A membrane computing based approach to deep graph representation learning

Dr. Katalin Anna Lázár [1]

[1]Department of Algorithms and their Applications, Faculty of Informatics, Eötvös Loránd University, Budapest, Hungary

Erasmus Mobility Program
Universidad de Sevilla, Escuela Técnica Superior de Ingeniería Informática (ETSII)
November 16, 2023

Topics

- Deep learning
- Overview of membrane computing [Riscos-Núñez, 2023].
- Tissue-like P systems
- Neural-like approach
- Outlook

Deep learning (DL)

- A field of machine learning (ML) algorithms based on artificial neural networks (ANNs) [Bengio et al., 2017].
- Results across a variety of domains [Ching, T. et al., 2018, LeCun et al., 2015].

ANNs

- Inputs are fed into the input layer,
- which feeds into one or more hidden layers,
- eventually linking to an output layer.

ANNs

- A layer consists of a set of nodes (features or units).
- Nodes of a layer are connected through edges to the immediately earlier and to the specific immediately deeper layers.

DL and ML

- supervised setting: the goal is to accurately predict one or more labels or outcomes associated with each data point,
- unsupervised setting: the objective is to summarize, explain or identify patterns in a dataset.
- can combine these steps.

Deep graph representation learning

- The idea is to learn a data transformation function that maps nodes to points in a low-dimensional vector space [Hamilton et al., 2017].
- The transformation techniques are based on nonlinear dimensionality reduction.

Deep graph representation learning

Advances:

- graph embeddings [Grover and Leskovec, 2016],
- graph convolutional networks [Zhang et al., 2019, Zitnik and Leskovec, 2017],
- transfer and meta-learning [Huang and Zitnik, 2020],
- adversarial attacks and defence on graphs [Zhang and Zitnik, 2020] and
- higher-order predictions [Alsentzer et al., 2020].

Overview of membrane computing

- Models covered
  - (Cell-like) P systems with active membranes
  - Tissue-like P systems with cell division / separation
  - Neural-like P systems

Overview of membrane computing

- Diversity of definitions: Syntax and semantics (objects, membrane, rules)
- Diversity of interpretations: Generative, computing, decision or simulation tools

Overview of membrane computing

Computational complexity [Pérez-Jiménez and Riscos-Núñez, 2017]

- Efficient solutions to hard problems
- P conjecture

Tissue-like P systems

Inspired by:

- intercellular communication
- cooperation between neurons

Tissue-like P systems

- Communication rules: symport/antiport
- Cells as nodes of a graph (and environment)
- +cell division +separation
- computational complexity

Multienvironment P systems

- Population dynamics P systems (probabilistic)
- Skeleton + Environment rules
- Algorithms for probabilistic behaviour
  - Binomial Block Based (BBB) simulation algorithm
  - Direct Non-Deterministic distribution algorithm with Probabilities (DNDP)
  - Direct Distribution based on Consistent Blocks Algorithm (DCBA) [Martínez-del-Amor et al., 2012]

Case studies

MeCoSim webpage:

- Bearded Vulture [Cardona et al.]
- Scavenger birds
- Avian scavengers
- Zebra mussel

Neural-like approach

- Spiking rules and Forgetting rules
- Applicability w.r.t. all spikes present in a neuron (although not all of them may be consumed).
- One rule is selected.
- Produced spikes are sent through all of the outgoing synapses (potential delay)
- Output neuron spikes into the environment

Neural-like approach

- fuzziness [Marín-Morejón, 2022, Pérez-Jiménez et al., 2017]
- evolutionary methods [Dong et al., 2021, Dong et al., 2023]

Outlook

- build bridges between membrane computing and DL,
- determine the different parameters in the model,
- computationally complete devices, non-Turing universal variants
- solve computationally hard problems in feasible time
- case studies (e.g. ecology)

References I

- Alsentzer, E., Finlayson, S., Li, M., Zitnik, M.: Subgraph neural networks. *Adv Neural Inf Process Syst* 33 (2020), 8017-8029.
- Bengio, Y., Goodfellow, I., Courville, A.: *Deep Learning*. MIT press, Cambridge, MA, USA, 2017.
- Cardona, M. et al.: Modeling ecosystems using P systems: The bearded vulture, a case study. In *Membrane Computing: 9th International Workshop, WMC 2008*, Edinburgh, UK, July 28-31, 2008, Revised Selected and Invited Papers 9 (pp. 137-156). Springer, Berlin-Heidelberg, 2009.
- Ching, T. et al.: Opportunities and obstacles for deep learning in biology and medicine. *J R Soc Interface* 15(141) (2018), 20170387.
- Dong, J. et al.: Automatic design of spiking neural P systems based on genetic algorithms. *IJUC* 16(2-3) (2021), 201-216.

References II

- Dong, J. et al.: Automatic design of arithmetic operation spiking neural P systems. *Nat Comput* 22(1) (2023), 55-67.
- Grover, A., Leskovec, J.: node2vec: Scalable feature learning for networks. *KDD* 2016, 855-864.
- Hamilton, W. L., Ying, R., Leskovec, J.: Representation learning on graphs: Methods and applications. *IEEE Data Eng Bull* 40(3) (2017), 52-74.
- Huang, K., Zitnik, M.: Graph meta learning via local subgraphs. *Adv Neural Inf Process Syst* 33 (2020), 5862-5874.
- LeCun, Y., Bengio, Y., Hinton, G.: Deep learning. *Nature* 521 (2015), 436-444.
- Marín-Morejón, J. A.: A new simulator for FRSNP systems. *IMCS Bulletin* 2022.

References III

- MARTÍNEZ-DEL-AMOR, M. A. ET AL.: DCBA: Simulating Population Dynamics P Systems with Proportional Object Distribution. *Int. Conf. on Membrane Computing 2012:* 257-276
- MeCoSim webpage: http://www.p-lingua.org/mecosim/doc/case_studies/multienvironment/population_dynamics_p_systems.html.
- ORELLANA-MARTÍN, D., VALENCIA-CABRERA, L., PÉREZ-JIMÉNEZ, M. J The environment as a frontier of efficiency in tissue P systems with communication rules. *TCS* 956 (2023), 113812.
- PÉREZ-JIMÉNEZ, M. J., RISCOS-NÚÑEZ, A.: New techniques to address the problem P vs. NP. *ISBBC 2017* June 28-30, 2017, Valencia
- PÉREZ-JIMÉNEZ, M. J. ET AL.: Fuzzy reasoning spiking neural P systems revisited: A formalization. *TCS* 701 (2017), 216-225.

References IV

- Riscos-Núñez, A.: An introduction to membrane computing. 3^{rd} *SCORE Workshop and 19^{th} BWMC January 24, 2023, Sevilla*
- Zhang, S., Tong, H., Xu, J., Maciejewski, R.: *Graph convolutional networks: A comprehensive review. Comput Soc Netw 6 (2019), 11.*
- Zhang, X., Zitnik, M.: *GNNGuard: Defending Graph Neural Networks against adversarial attacks. Adv Neural Inf Process Syst 33 (2020), 9263-9275.*
- Zitnik, M., Leskovec, J.: *Predicting multicellular function through multi-layer tissue networks. Bioinformatics 33 (2017), i190-i198*