

An Artificial Molecular Model To Foster Communities

C. Schommer

University Luxemburg

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What's about?

■ Our Goals:

- Adaptive System that fosters on fluid data situation.
- Autonomous System that communicates with its environment.
- Intelligent System that maintains *interesting* patterns.

What's about?

■ Our Concept:

- Data = Atomic nodes α_{A_i} .
- Information = Collection of α_{A_i} forms a molecular structure.
- Insights = Interesting patterns of relevance.
- Knowledge = Relevant patterns of temporal existence.

■ Our Approach:

- Need for a fundamental description of the model.
- What are relevant patterns?
- Introducing catalytic reactions: autonomous modifications on molecules.

What's about?

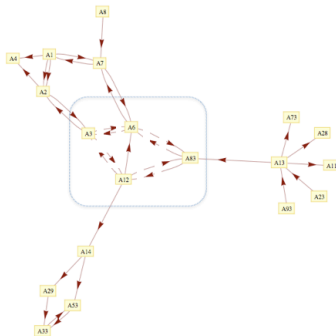


Figure: Snapshot of a fluid data situation.

The Model – A Shape Of Molecules

A single molecular bond $sBond(\alpha_{A_i}, \alpha_{A_j})$ exists between atomic nodes α_{A_i} .

$$sBond(\alpha_{A_i}, \alpha_{A_j}) = \begin{cases} \omega_{A_i \rightarrow A_j} & : \alpha_{A_j} \rightarrow \alpha_{A_i} \\ \vee \alpha_{A_i} \rightarrow \alpha_{A_j} & \\ 0 & : else \end{cases}$$

A single molecular bond has a weight of $\omega_{A_i \rightarrow A_j}$, which is expressed by the conditional probability $P(A_j | A_i)$. If the relationship between the two actor nodes is directed in both directions, then we call this bi-relationship a *double molecular bond*.

$$dBond(\alpha_{A_i}, \alpha_{A_j}) = \begin{cases} \omega_{A_i \rightarrow A_j} \times \omega_{A_j \rightarrow A_i} & : \alpha_{A_j} \rightarrow \alpha_{A_i} \\ \wedge \alpha_{A_i} \rightarrow \alpha_{A_j} & \\ 0 & : else \end{cases}$$

The Model – A Shape Of Molecules

If an atomic node α_{A_i} is being arranged as a centre of k adjacent nodes α_{A_j} , then this unary structure is called a *molecule star*.

$$\mathbf{mStar}(\alpha_{A_i}) = \begin{cases} 1 & : \neg sbond(\alpha_{A_i}, \alpha_{A_j}) \wedge (\bigwedge sBond(\alpha_{A_i}, \alpha_{A_j}) \vee \bigwedge dBond(\alpha_{A_i}, \alpha_{A_j})) \\ 0 & : else \end{cases}$$



Figure: A molecular star.

The Model – A Shape Of Molecules

In case that two *actor nodes* α_{A_i} and α_{A_j} share a *double molecular bond*, we call this a *molecular bridge*.

$$\mathbf{mBridge}(\alpha_{A_i}, \alpha_{A_j}) = \mathbf{dBond}(\alpha_{A_i}, \alpha_{A_j})$$

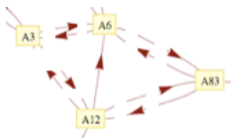


Figure: A molecular bridge.

The Model – A Shape Of Molecules

- *Atomic actor nodes* may play a role inside each molecule, being either a node that actively stimulates another node or a node that is passively stimulated by another node.
- A decomposition of a molecule concerning a semantic assignment may then be as follows: let α_{A_i} , α_{A_j} and α_{A_k} disjunctive *atomic actor nodes*, $1 \leq i \neq j \neq k \leq n$ natural numbers, and n the total number of nodes, then an *atomic actor node* α_{A_i} is a *atomic reactor* and/or an *atomic trigger*.

$$\mathbf{mReactor}(\alpha_{A_i}) = \exists \alpha_{A_j} : sBond(\alpha_{A_j}, \alpha_{A_i})$$

$$\mathbf{mTrigger}(\alpha_{A_i}) = \exists \alpha_{A_j} : sBond(\alpha_{A_i}, \alpha_{A_j})$$

The Model – A Shape Of Molecules

Some examples of molecule structures are:

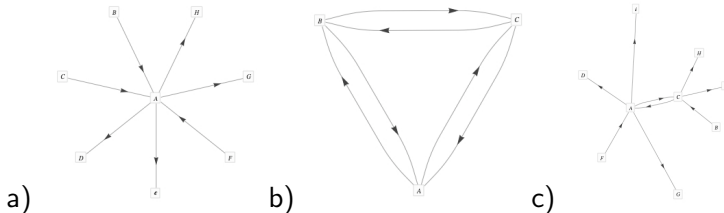


Figure: Selected molecular forms with a) a molecular star, b) a collection of molecular bridges (diamond) and c) a molecular bridge with single/double molecular bonds (bottom).

The Model – A Shape Of Molecules

Introducing operational functions like the distance $d(\alpha_{A_i}, \alpha_{A_j})$

$$\mathbf{d}(\alpha_{A_i}, \alpha_{A_j}) = \begin{cases} \sum_{k=i}^j \sigma_{A_k} & : A_i \rightarrow A_j \\ \text{undefined} & : \text{else} \end{cases}$$

or the strength $s(\alpha_{A_i}, \dots, \alpha_{A_j})$ of a relationship. For example, a *molecular star* is certainly depending on the number of associated actor nodes α_{A_j} , their activation states σ_{A_j} , and the connection weights $\omega_{A_i \rightarrow A_j}$ and $\omega_{A_j \rightarrow A_i}$, respectively, among them:

$$\mathbf{s}_{mStar}(\alpha_{A_1}, \dots, \alpha_{A_n}) = \prod_{k,l=1; k \neq l}^n \omega_{A_k \rightarrow A_l}$$

The Model – Reaction Rules

- A functional protein Π_k is therefore unlike a static collection of nodes but moreover a vivid (artificial) and autonomous system.
- Besides, we understand these functional proteins as an operating structure that is commissioned to complete tasks:
 - it is conceivable to send information
 - it describes the structure it obsesses.
- Functional proteins may be forced to continuously improve its own structure:
 - such an improvement may be the update of existing single or
 - double bonds or atomic nodes (decrease/increase).

The Model – Reaction Rules

Each α_{A_i} shares an activation σ_{A_i} and owns a set of items Γ_{A_i} .

- Each *atomic actor node* is allowed to *react* with another α_{A_j} through a catalyst τ .
- In case that an actor node α_{A_i} with a set of items ξ_i owns the same or a subset of interests than another actor node α_{A_j} , then both may react, merge and establish a *catalytic bridge* τ_{A_i, A_j} .

The Model – Reaction Rules

- With Γ_{A_i} , we allow each actor to own a number of *items*, for example interests that are organized within a hierarchical system.
- We then receive levels of different granularity with for example

$$\begin{aligned} \gamma^0 = \{Root\} \leftarrow \gamma^1 = \{A, \dots, Z\} \leftarrow \gamma^2 = \{A_1, \dots, Z_n\} \\ \leftarrow \dots \leftarrow \gamma^3 = \{A_{1,1}, \dots, Z_{n,m}\} \end{aligned}$$

- The concept is that each time an association is performed, the actor's interest γ^j may be extended by another interest.

The Model – Reaction Rules

For example, if an actor A_i is interested in

$$\gamma^3 = \{A_{1,1}, A_{1,2}, A_{1,3}, A_{1,4}\}$$

then the interest level is replaced to $\gamma^2 = \{A_1\}$ in case that a threshold \min_{γ}^k is reached.

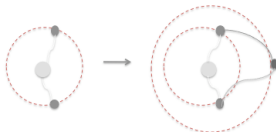


Figure: Generalization of the interest level of actor A_i .

Application Example

- We target on Bibliographic Databases like *DBLP*.
 - A publication is a molecule of atomic author nodes.
 - Each atomic author node holds a list of interests (ACM classification).
 - If the interests between authors match then a catalytic bridge is established.

Application Example

The merge evolves because of a common interest $B.1$: in this case, it is an identical classification chapter in the ACM classification system.

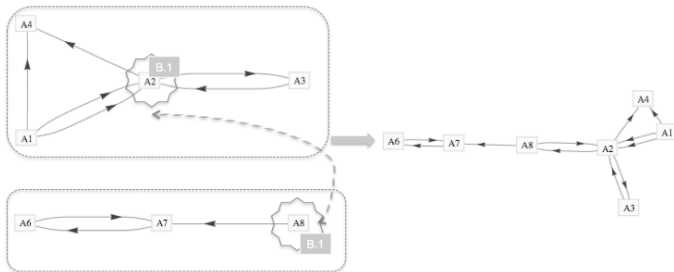


Figure: Reaction of two independent molecules to a functional protein. The merge is initiated by a catalyst τ that forms a catalytic bridge between α_{A_2} and α_{A_8} .

Application Example

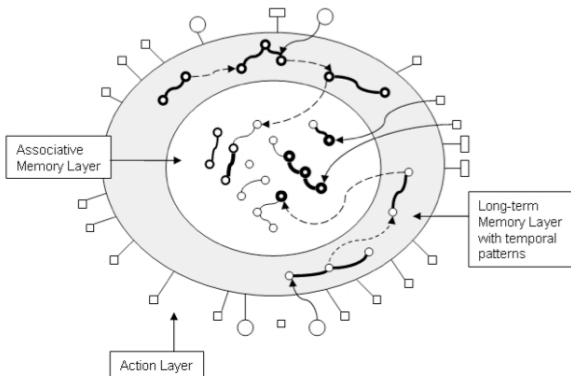


Figure: Fluid management architecture simulating the human mind – with STM (information), LTM (insights/knowledge), and Action Layer (Communication).

Conclusions

Towards a **bio-inspired machinery** that...

- fosters on fluid data situation (Adaptivity, Associativity).
- communicates with its environment (Autonomy).
- maintains *interesting* patterns (Intelligence).

The Final Side

Thank you for your attention!

Questions?