# Lecture 8: Applications of Graph Neural Networks

## Relational Learning

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## Overview

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- Life science applications
    - Biomedical data and drug discovery
    - Particle physics

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- Summary of the relational learning theme

## Life Science Applications

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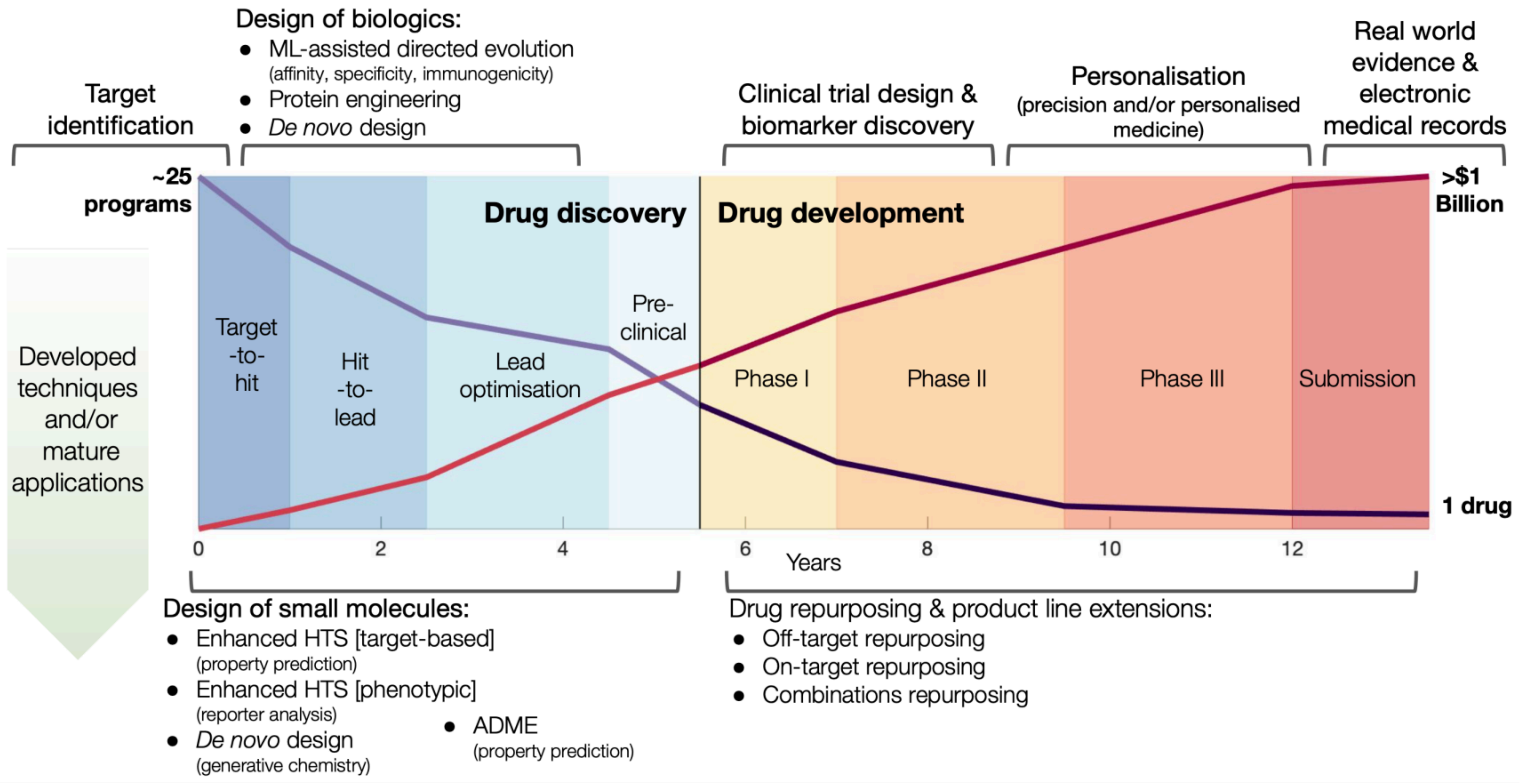
    - **Abstract scale**: Knowledge graphs can represent the complex relationships between drugs, side effects, diagnosis, associated treatments, and test results etc.
- Drug discovery is a long and expensive process — There is a greater interest in applying computational methodologies to enhance the drug discovery process and make it more efficient.

# Timeline of Drug Development



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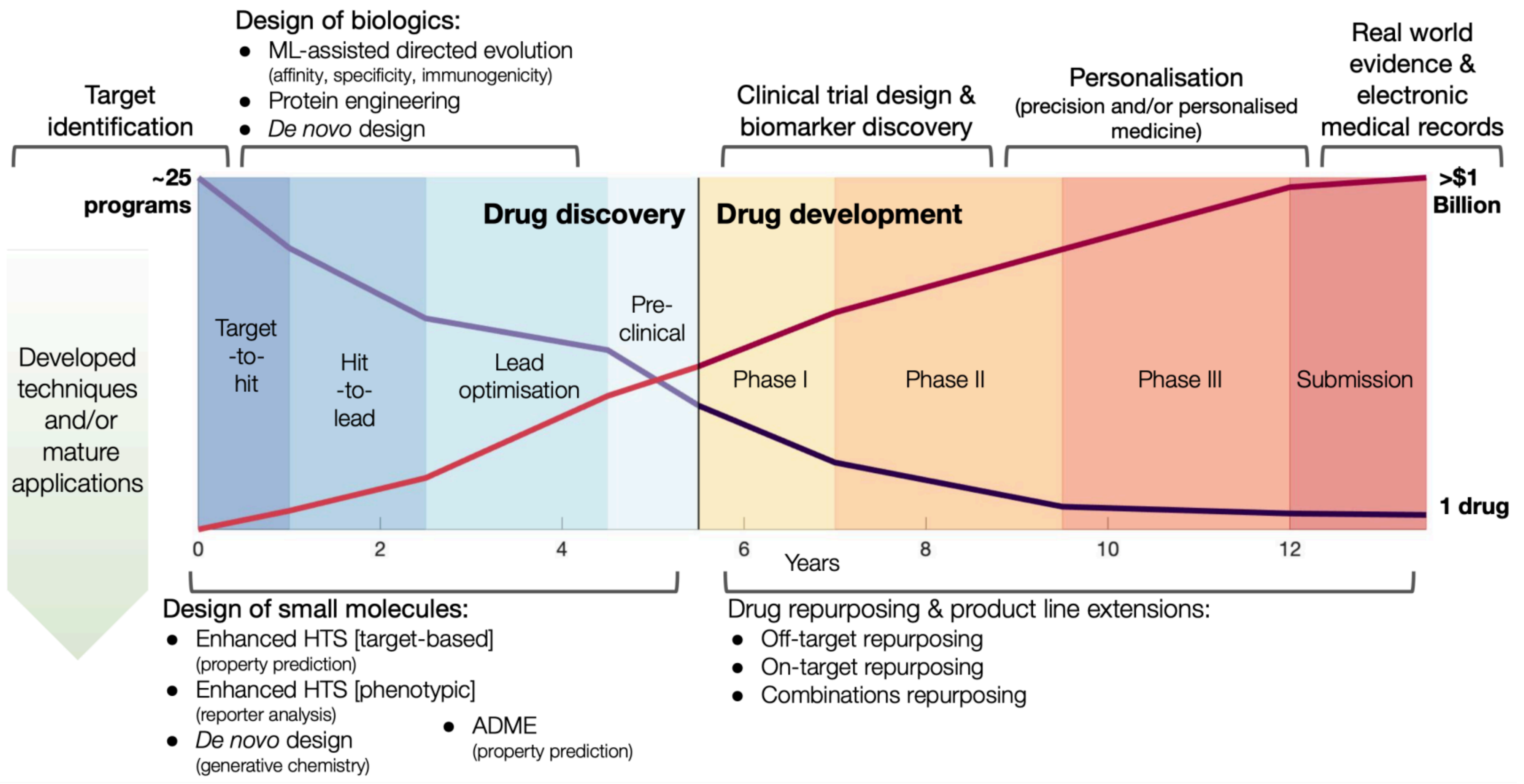

Target identification
Design of biologics:
ML-assisted directed evolution (affinity, specificity, immunogenicity)
Protein engineering
*De novo* design
Clinical trial design & biomarker discovery
Personalisation (precision and/or personalised medicine)
Real world evidence & electronic medical records
~25 programs
>$1 Billion
Drug discovery
Drug development
Developed techniques and/or mature applications
Target -to- hit
Hit -to- lead
Lead optimisation
Pre- clinical
Phase I
Phase II
Phase III
Submission
1 drug
0
2
4
6
8
10
12
Years
Design of small molecules:
Enhanced HTS [target-based] (property prediction)
Enhanced HTS [phenotypic] (reporter analysis)
*De novo* design (generative chemistry)
ADME (property prediction)
Drug repurposing & product line extensions:
Off-target repurposing
On-target repurposing
Combinations repurposing

Figure from (Gadoulet et al, 2021) showing the timeline of drug development linked to potential areas of application of GRL.

## Drug Development Applications

| Relevant application | Reference | Method type | Task level | ML approach | Data types | Exp. val? |
|---|---|---|---|---|---|---|
| 4.1 Target identification | | | | | | |
| — | [47] | Geometric (§3.2) | Node-level | Unsupervised | Di, Dr, GA | |
| 4.2 Design of small molecules therapies | | | | | | |
| Molecular property prediction | [21] | GNN (§3.4) | Graph-level | Supervised | Dr | |
| | [101] | GNN (§3.4) | Graph-level | Supervised | Dr | |
| | [22] | GNN (§3.4) | Graph-level | Supervised | Dr | |
| Enhanced high throughput screens | [50] | GNN (§3.4) | Graph-level | Supervised | Dr | ✓ |
| De novo design | [102] | GNN (§3.4) | Graph-level | Unsupervised | Dr | |
| | [48] | Factorisation (§3.3) | Graph-level | Semi-supervised | Dr | ✓ |
| 4.3 Design of new biological entities | | | | | | |
| ML-assisted directed evolution | — | — | — | — | — | |
| Protein engineering | [49] | GNN (§3.4) | Subgraph-level* | Supervised | PS | |
| De novo design | [103] | GNN (§3.4) | Graph-level | Supervised | PS | ✓ |
| 4.4 Drug repurposing | | | | | | |
| Off-target repurposing | [104] | Factorisation (§3.3) | Node-level | Unsupervised | Dr, PI | |
| | [105] | GNN (§3.4) | Graph-level | Supervised | Dr, PS | |
| On-target repurposing | [106] | Factorisation (§3.3) | Node-level | Unsupervised | Dr, Di | |
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# Drug Development Applications

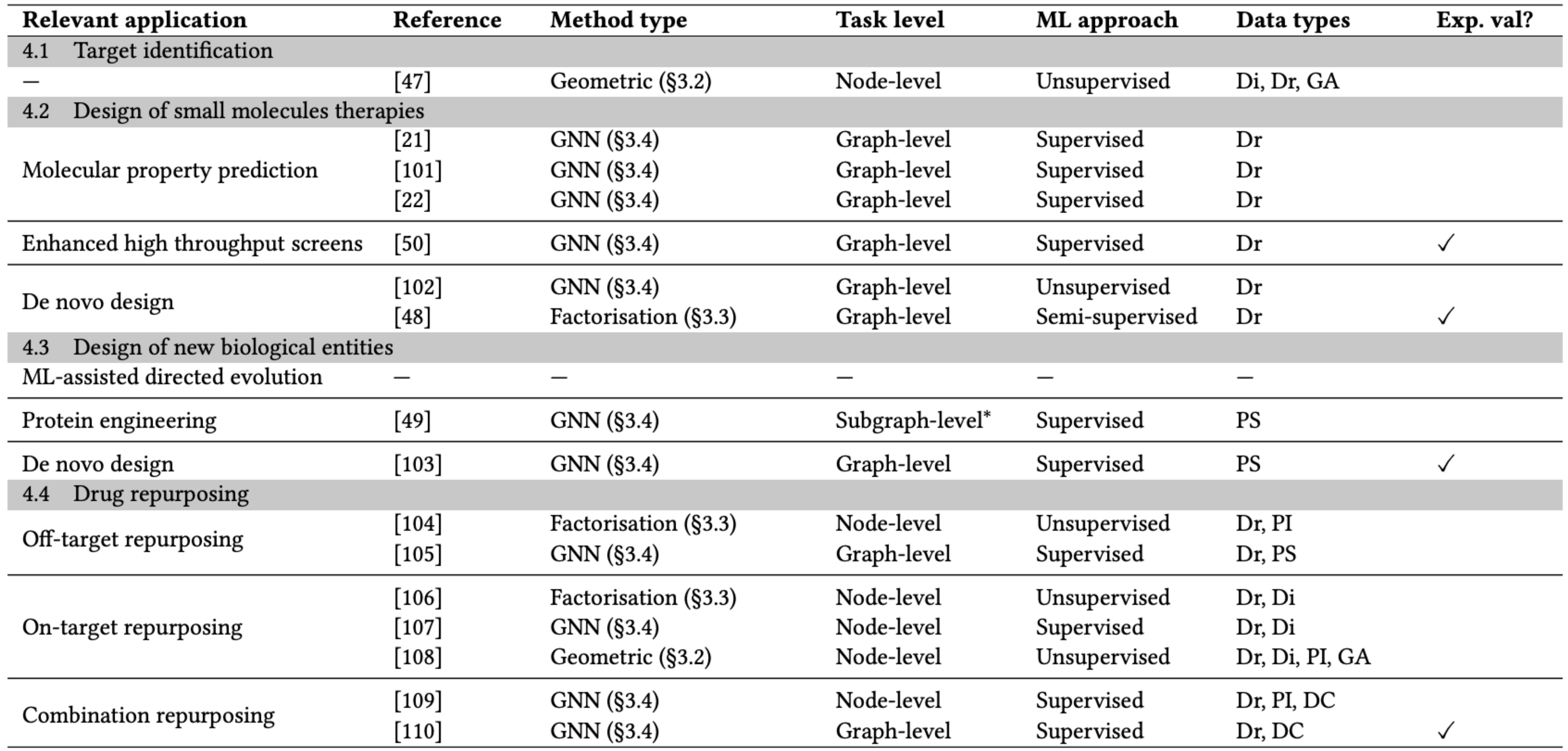

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Table from (Gadoulet et al, 2021) listing exemplar applications of GNNs in drug discovery. The acronyms stand for Dr: Drugs, DC: Drug combinations, PS: Protein, PI: Protein interactions, GA: Gene annotations, Di:Diseases, respectively.

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- After ranking the candidates according to the model's predicted score, select a list of promising candidates (only, 23 compounds) that can potentially inhibit the growth of E. coli.

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"This work highlights the significant impact that machine learning can have on early antibiotic discovery efforts by simultaneously increasing the accuracy rate of lead compound identification and decreasing the cost of screening efforts."

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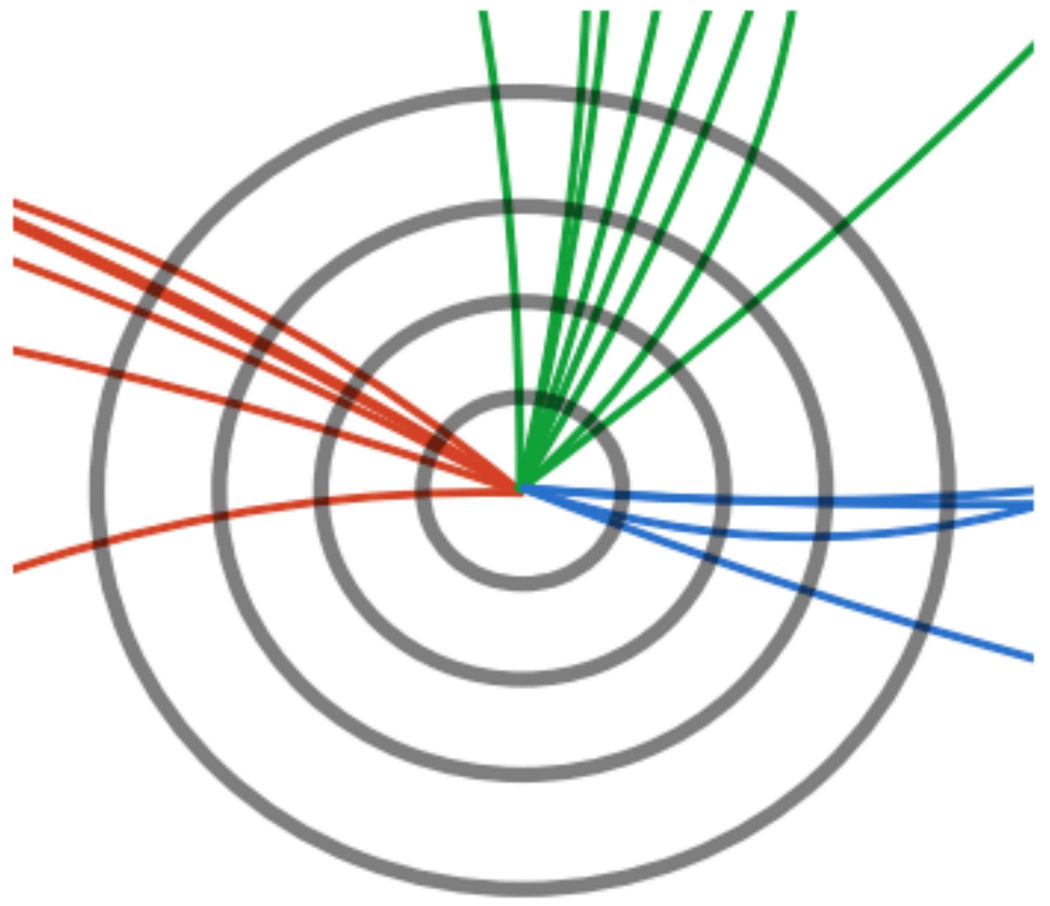
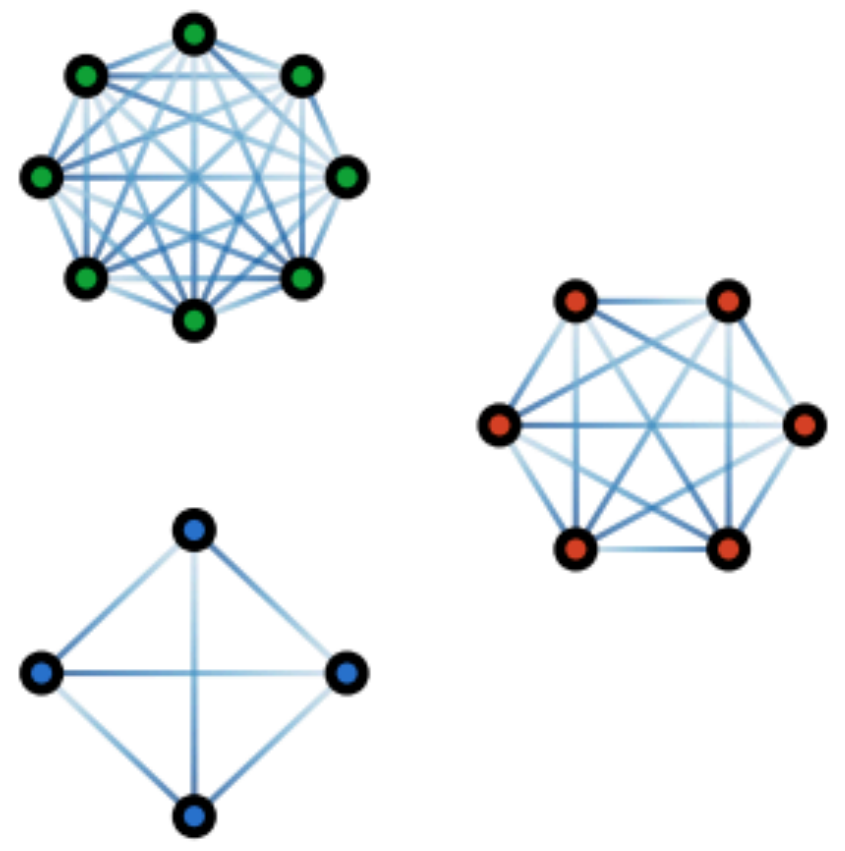
“Indeed, modern neural molecular representations have the potential to: (1) decrease the cost of lead molecule identification because screening is limited to gathering appropriate training data, (2) increase the true positive rate of identifying structurally novel compounds with the desired bioactivity, and (3) decrease the time and labor required to find these ideal compounds from months or years to weeks.”

(Stokes et al., 2020)

# Particle Physics





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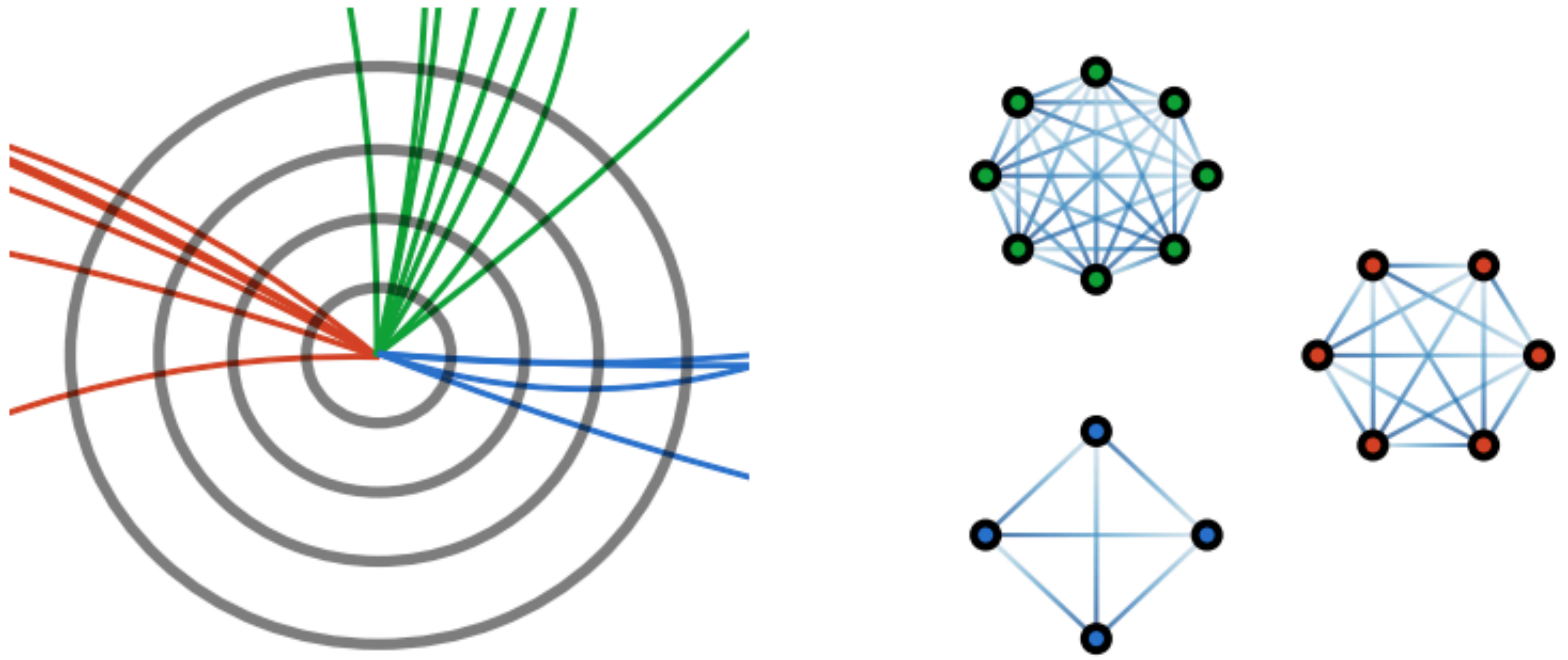

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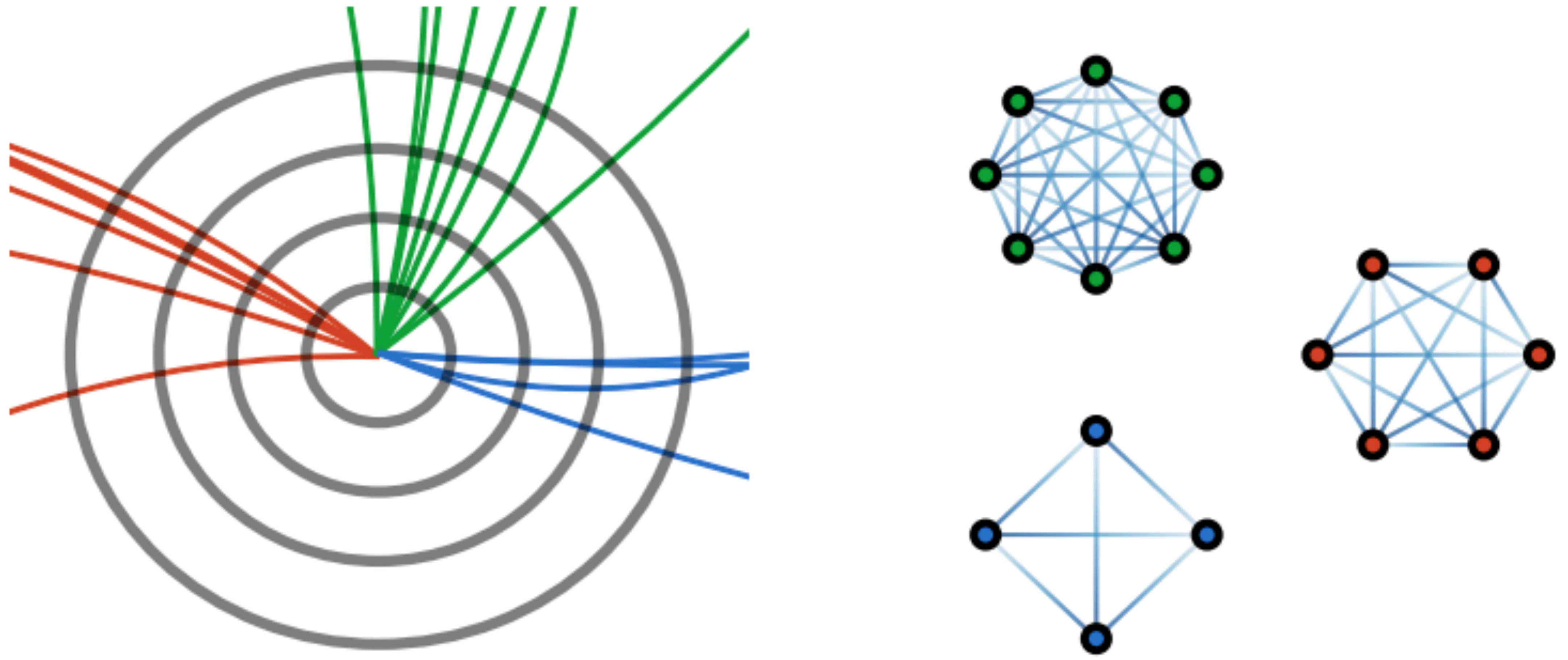

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We follow the survey by (Shlomi et al., 2021), and briefly highlight some applications of graph representation learning in particle physics.

# Particle Physics: Jet Classification

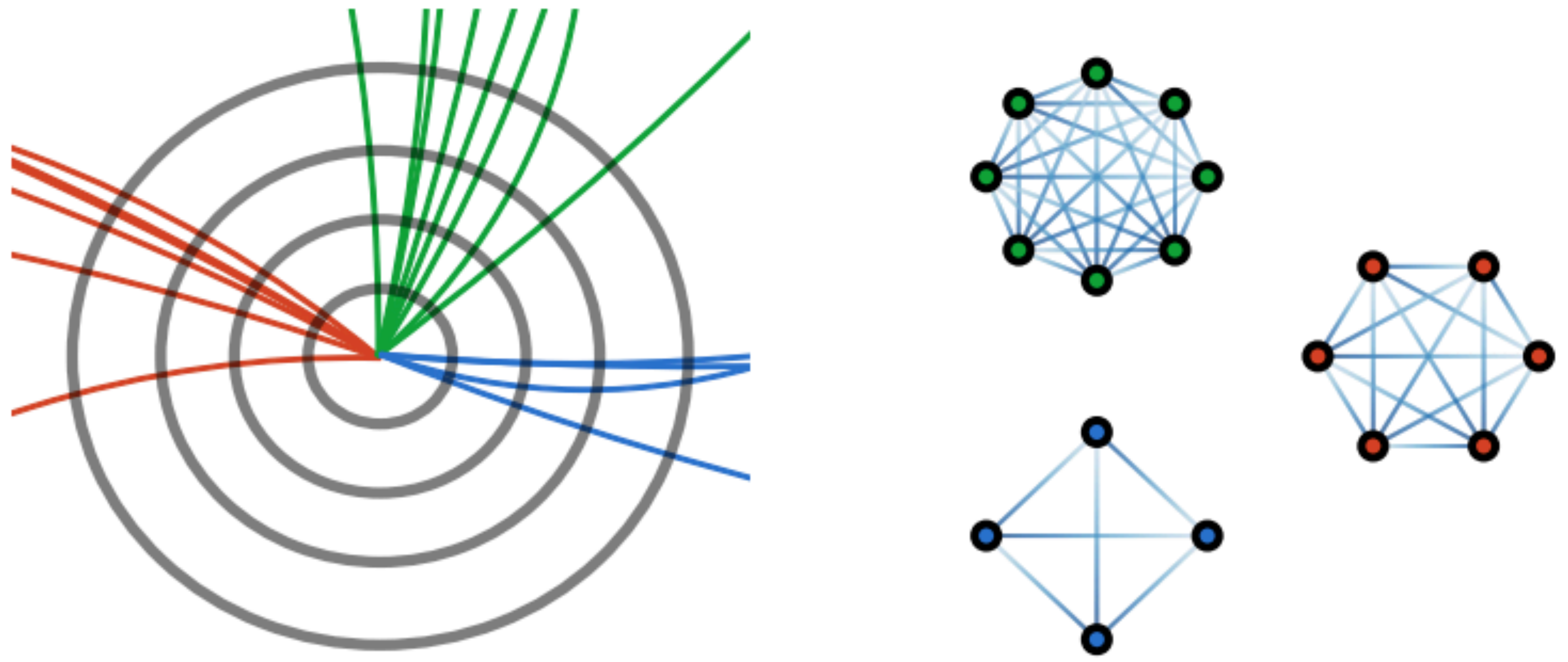

Figure from (Shlomi et al., 2021), depicting jet classification based on the particles associated to the jet.

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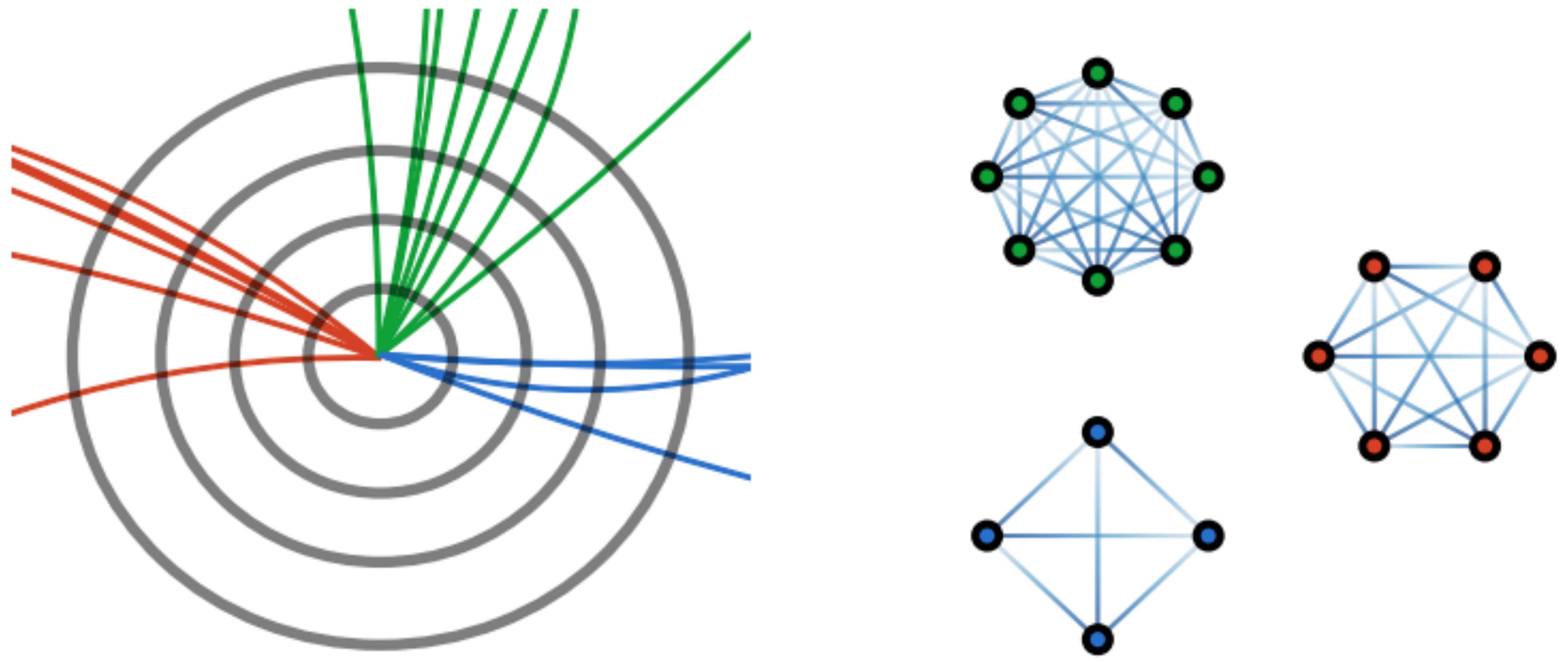

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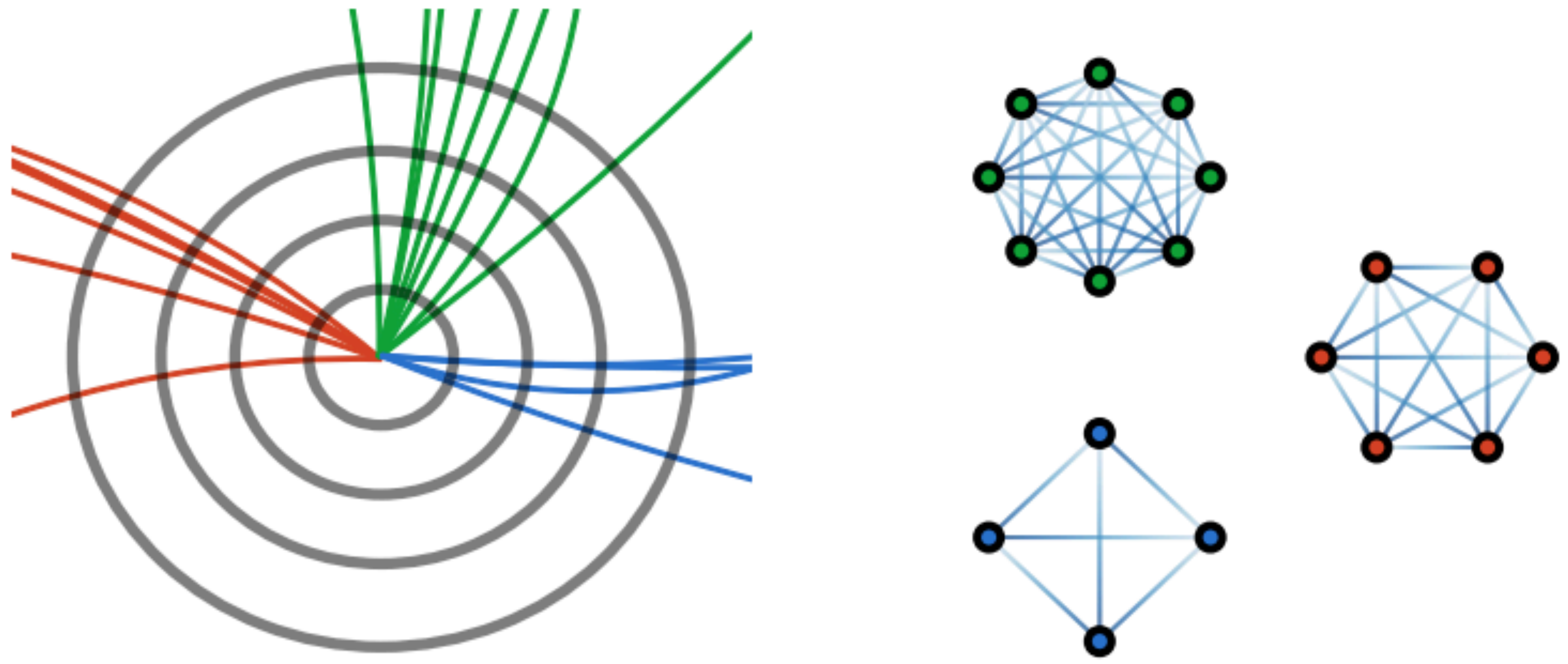

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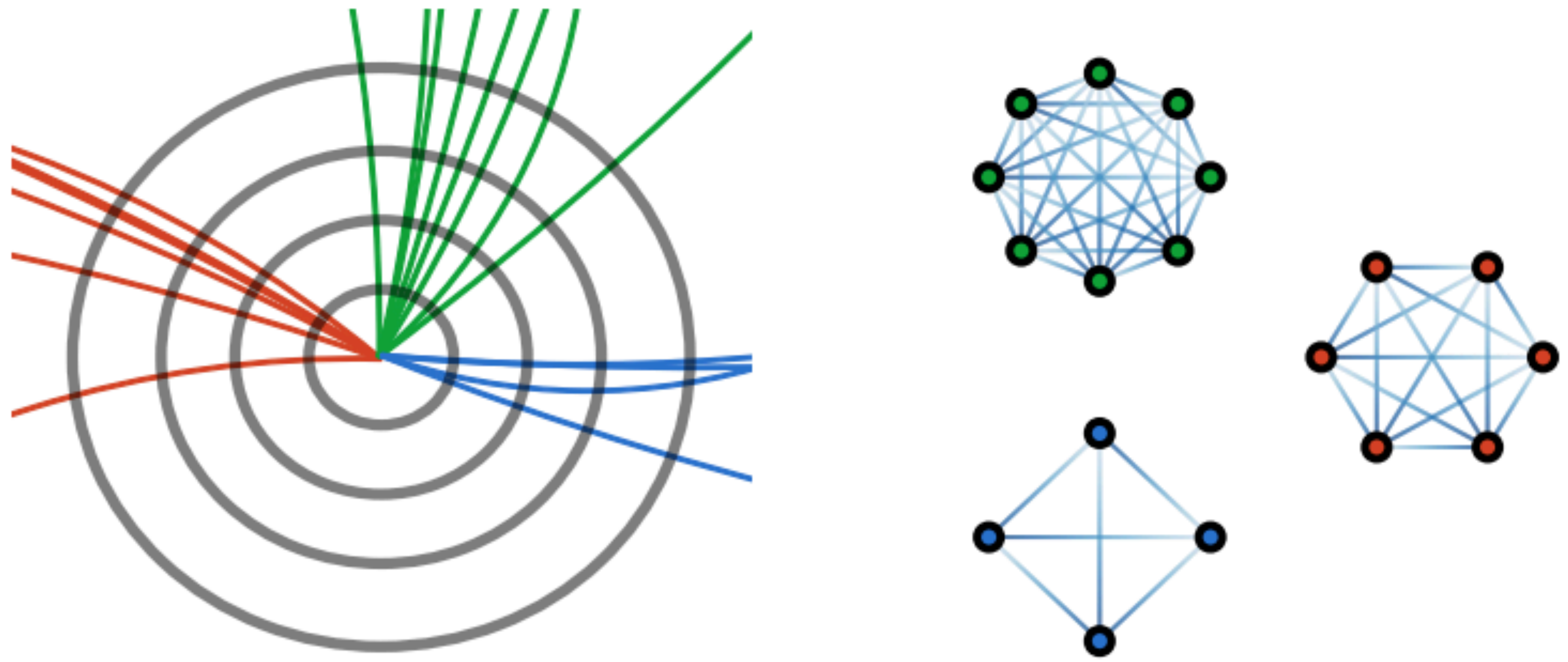
One approach is to view a jet as a graph, where nodes are particles (with features) and edges represent interactions, and apply graph classification.



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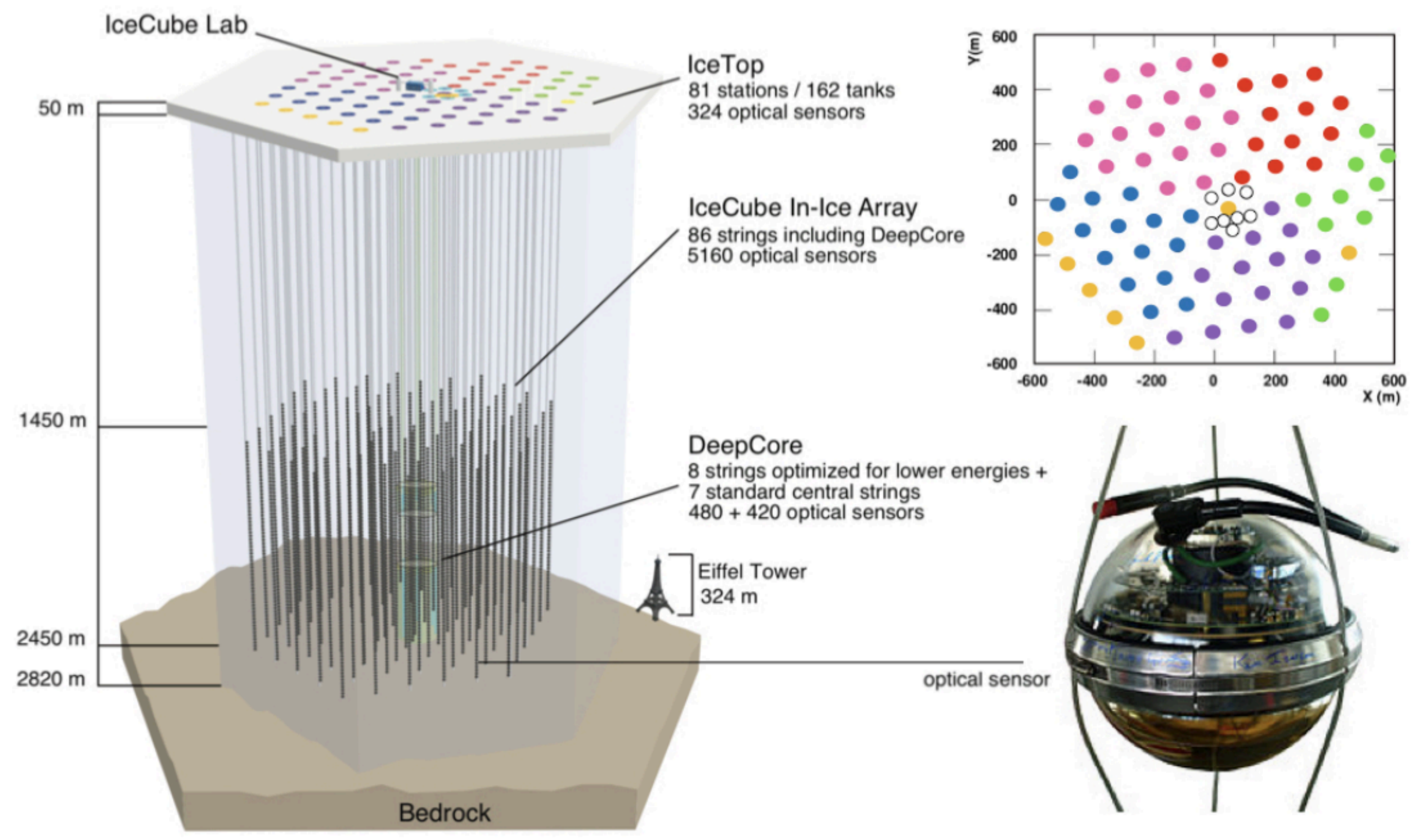

Figure from (Choma et al., 2018) depicting the IceCube Neutrino Observatory with the in-ice array, its subarray DeepCore, and the cosmic-ray air shower array IceTop.

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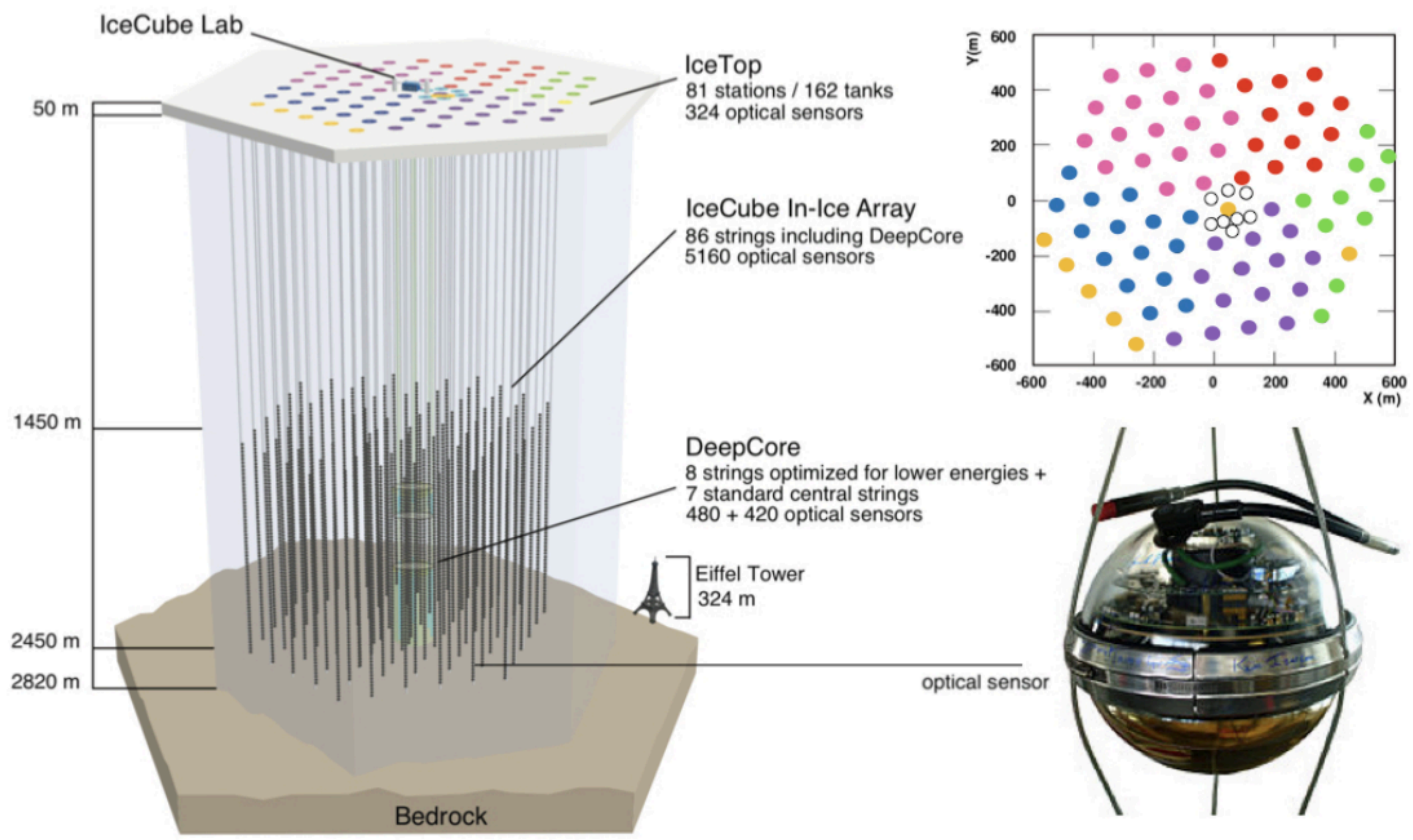
**Event Classification**. The task of predicting the physics process at the origin of the recorded data.



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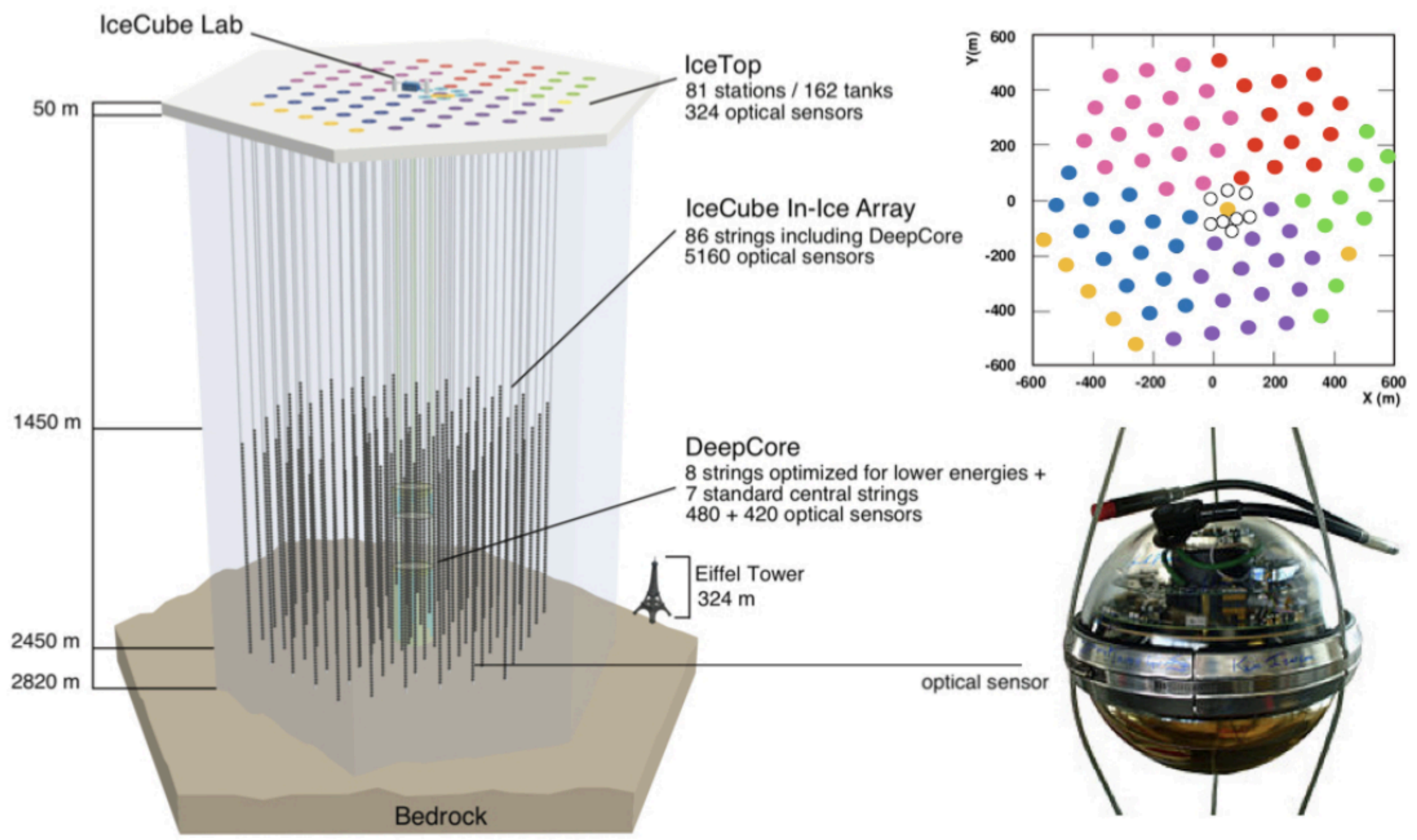

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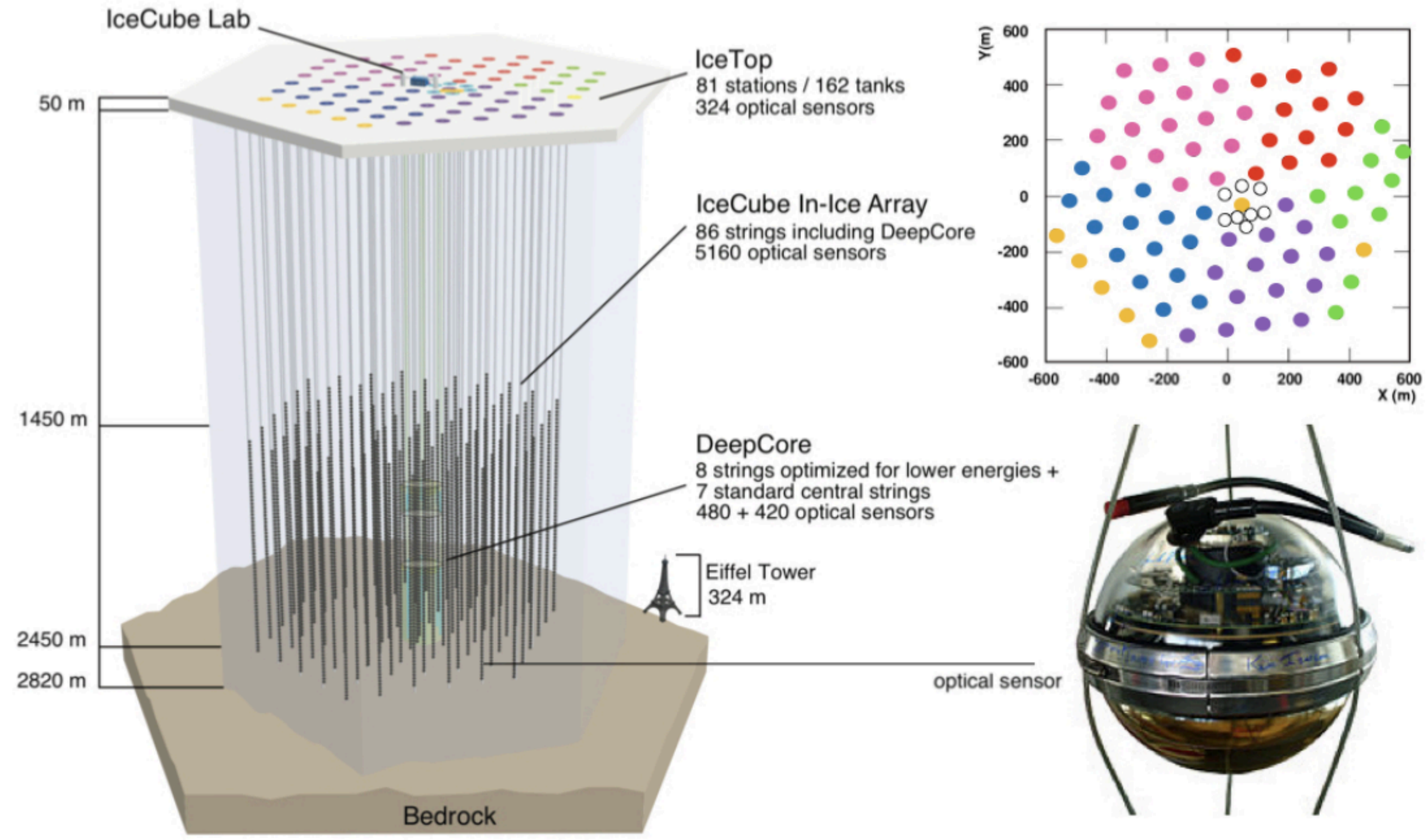

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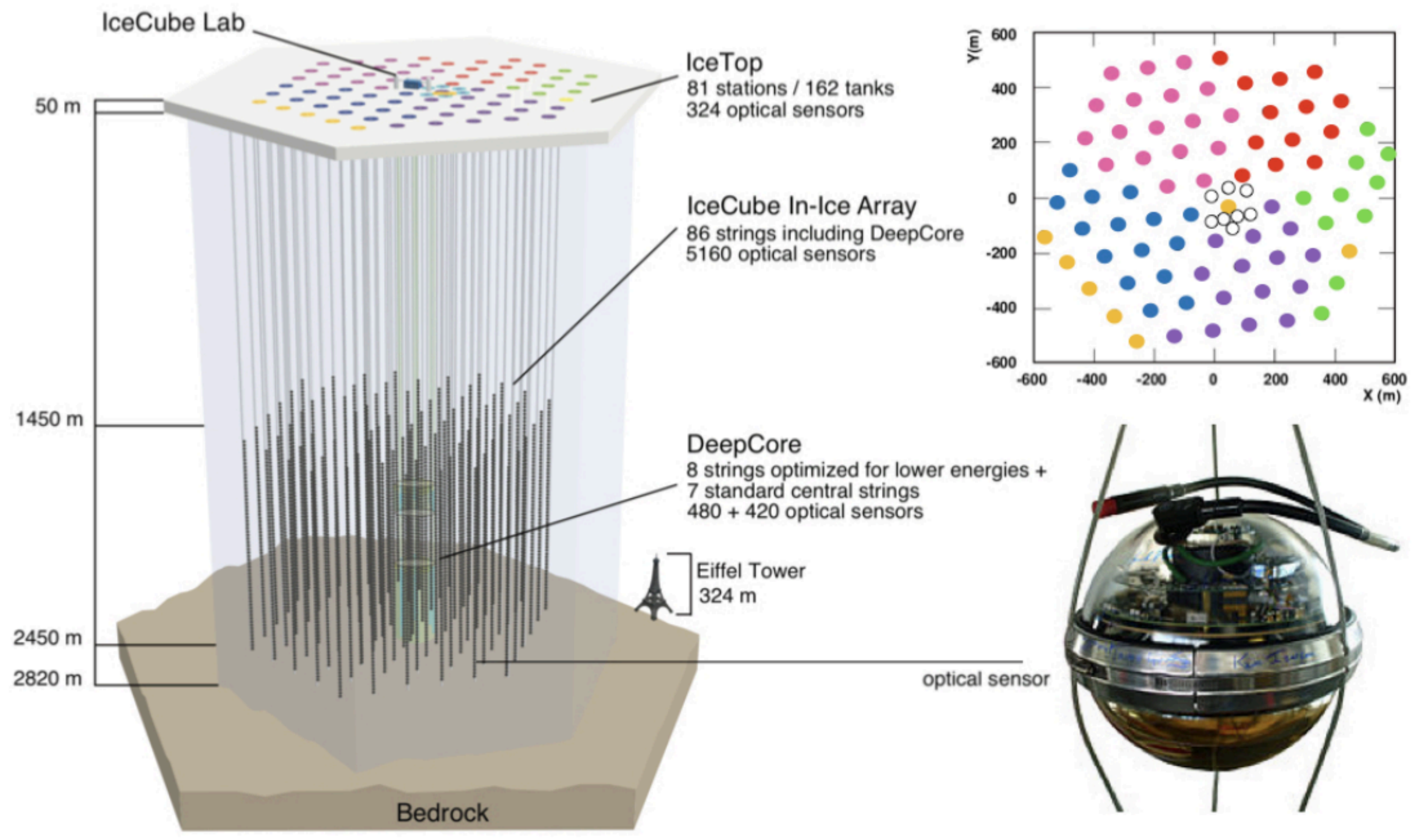
The goal is the classification of the signal in the IceCube detector, to determine if a muon originated from a cosmic neutrino, or from a cosmic ray showering in the earth atmosphere.



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## Combinatorial Optimisation and Reasoning

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    - Train the graph neural network, and predict satisfiability status of novel formulas, given as graphs.

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- Naming-invariance, e.g., $(x \wedge y) \vee (\neg x \wedge \neg y) \equiv (\neg z \wedge \neg u) \vee (z \wedge u)$,

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Many other problems, beyond SAT, such as TSP, #SAT, etc. are investigated in this context.

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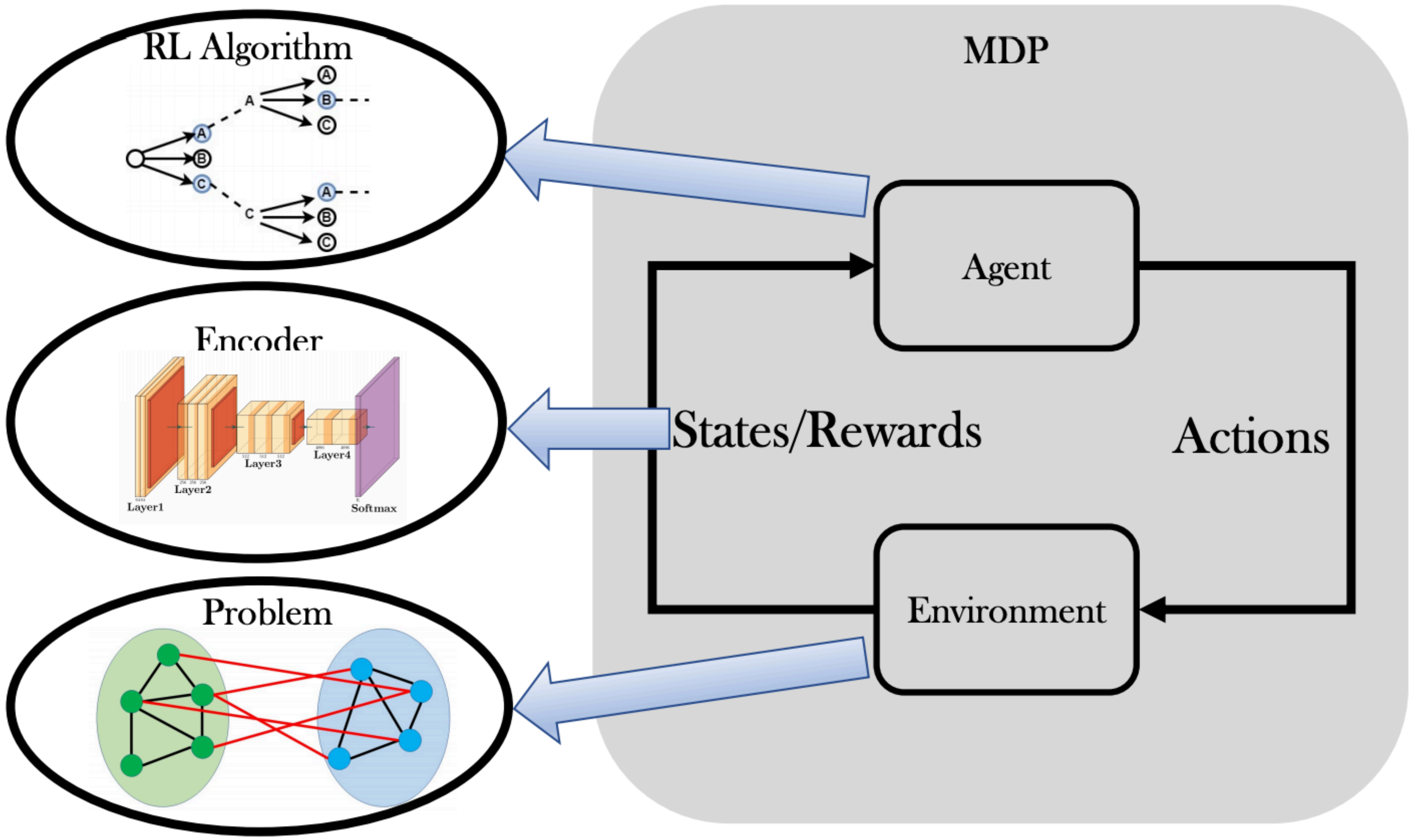

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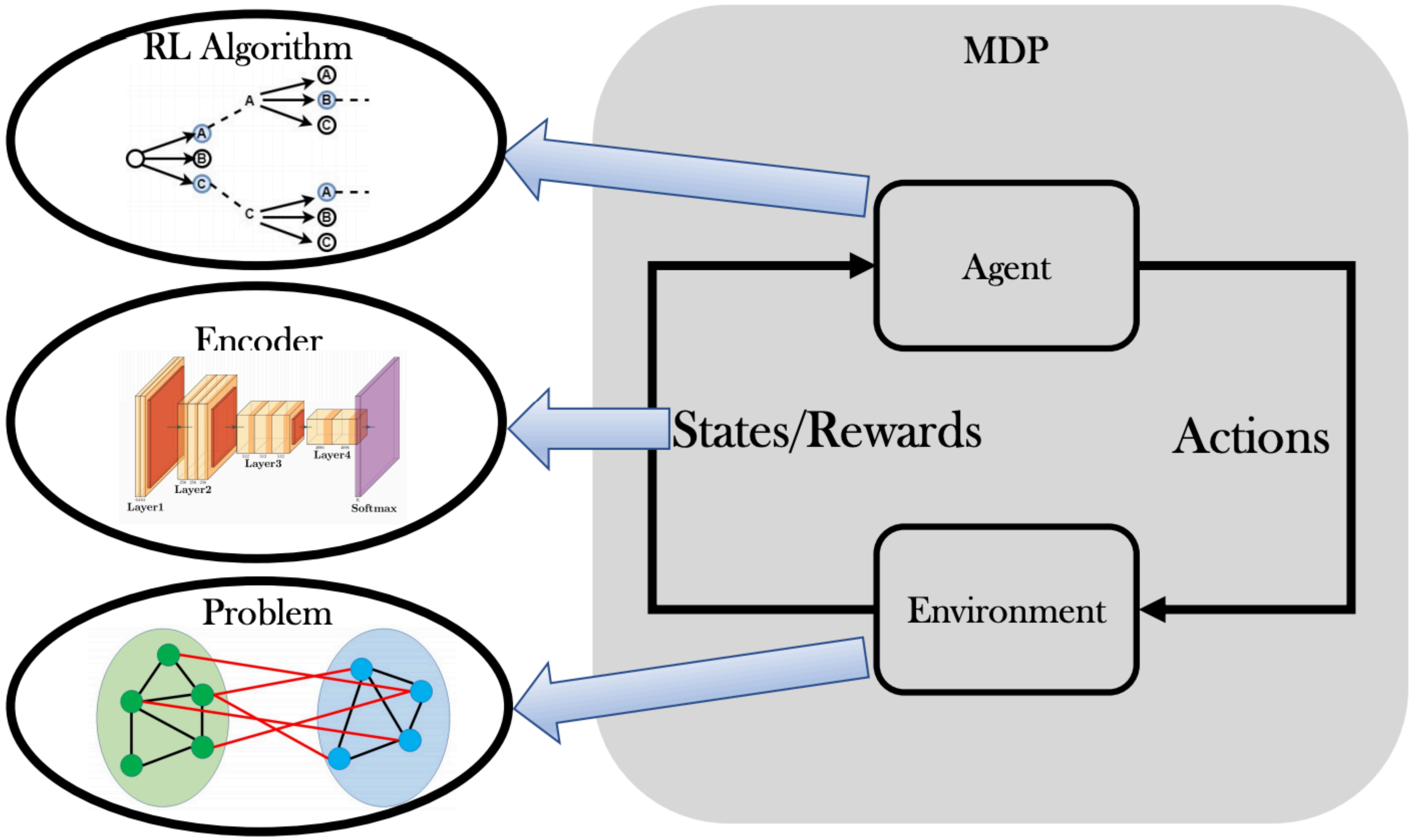

Graph neural networks alone are quite limited to attack such problems, and a line of work combines the power of graph neural networks with reinforcement learning for solving combinatorial optimisation problems. Figure is taken from a survey paper (Mazyavkina et al., 2020) and shows the pipeline.

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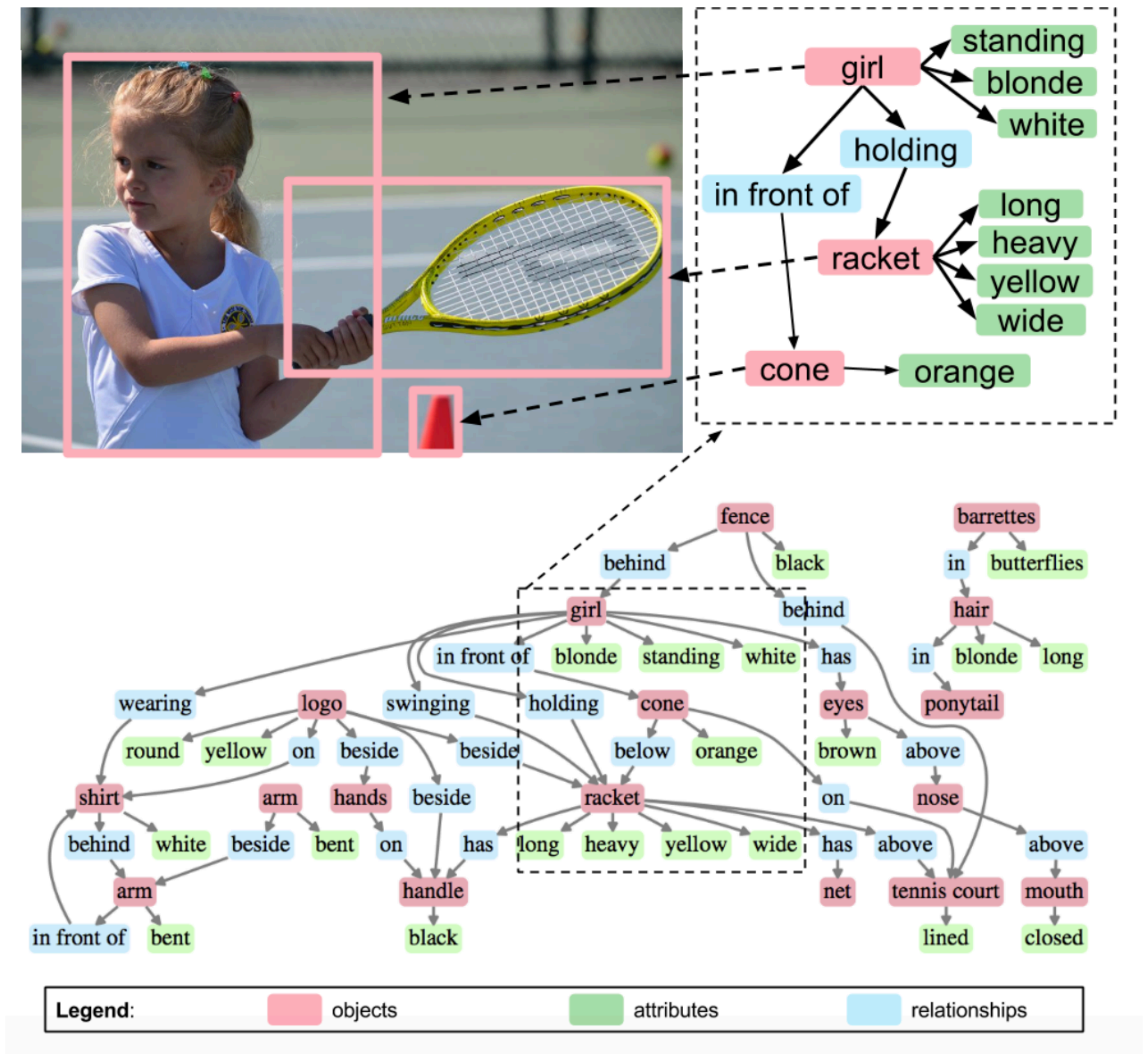
- Once the parameters of the model have been trained, the agent is capable of searching the solutions for unseen instances of the problem.

## Computer Vision: Scene Graphs and Question Answering

# Scene Graphs



Scene graph from (Johnson et al., 2015).

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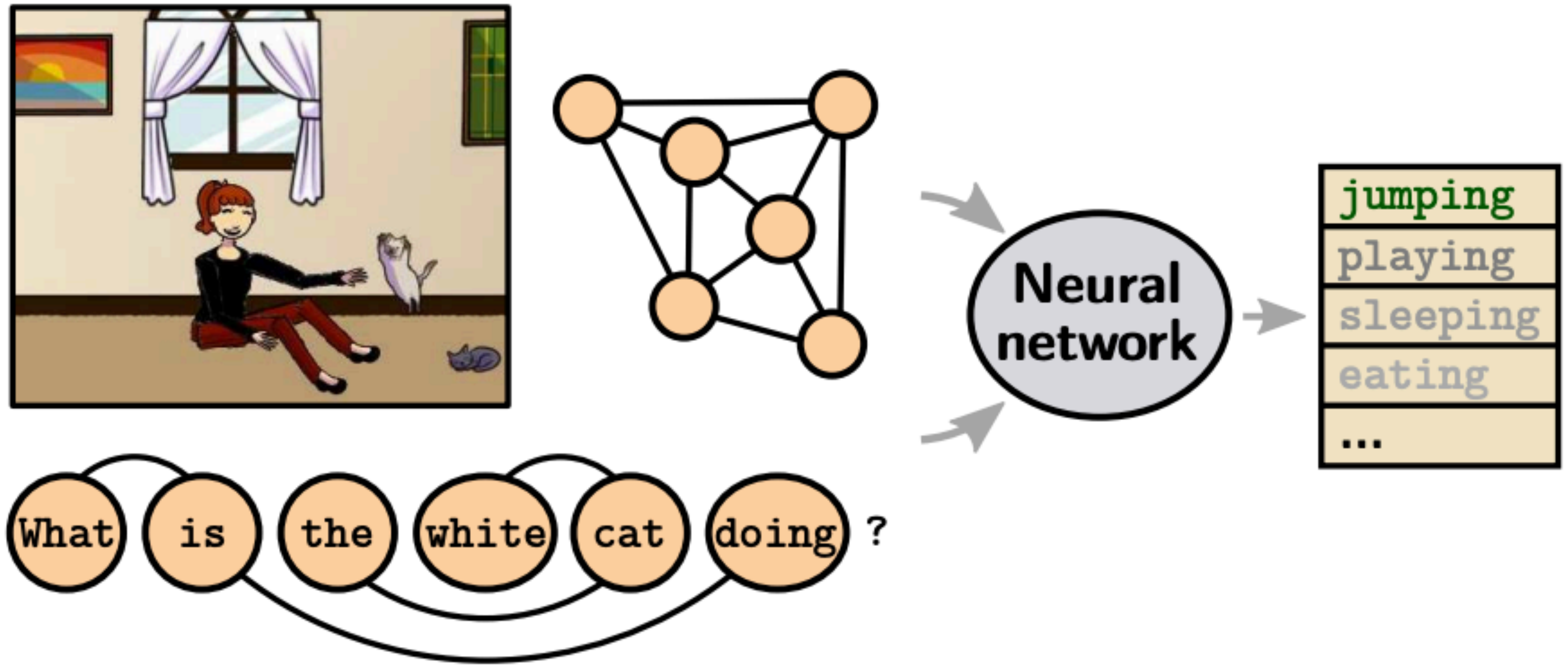
Graph neural networks are used in both generating scene graphs and for high-level tasks that one would be interested in performing on them, e.g., visual question answering.

## Visual Question Answering



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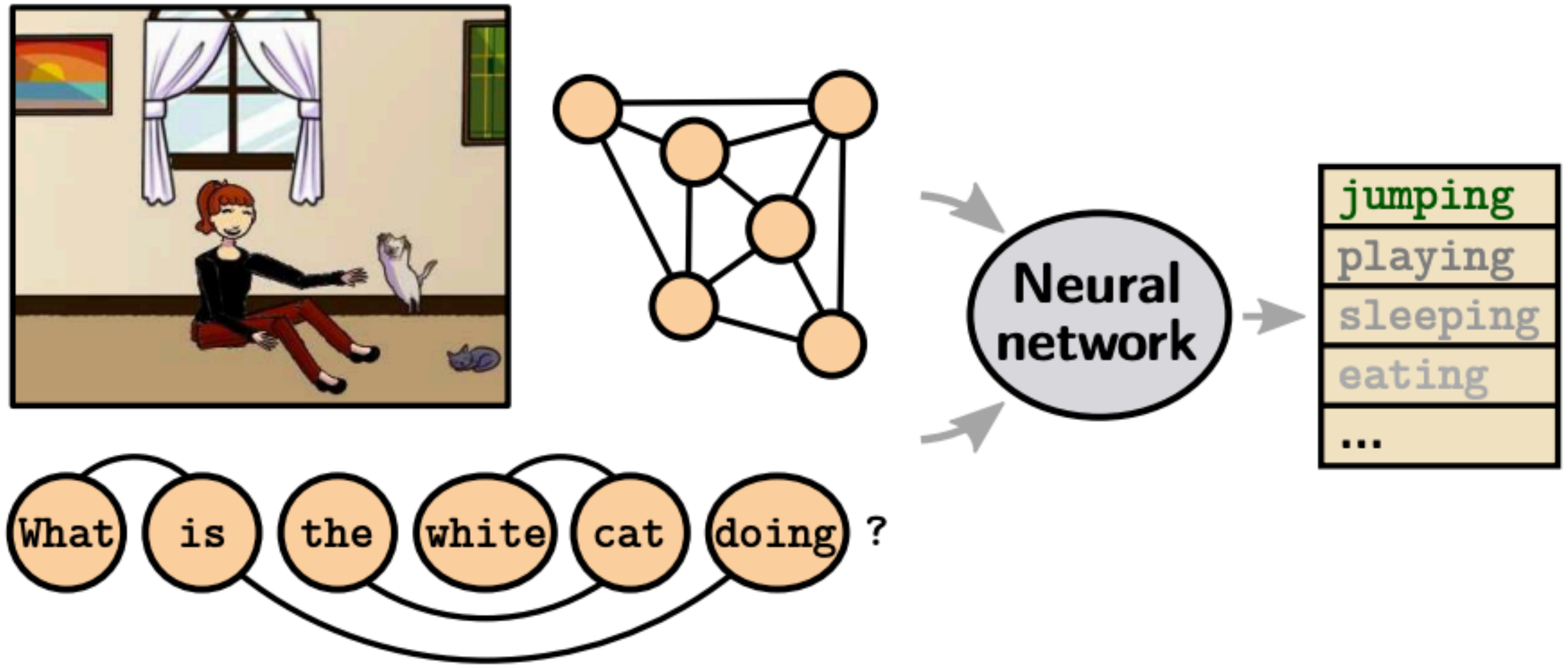

Encode the input scene as a graph representing the objects and their spatial arrangement. Encode the input question as a graph representing words and their syntactic dependencies. Train a neural network to reason over these representations, and to produce a suitable answer as a prediction. (Tenet et al., 2016)

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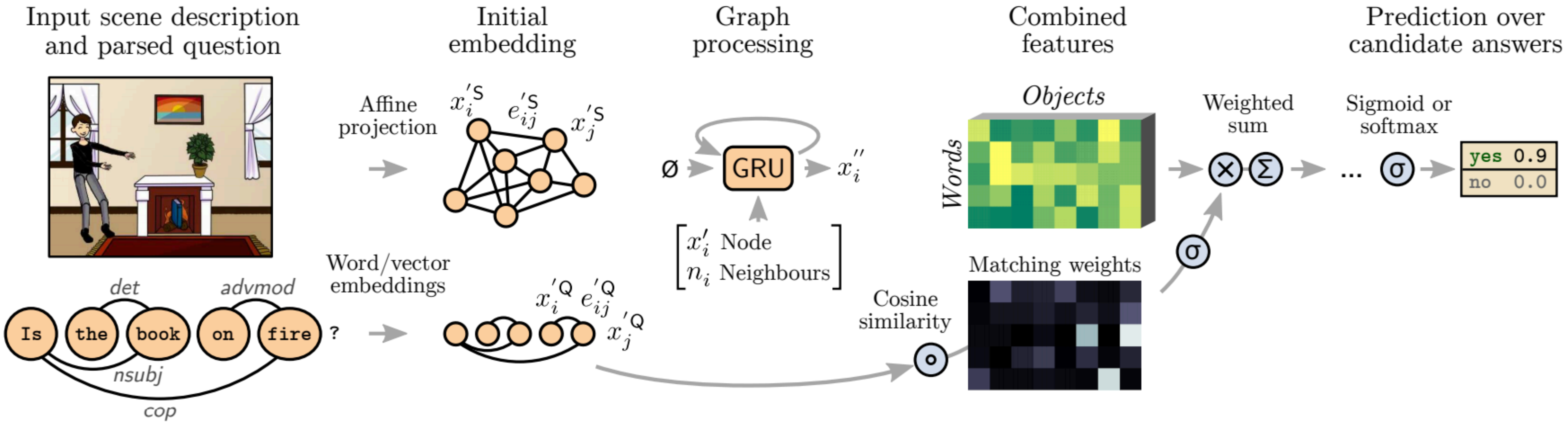

Figure from (Tenet et al., 2016) illustrating a pipeline for visual question answering using gated GNNs.

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This is the primary intuition behind rGCNs (Schlichtkrull et al., 2018).

## Knowledge Graph Completion with GNNs

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Specifically, rGCNs (Schlichtkrull et al., 2018) builds on GNNs and incorporate relation-specific weight matrices in aggregation:

$$\mathbf{h}_u^{(t)} = \sigma\Big(\sum_{r \in \mathbf{R}} \sum_{v \in N(u)} \big(\frac{1}{c_{u,r}}\big)\mathbf{h}_v^{(t-1)}\mathbf{W}_r^{(t)} + \mathbf{h}_u^{(t-1)}\mathbf{W}_{self}^{(t)}\Big),$$

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Note that rGCNs combine many aspects of this course: shallow KGC models and GNNs!

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GrAIL then performs message passing in this subgraph to make predictions. Since it relies on a local subgraph, and introduces its own labels, it can be applied to new unseen entities.

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## Thanks!

## Good luck with your projects...

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