$: set of edges incident on v
- **Neighbors of v :**

$$N(v) = \{u \in Vert(g) \mid (u,v) \vee (v,u) \in edg(v)\}$$ Directed

$$N(v) = \{u \in Vert(g) \mid (u,v) \in edg(v)\}$$ Undirected



- Contex of v is the set of vertexes with a path to/from v affecting the output of v.

NN4G: Hidden Units

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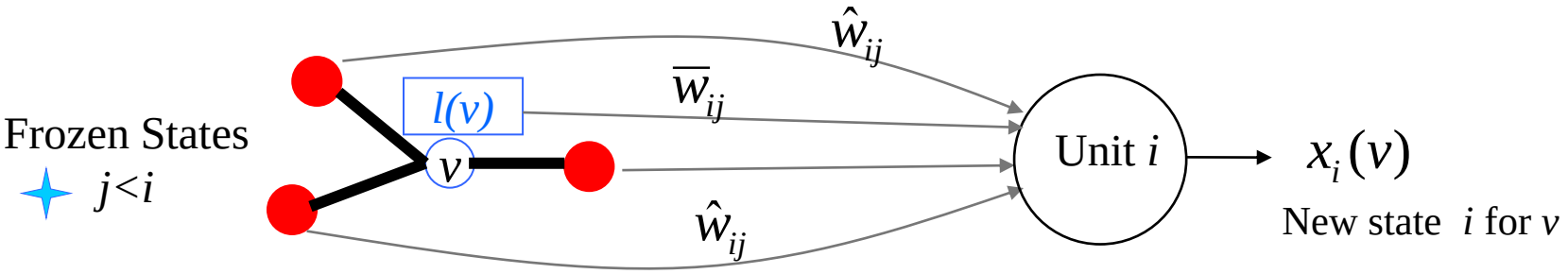
- NN4G compute a state variable for each vertex

$$x(v) = \begin{cases} x_1(v) = f\left(\sum_{j=0}^{L^v} \overline{w}_{1j} l_j(v)\right) \\ x_i(v) = f\left(\sum_{j=0}^{L^v} \overline{w}_{ij} l_j(v) + \sum_{j=1}^{i-1} \hat{w}_{ij} \sum_{u \in \boldsymbol{N}(v)} x_j(u)\right) \end{cases} \quad i = 2,\ldots, N$$

Current Label

Context

It was the sum over the children 1..*k* for RecNN



- Note: ***Not Recursive*** (no feedbacks): $x_i(v)$ dependes only on frozen values (j<i)
  - No cyclic dependencies are introduced in the defintion of the state transition system
- No topological order to follow: $x_i(v)$ can be computed in parallel for vertexes of *g*

NN4G: Hidden Units Generalization (edges)

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- NN4G define a very general computational framework, e.g.

$$x(v) = \begin{cases} x_1(v) = f\left(\sum_{j=0}^{L^v} \overline{w}_{1j} l_j(v)\right) \\ x_i(v) = f\left(\sum_{j=0}^{L^v} \overline{w}_{ij} l_j(v) + \sum_{j=1}^{i-1} \sum_{u \in \boldsymbol{N}(v)} \hat{w}_{ij}^{(v,u)} x_j(u)\right) \end{cases} \quad i = 2,\ldots, N$$

W for edge (v,u)

- (v,u) is unordered (for undirected graphs)
- Stationarity (weight sharing) strategy: association between weights and edges
  - Entering/leaving edges for directed graphs
  - Position for positional/ordered graphs
  - **Label of the arc** more in general: $W^{(u,v)} = W^{(t,v)}$ *if* $L(u,v)=L(t,v)$

- First trials: full stationarity: 1 weights for each edges:
  - unordered and undirectd graphs and
  - strong parameters reduction

NN4G: Output unit

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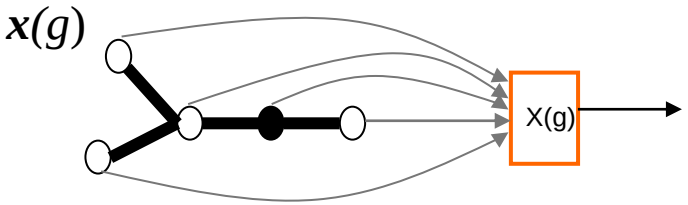
1. From states to the output layer
   - IO- isomorphic transduction (an output for each vertex) or
   - A scalar value for a whole graph can be emitted, using an operator X, ***e.g.***:

States mapping function



Can be even a simple global sum or average or selection from relevant vertices etc.

2. Output layer: e.g. A single standard neural unit

$$y(g) = f\left(\sum_{j=0}^{N} w_j X_j(g)\right)$$

- Learning: as in (feedforward) Cascade Correlation: adding hidden units and interleaving min. of error at the output layer and max. of the correlation score for each hidden unit.

Algorithm

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1. For i=1 to *N*
2. For all *g* in *G*
3. For all *v* in *Vert(g)*
4. Compute $x_i(v)$ *(even in parallel *)*
5. Compute $X_i(g)$
6. For all *g* in *G*
7. Compute *y(g)*

(*) I.e. a traversal of the input graph: the result does not depend on the visiting order

NN4G: 2) Hidden Units and Context

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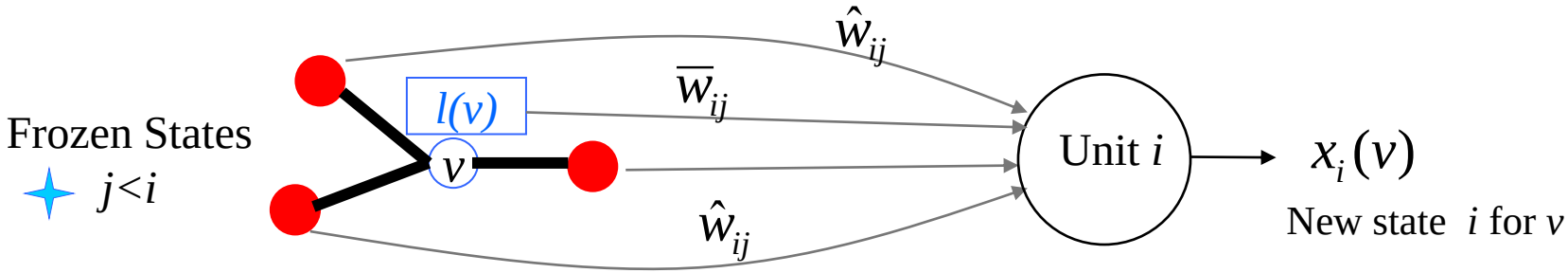
- Is NN4G just a relational approach taking only a local neighborhood (for each hidden unit) **?**



- ***No***, because through layering NN4G extend the context of each vertex to all the vertices in graph
- Because progressively, ***by composition***, the model extends the context of influence to other vertices through the context developed in the previous frozen hidden units (layers) → *see the next slide*

Evolution of the Context (Compositional)

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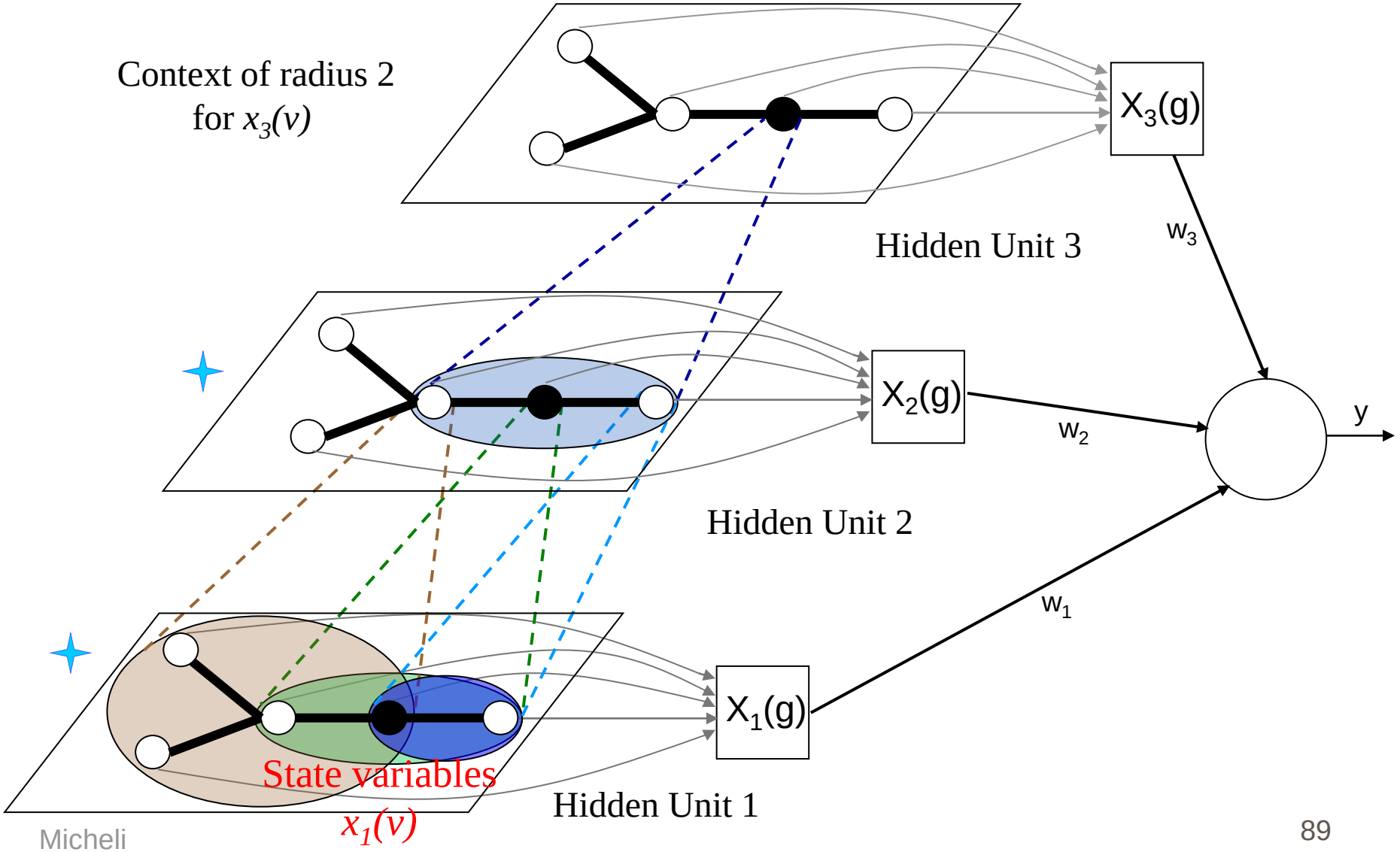

NN4G: Context Growth

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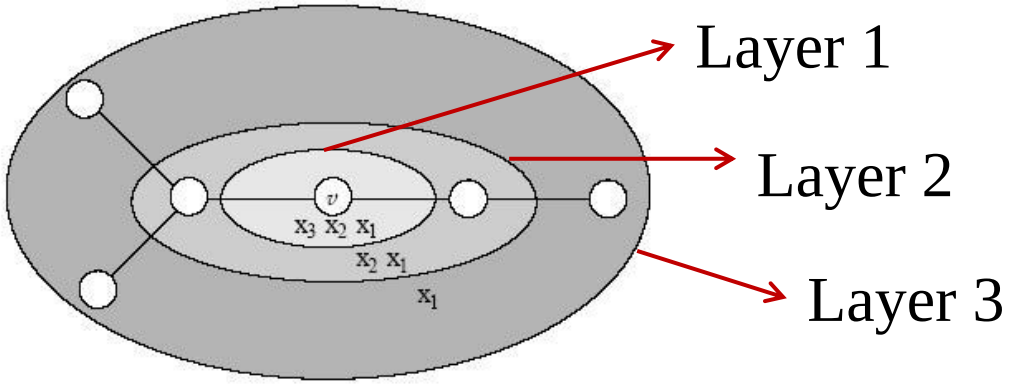
- The growth of the context is symmetric in each direction starting from each vertex, and grow with layers



- In such a way, the size of the context window can grow and we do not need to fix it prior to learning.
- *The **depth** of networks is functional to context development*

Context Scope:

Formal Properties relating *h* and *C*

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- It has been **formally proved** that that the context $C(x_h(v))$ grows one step ahead, for each added unit (layer *h*), as $N^h(v)$:
  - the dimension of the context is proportional to the number of units,
  - and the structure of the composition is given by the topology of the input graph

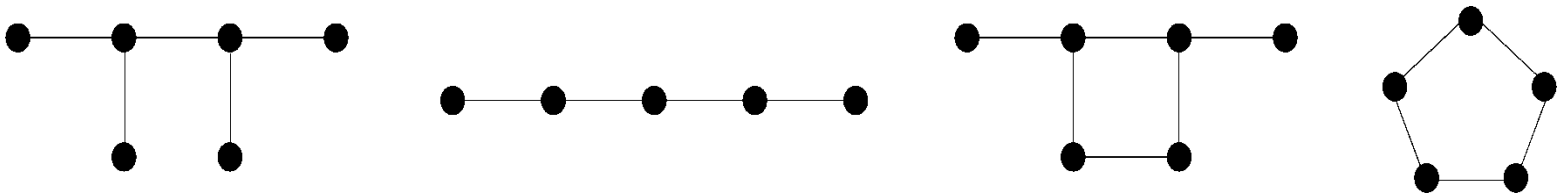
1. And that $C(x_h(v))$ can involve all the vertices of the graph:

   Theorem [NN4G]: Given a finite size graph *G*, there exists a finite number *h* of state variables (hidden layers) such that for each *v* in *G* the context of *v* involves all the vertices of *G*.
   - In particular, *h* > "diameter" of the graph satisfy the proposition.

   Micheli. IEEE TNN, 2009.

Example of experimental assesment: Cyclic versus Acyclic Undirected Graphs

- Artificial task: test NN4G capability to learn a relevant topological feature, i.e the **occurrence of cycles** in the input undirected graphs, which cannot be directly treated by RNN.
- **Input domain**: 150 cyclic graphs and 150 acyclic graphs with 3 up to 10 vertexes (2670 Vertexes)



- **100% test classification accuracy** over all the folds of 10-fold cross-validation with 5 trials for each fold.
- Just **2 hidden units**.
- In fact, the second unit is able to distinguish the ratio between the number of edges and vertexes in the graph, which is a sufficient feature to discriminate the input graphs on the basis of the occurrence of cycles in its topology.

NN4G Recap

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- NN4G: *A deep model for graphs*
- Characteristics:
  - Direct/undirected cyclic/acyclic labeled graphs
    - W.r.t. RecNN does not assume **causality** over directed structure;
      in particular, no assumption on the topological order is needed;
  - ☆ Incremental, layer by layer learning & automatic model design
  - **Depth** functional to contextual encoding: Dimension of context grows with layers (*formally proved*)
  - ☆ **Efficient**: no cyclic def. of state var., divide et impera on the task
    - Scaling: Current model (full stationarity): *O(|G|Vh² epochs):* Linear in the number of vertices
  - ☆ Generality: No constraints on weights values (vs GNN)
  - Pool strategy (Cascade corr. Training): local minima avoidance, supervised architecture optimization .

A first comparison
NN4G / Conv.NN for Graphs

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Concepts in common:

- *Traversal of the input graph:* Visiting (the nodes of) input graphs through units with weight sharing (stationarity)
  - This correspond for CNN to the *convolution* over (the nodes of) input graphs,
  - i.e. constrained to graph topology instead of 2D matrix
- Layering and hence *moving to deep architecure* (functional to contextual processing)
- Composition for the (no causal) context learning, parsimony, and adaptivity are achieved and extend to *any kind of graphs*
- Node-centric learning can exploit the *Collective inference*

A first comparison
NN4G / Conv.NN for Graphs

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Main differences are more related to the *training*:

- **CNN-G**s typically use CNN architecture/training approaches,
  - Fixed architecture (few hidden layers)
  - Top-down back-prop (end-to-end): can be quite computational demanding using many layers

- **NN4G**: Incremental, layer by layer learning & automatic model design
  - Advantages: No gradient vanish issue, *divide et impera*, automatic number of layers, etc.

Learning in Structured Domain
Plan in 2 lectures

1. Recurrent and Recursive Neural Networks

Extensions of models for supervised and unsupervised learning in structured domains

- 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

- Recap SD1
- Causality for Recurrent and Recursive models &
- Contextual approaches (BRCC/CRCC and DPAGs)
- Neural Networks for graphs
- **Other models and looking ahead**

By a journey through the causality assumption!

NN4G+ HTMM

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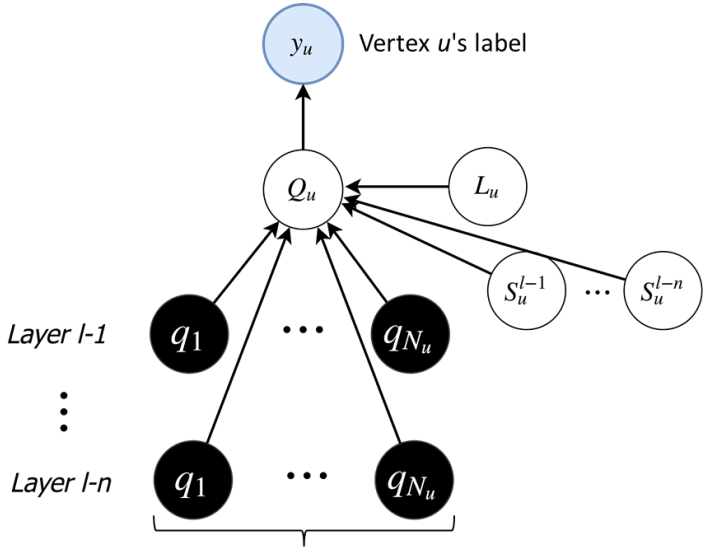
- We can extend such contextual ideas also to RC and HTMM approaches making them *deep and for graphs*

- *E.g. ICML 2018* A NN4G realized by a *generative* approach
- trained by a mix of unsupervised (Markov models for hidden layer) and supervised (output layer) approaches
- Also for unsupervised / semi-supervised probabilistic learning

- *Contextual Graph Markov Models*



Bacciu , Errica, Micheli, ICML 2018.

And Kernels?

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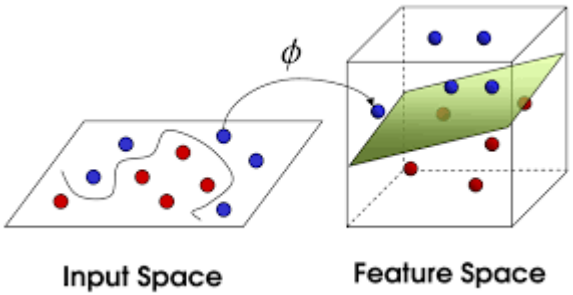
- Kernels for SD from RC [1] and HTMM [2] for SD, e.g. (by CIML):

- Kernels for SD from RC

1. D. Bacciu, C. Gallicchio, A. Micheli, *A reservoir activation kernel for trees.* ESANN 2016

- Kernels for SD from HTMM (adaptive kernels + generative & discriminative)

2. D. Bacciu, A. Micheli, A. Sperduti. *Generative Kernels for Tree-Structured Data,* IEEE TNNLS (Transactions on Neural Networks and Learning Systems), 2018



Summarizing the MODELS panorama for SD (examples)

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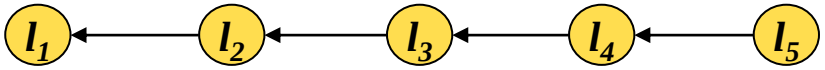
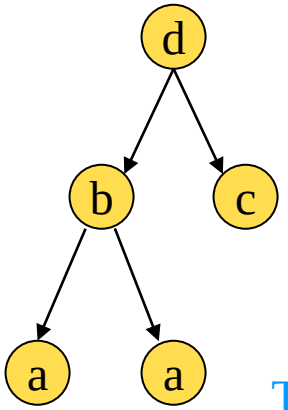
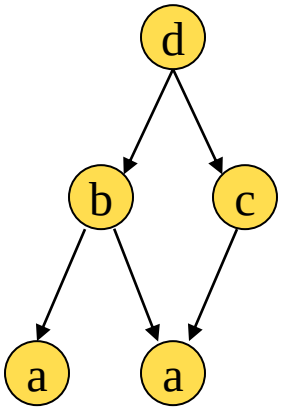


Standard ML models for flat data

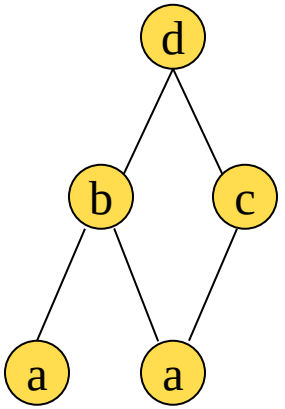
- Recurrent NN/ESN
- HMM
- Kernel for strings …



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



DPAG:
- CRCC



- GNN/GraphESN
- NN4G
- Conv.NN for G.
- Graph Kernels
- SRL
- …

See references for models in the bibliography slides (later)

Future – just ahead

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- **New models for SD** (discussed so far)
- **New applications**
- **…**

Future applications

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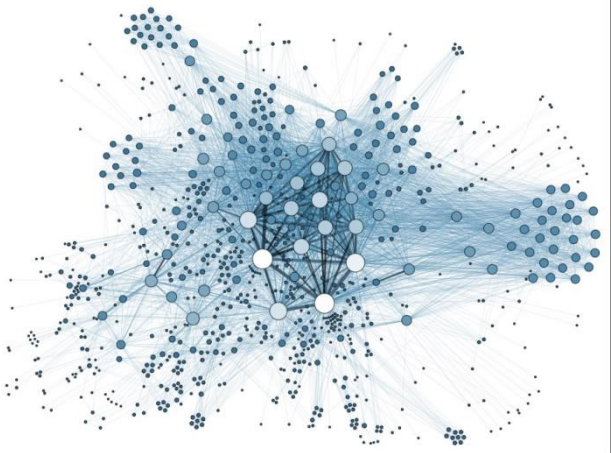
Under construction! Ready to apply for tree/graph data on:

- Network data → next slide
- Parallel programming: Skeleton application description (trees) → estimation of execution time and energy (with M. Danelutto)
- System biology (graphs/networks) (with P. Milazzo) *on-going*
- Bioinformatics:
  - Coarse grained models for Proteins (next slide)
  - Prediction of protein function (Gene Ontology graphs)
  - Pan-genome analysis (by graph represenation)
- SW engineering (DPAGs) (with V. Gervasi)



Coarse grained models for Proteins (Biophysics)

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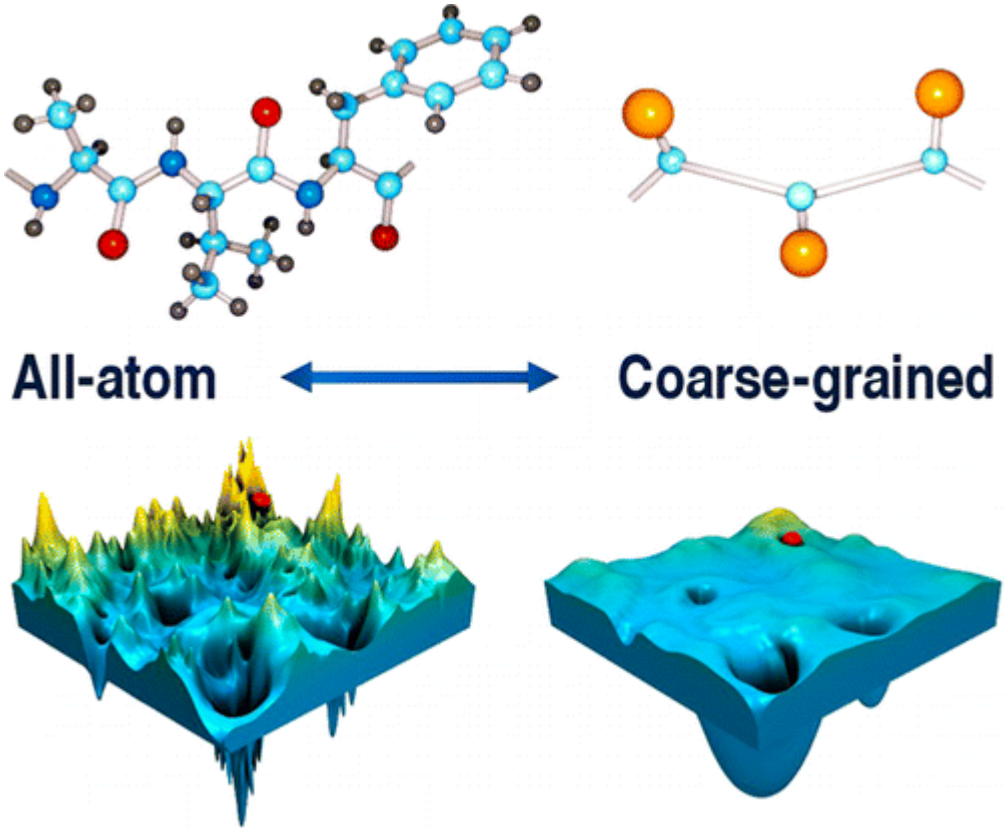

By NN for graphs!

On-going: Thesis available!

Processing/Learning Aims

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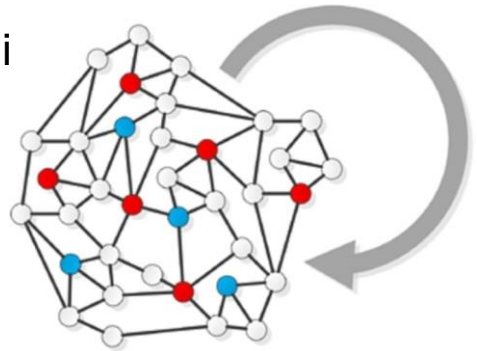
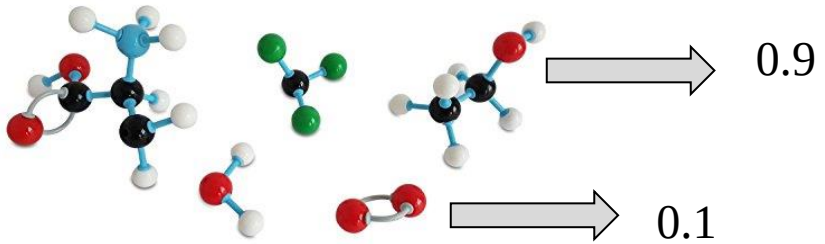
Also task changes according to the data which can be:

- A single graph (typically a network): in-graph learning
  - For instance to classify the nodes of a partially labeled network (as a social network or a graph in semi supervised learning problems)
  - Belong to input-output isomorphic transductions



- A collection of variable size graphs: between-graphs
  - For instance, classify different graphs starting from a training set of know couples as in the molecules example

Given a set of examples $(graph_i, target_i)$
Learn an hyphotesis mapping $T(graph)$



Networks, an example: *within* or *in-graph* learning

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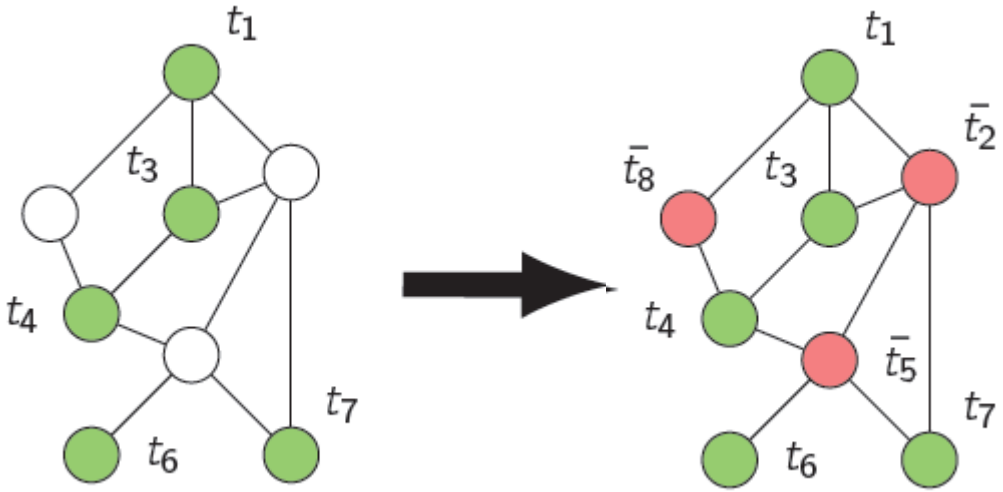
Network data: entities are interconnected

Within-network learning: training entities are connected to entities whose classifications are to be estimated



An instance of IO-isomorphic transduction for graphs!

- Example: web spam (host) classification
- ~10K vertices (hosts) and 500K links (web pages links)
- Classify each vertex as spam/not spam given the target is know for some of them (*in the same unique graph*!)

A more general aim (CIML -Pisa)

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- Adaptive processing of SD
- **A theoretical and pratical framework for the automatic design of *efficient* models** for sequences, trees and graphs (both generative and discriminative) exploiting DL approaches
  - Able to answer the main issue of DL frameworks: how many layers? How many units? Which hyper.? Etc.
  - Open to *semi-supervised* learning and different graph and network tasks
  - *Efficient* by incremental NN and RC approaches

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Bibliography: aims

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Different parts in the following:

- Basic/Fundamentals
- * Possible topic for seminars
- May be useful also for future studies

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

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

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DRAFT, please do not circulate!

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