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AI at the Faculty of Mathematics

Mladen Nikolić





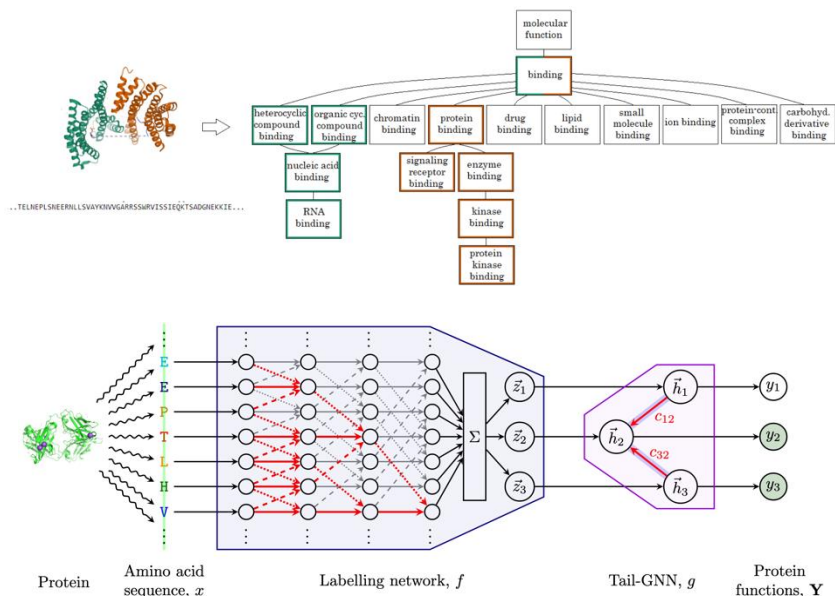
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AI AT THE FACULTY OF MATHEMATICS

Deep Learning

GNNs for Protein Function Prediction

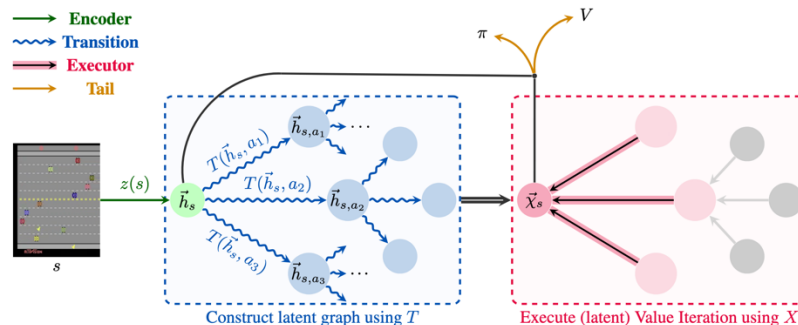
- Protein functions are organized in an ontology which is a rooted DAG
- Functions of a protein are represented by an upward closed subgraphs
- Task: given an amino acid sequence of a protein, predict the subgraph
- Tail-GNN – a CNN encoder providing latent representations for graph nodes, followed by a GNN classifier



Spalević S., Veličković P., Kovačević J. & Nikolić M. (2020). «Hierarchical Protein Function Prediction with Tail-GNNs», ICML, GRL+.

GNNs for Planning in Reinforcement Learning

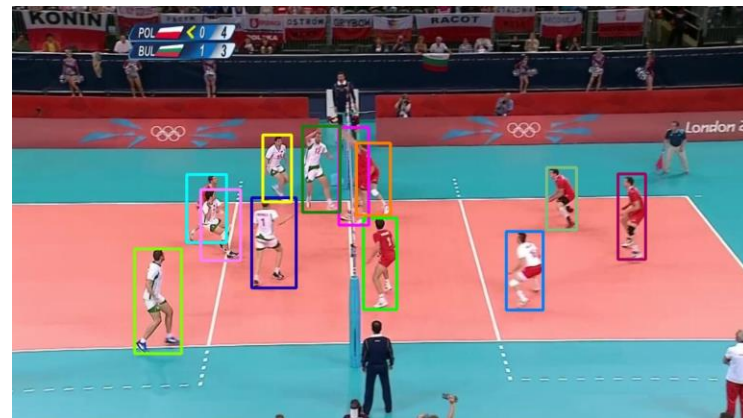
- Planning is about building the model of the agent's environment and using it to enhance the learning process
- Environment can be described by a (usually unknown) state-transition graph
- We learn a mapping of such a graph into a high-dimensional latent space
- We incentivize a GNN policy network to learn planning in that latent space
- Applicable to arbitrary state spaces
- More robust than previous methods



Deac A., Veličković P., Milinković O., Bacon P.-L., Tang J. & Nikolić M. (2021). «*Neural Algorithmic Reasoners are Implicit Planners*», NeurIPS.

Object Tracking in Videos

- Kalman filters are not the best choice for nonlinear motion
- They also require domain specific choices
- We propose deep learning models for motion modeling and noise filtering, lifting most of these limitations
- We explore RNN, NODE, CNP, and transformer models
- We propose various heuristics which yield state-of-the-art tracker for non-linear motion



From SportsMOT dataset

Adžemović M., Tadić P., Petrović A. & Nikolić M. (2025). «*Beyond Kalman Filters: Deep Learning-Based Filters for Improved Object Tracking*», Machine Vision and Applications.

Adžemović M., Tadić P., Petrović A. & Nikolić M. (2025). «*Engineering an Efficient Object Tracker for Non-Linear Motion*», Under review.

Fairness in AI

- Human-produced data is biased and hence the models, too
- Bias is often addressed by weighting the samples in preprocessing
- We propose an adversarial training method which can determine such weights in an end-to-end fashion
- Fairness metrics are non-differentiable and are often optimized indirectly by surrogate functions
- We propose a reinforcement learning method which optimizes them directly

$$\mathbf{AEOD} = |TPR_{z=0} - TPR_{z=1}|$$

$$\mathbf{ASD} = |P(\hat{y} = 1|z = 0) - P(\hat{y} = 1|z = 1)|$$

Petrović A., Nikolić M., Radovanović S., Delibašić B., Jovanović M. (2022). «FAIR: Fair Adversarial Instance Re-Weighting», Neurocomputing.

Petrović A., Nikolić M., Jovanović M., Bijanić M., Delibašić B. (2021). «Fair Classification via Monte Carlo Policy Gradient Method», Engineering Applications of Artificial Intelligence.

Applications - Credit Risk Scoring

- Estimate 12 month probability of default for new and existing clients
- Data on real companies in Serbia in 2012-2018 (financial statements and credit settlement status)
- Proposed a deep learning model which directly consumes financial statements and predicts probabilities of default
- Considerably outperforms logistic regression (AUC 0.87 vs. 0.72)

Jordanski M., Jović Ž., Marić M., Lutovac M., Marić V. (2025). «*Credit Risk Scoring: Altman vs. Machine Learning*», Under review.

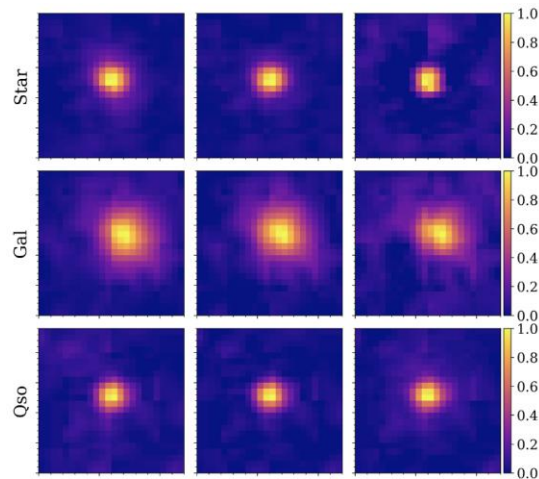
Applications – Rapid Earthquake Loss Assessment

- An important step in recovery from earthquakes
- Needs to be quick and precise
- We use DeepSets over CNN encoder to assess the damage from a set of photos of a building
- Photos are from mobile phone cameras



Applications - Astronomy

- A part of Large Synoptic Survey Telescope project (LSST / Vera C. Rubin observatory)
- Analysis of quasar lightcurves using conditional neural processes
- Classification of galaxies, stars, and quasars using various machine learning methods (won LSST AGN Data Challenge)



Kovačević A., Ilić D., Popović L., Andrić-Mitrović N., Nikolić M., Pavlović M., Čvorović-Hajdinjak I., Kežević M., Savić Đ. (2023). «Deep Learning of Quasar Lightcurves in the LSST Era», Universe.

Savić Đ. et al. (2023). «The LSST AGN Data Challenge: Selection Methods», Astrophysical Journal.



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AI AT THE FACULTY OF MATHEMATICS

Computational Intelligence

Computational Intelligence

CI Techniques

- Metaheuristics: Variable Neighborhood Search (VNS), GRASP, Tabu Search
- Fuzzy Systems: For modeling imprecise knowledge and decision-making
- Hybrid Approaches: Combining heuristics with exact methods (e.g., MIP + VNS)
- Mathematical Programming: Linear, integer, and nonlinear optimization

Applied Problem Domains

- Community Detection
- Hybrid Flow Shop Scheduling
- Multi-Level Uncapacitated Facility Location Problem
- Bus Terminal Location Problem
- Vehicle Routing Problem
- Forming Heterogeneous Groups for Computer-Supported Collaborative Learning

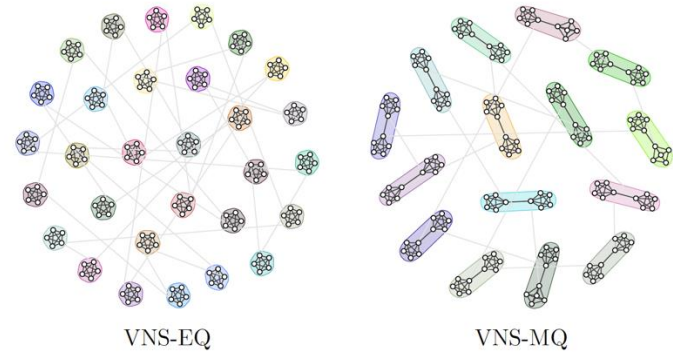
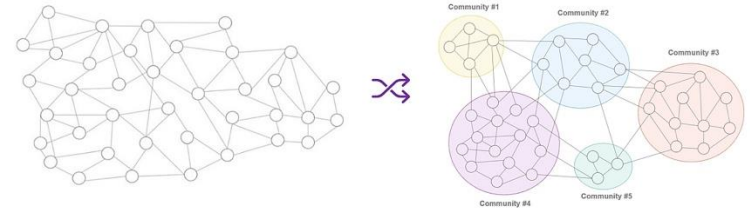
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RIMO – Research Group in Computational Intelligence and Mathematical Optimization

<http://poincare.matf.bg.ac.rs/~maricm/research-group.html>

Community Detection

- Community detection (graph clustering) aims to partition a graph into groups of nodes with dense internal and sparse external connections
- Modularity (MQ) is a popular quality function, but it fails to detect small, well-defined communities in large networks
- The proposed EQ function quantifies community quality as the exponential difference between internal and external density
- Optimization is performed using Variable Neighborhood Search (VNS)
- Results show EQ identifies more accurate community structures on both artificial and real-world networks



Džamić D., Pei J., Marić M., Mladenović N., Pardalos P.M. (2018). Exponential quality function for community detection in complex networks. *International Transactions in Operational Research*.



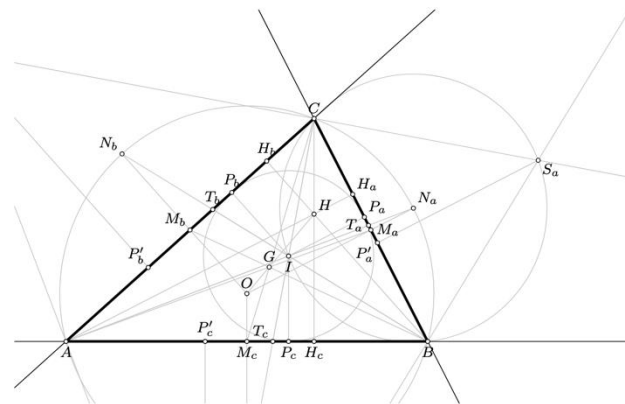
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Logic-Based Reasoning

Development of new Solvers and Provers

- Boolean satisfiability problem (SAT) and related SMT problem
- Constraint satisfaction problems
- Fragments of first order logic (e.g., coherent logic)
- Triangle construction problems



Marić F. (2009). «*Formalization and Implementation of Modern SAT Solvers*», Journal of Automated Reasoning.

Stojadinović M., Marić F. (2014). «*meSAT: Multiple Encodings of CSP to SAT*», Constraints.

Janičić P., Narboux J. (2022). «*Theorem Proving as Constraint Solving with Coherent Logic*», Journal of Automated Reasoning.

Banković M., Marić F. (2021). «*Faradžev Read-Type Enumeration of Non-Isomorphic CC Systems*», Computational Geometry.

Marinković V. (2017). «*ArgoTriCS – Automated Triangle Construction Solver*», Journal of Experimental and Theoretical Artificial Intelligence.

Formal Theorem Proving

- Human proofs of mathematical theorems are often not quite formal
- We prefer formal, machine-verifiable, and human-readable proofs
- Performed in automated or interactive fashion
- Relies on Isabelle and Coq proof assistants
- Most often applied to geometry

$$\frac{\frac{\frac{[(\forall y)p(x', y)]^1}{p(x', y')} \forall E}{(\exists x)p(x, y')} \exists I}{[(\exists x)(\forall y)p(x, y)]^2 \quad (\forall y)(\exists x)p(x, y)} \forall I}{(\forall y)(\exists x)p(x, y)} \exists E, 1}{(\exists x)(\forall y)p(x, y) \Rightarrow (\forall y)(\exists x)p(x, y)} \Rightarrow I, 2$$

Stojanović Đurđević S., Narboux J., Janičić P. (2015). «Automated Generation of Machine-Verifiable and Readable Proofs: A Case Study of Tarski's Geometry», Annals of Mathematics and Artificial Intelligence.

Banković M., Drečun I., Marić F. (2023). «A Proof System for Graph (Non)-Isomorphism Verification», Logical Methods in Computer Science.

Practical applications

- Formal verification of blockchain protocols in higher order logic
- Verification of refactored embedded SQL code (equivalence before and after refactoring) using SMT solvers
- Solving practical combinatorial problems (e.g., making timetables)

Marić F., Scholz B., Subotić P. (2025). «*Formal Verification of Fail-Safe Cross-Chain Bridge*», FMBC.

Spasić M., Vujošević Janičić M. (2021). «*Verification Supported Refactoring of Embedded SQL*», *Software Quality Journal*.

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