

Computational Geometry meets Machine Learning

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Introduction

- We are interested in straight skeletons of (non-convex) polytopes in ℝ³
- Straight skeleton structure *R* is defined by a mitered boundary offsetting process
- For each vertex *v* with deg(*v*) > 3, its offset surface
 Σ is computed by the offset plane arrangement A(*v*)
- Boundary of union of all relevant unbounded arrangement cells defines Σ, but ...
 - Σ may not be valid
 - Σ may contain bounded facets \Rightarrow complicates $\mathcal R$

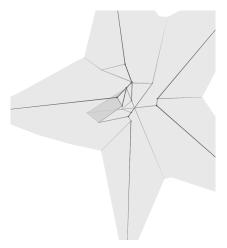


Cell Adding Process (CAP)

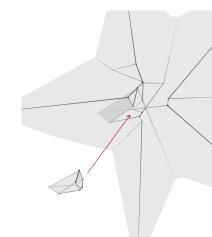
```
Let \mathcal{F} be the set of bounded facets in \Sigma
while \mathcal{F} is not empty:
Choose f \in \mathcal{F}
Let c be the bounded cell upon f
\Sigma \leftarrow \Sigma \cup c
Update \mathcal{F}
```

- Add bounded arrangement cells to Σ until all facets become unbounded
- This is always possible by the structure of $\mathcal{A}(v)$
- After CAP, Σ is valid and contains only unbounded facets

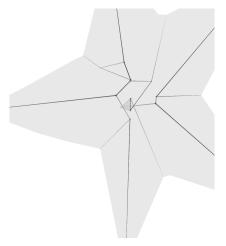




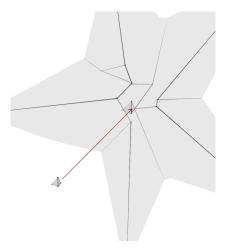




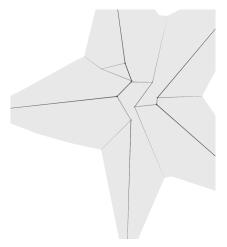




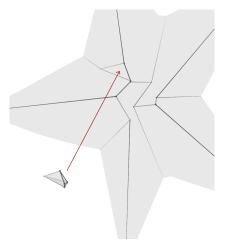




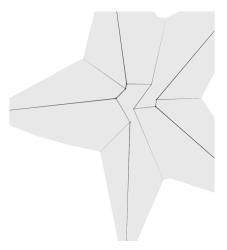














Let \mathcal{F} be the set of bounded facets in Σ while \mathcal{F} is not empty: Choose $f \in \mathcal{F}$ Let c be the bounded cell upon f $\Sigma \leftarrow \Sigma \cup c$ Update \mathcal{F}

- \mathcal{F} can easily be found
- Iteration over all facets in Σ



```
Let \mathcal{F} be the set of bounded facets in \Sigma
while \mathcal{F} is not empty:
Choose f \in \mathcal{F}
Let C be the bounded cell upon f
\Sigma \leftarrow \Sigma \cup C
Update \mathcal{F}
```

- There may be many facets in ${\cal F}$
- Which $f \in \mathcal{F}$ should we choose?
- Does it even matter which f we choose? Yes!



CAP Algorithm Analysis: Choose $f\in\mathcal{F}$

- For a bounded facet f there is a unique cell c upon f
- Σ ∪ c may create new bounded facets f', f", ... on Σ
 ⇒ F is extended by f', f", ...
- Order of the facets we choose in CAP is crucial for the updated or final $\boldsymbol{\Sigma}$
- If the order is chosen in an unfavorable way, it is no longer possible to get rid of all bounded facets! Why?
 - c may be <u>un</u>bounded for some f
 - If *c* is <u>un</u>bounded \Rightarrow we must not $\Sigma \cup c$ $\Rightarrow f$ may remain forever on Σ and in \mathcal{F}



```
Let \mathcal{F} be the set of bounded facets in \Sigma
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Update \mathcal{F}
```

- There is always a unique cell c upon f
- *c* can easily be determined from the structure of $\mathcal{A}(v)$
- If $f \in \mathcal{F}$ is chosen properly $\Rightarrow c$ is always bounded



```
Let \mathcal{F} be the set of bounded facets in \Sigma
while \mathcal{F} is not empty:
Choose f \in \mathcal{F}
Let c be the bounded cell upon f
\Sigma \leftarrow \Sigma \cup c
Update \mathcal{F}
```

- Merging c to Σ is always doable
- Updated Σ is always unique



```
Let \mathcal{F} be the set of bounded facets in \Sigma
while \mathcal{F} is not empty:
Choose f \in \mathcal{F}
Let c be the bounded cell upon f
\Sigma \leftarrow \Sigma \cup c
Update \mathcal{F}
```

- Σ was only updated locally around c
- \mathcal{F} can thus be updated efficiently



⁷ Problem Definition

- Given is a (not necessarily valid) surface Σ that contains bounded facets
- We are looking for a set of cells $\mathcal C$ such that $\Sigma'=\Sigma\cup\mathcal C$ contains unbounded facets only $\Rightarrow\Sigma'$ is valid
- C certainly exists due to the structure of A(v)
- ${\mathcal C}$ does not have to be unique $\Rightarrow \Sigma'$ may not be unique
- \hfill We are already satisfied with one instance of ${\cal C}$
- For a given Σ , how to find C?



Current Solution Approach

- We extend C step by step according to the rules:
 - (1) If $f \in \mathcal{F}$ is not visible from $v \Rightarrow f$ cannot belong to $\Sigma' \Rightarrow \text{add } c \text{ to } C$, for c upon f, to make f disappear
 - (2) Add any c to C for which no new bounded facets are created (c fits perfectly to the surface)
 - (3) Add any c to C that have at least 2 facets in common with the surface and all of them are connected
 - (4) If none of the above 3 criteria apply \Rightarrow select any $f \in \mathcal{F}$ and add the corresponding bounded *c* to C



Solution Discussion

- If rule (1) is applicable ⇒ c surely belongs to the solution set C
- Otherwise, (2), (3) or (4) is applicable (descending priority)
- There is room for improvement in the remaining three rules
- Current approach does not lead to the goal for all problem instances
- It is likely that a better heuristic algorithm exists



Different Solution Approach

- Given is a combinatorial optimization problem
- Finding C is probably NP-hard (open question)
- Different problem instances (data) but same problem structure
- Idea: Apply Machine Learning to learn patterns in the data to exploit problem structure
- Machine learning based methods are able to find new, previously unknown heuristics
- Automatically learn good heuristic algorithms for finding $\ensuremath{\mathcal{C}}$



Machine Learning

- Machine Learning (ML) is a sub-discipline of Artificial Intelligence in which a machine learns intelligent behaviour
- "A computer program is said to learn from experience *E* with respect to some task *T* and some performance measure *P*, if its performance on *T*, as measured by *P*, improves with experience *E*." [1]
 - T: Driving on highways using vision sensors
 - P: Average distance traveled before an error
 - E: Images sequence & steering commands by humans [1]

[1] Mitchell, T. (1997). Machine Learning. McGraw Hill. p. 2. ISBN 978-0-07-042807-2.



Machine Learning Paradigms

- Unsupervised Learning: Learning properties and patterns in unlabeled data
- Supervised Learning: Learning a mapping of data (input) to labels (output)
- Reinforcement Learning: Learning the optimal policy of an agent interacting with an environment



The three basic paradigms

of ML

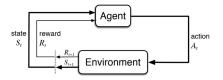


Reinforcement Learning (RL)

- An agent interacts with an environment
- During this time, the agent makes decisions in the form of actions
- Environment changes its internal state and emits a reward (weak feedback)
- Goal is to maximize the accumulated reward during the agent's lifetime
 - ⇒ Agent's behaviour is *reinforced* (therefore "reinforcement learning")
 - \Rightarrow Optimal **policy** is learned



Agent-Environment Interaction



- In a discrete timestep t the environment is in state S_t
- Agent chooses and performs an action A_t
- Environment changes its state to S_{t+1} and emits a reward R_{t+1} (next timestep)
- Based on that, the agent chooses the next action A_{t+1} , etc... $\Rightarrow S_0, A_0, R_1, S_1, A_1, R_2, S_2, A_2, ...$



Our Agent & Environment

- Agent is "an invisible character"
- Agent decides on a specific *f* ∈ *F* ⇒ associated *c* is merged onto Σ
- Environment is "anything outside of the agent"
- Environment includes
 - surfaces
 - plane arrangements
 - merging dynamics
 - everything else



Episode

- When our agent interacts with our environment, an episode is generated
- Episode starts in an initial state (at t = 0) and ends in a terminal state (at t = T)
- Sequence: $S_0, A_0, R_1, S_1, A_1, ..., A_{T-1}, R_T, S_T$
- Initial state S₀ is represented by Σ
- Terminal state S_T is represented by $\Sigma' = \Sigma \cup \{c_1, ..., c_T\}$



⁷ POMDP

- Partially Observable Markov Decision Process
- 6-tuple (S, A, Ω, T, O, R)
 - S: State space
 - A: Action space
 - Ω: Observation space
 - $T: S \times A \times S \rightarrow [0, 1]$: Transition function
 - $O: S \times A \times \Omega \rightarrow [0, 1]$: Observation function
 - $R: S \times A \times S \rightarrow \mathbb{R}$: Reward function

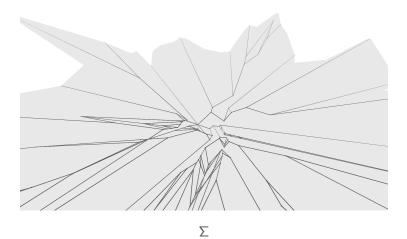


State

- A state describes the current situation in the environment
- A state of our environment is represented by Σ
- ∑ is described by its vertices, edges and facets and their connectivity information
- Note that state space S comprises all possible surfaces than can occur in the environment (S is infinite)



State Example





Observation

- For each state $s \in S$ there is an **observation** $o \in \Omega$
- Typically, *o* does not provide all information of *s*, *o* only contains hints about how *s* looks like
- We already know s, so why are we interested in o?
 - *s* provides too much information
 - Scaling/Translation/Rotation of Σ is irrelevant in our problem
 - Exact position of each vertex on Σ is redundant



Observation

- What part of ∑ might be important for encoding the problem structure?
 - Connectivity information between facets
 - Relation between facets in the space
 - Sharing planes of facets
- Formulating *o* as a **graph** *G*
- Think of G as a reduced special dual representation of Σ
- Let ${\mathcal N}$ be the nodes and ${\mathcal E}$ the edges of ${\boldsymbol G}$

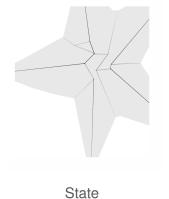


² Graph Nodes

- Each facet $f \in \Sigma$ corresponds to a node $n \in \mathcal{N}$
 - If *f* is bounded and its associated *c* is bounded \Rightarrow type $n_t = 1$
 - If *f* is bounded but *c* is unbounded \Rightarrow *n*_t = 2
 - If *f* is unbounded \Rightarrow *n*_t = 3
- Each plane on Σ corresponds to a node $n \in \mathcal{N}$ with $n_t = 4$



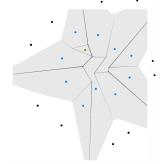
Graph Nodes Example



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Graph Nodes Example



State together with N (green for $n_t = 1$, blue for $n_t = 3$, black for $n_t = 4$)



Graph Nodes Example



\mathcal{N}

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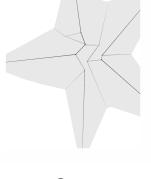


Graph Edges

- Each edge $e' \in \Sigma$ corresponds to an edge $e \in \mathcal{E}$, connecting the nodes of neighbouring facets
- Each facet $f \in \Sigma$ corresponds to an edge $e \in \mathcal{E}$, connecting the facet's node with its supporting plane's node
- Each $e \in \mathcal{E}$ has weight e_w , corresponding to the interior angle between the two facets on Σ
 - If *e* is adjacent to a plane node $\Rightarrow e_w = 0$, since in the imagination the facet encloses no angle with its plane



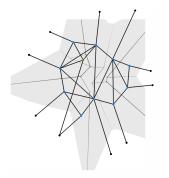
⁷ Graph Edges Example



State



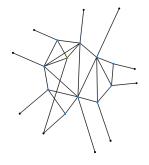
Graph Edges Example



State together with \mathcal{N} and \mathcal{E} (without weights)



Graph Edges Example



 ${\mathcal N}$ and ${\mathcal E}$

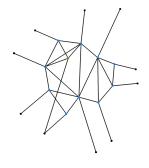


⁴⁰ Action

- Based on the current observation, the agent chooses an action
- An action expresses what the agent can do in the current observation of the environment
- An action of our agent is represented by selecting a node n ∈ N of type n_t = 1
- *n* is associated with a (bounded) facet $f \in \Sigma$
- *f* is associated with a (bounded) cell $c \in \mathcal{A}(v)$
- The action causes merging of *c* onto Σ ⇒ state and observation transition



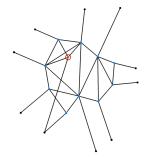
Action Example



G



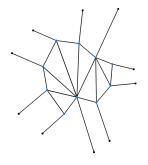
Action Example



Selecting a node of type $n_t = 1$



Action Example



Next G



⁴⁴ Reward

- Based on the current state and selected action, the environment emits a reward
- The reward tells the agent how good its action was
- It is often represented by a scalar r
- The higher r, the better the action was
- What does our reward look like?
- Can we give a reward after each action?



⁴⁵ Reward

- There might be cells c₁, c₂, ... ∈ A(v) that certainly belong to our solution set C
- But instead of giving these actions a higher reward and learn from this, we can directly insert c₁, c₂, ... into C ⇒ Expert Policy (discussed later)
- Actions that directly lead to the success/failure state, should get a high/low reward
- For all intermediate actions, we cannot state in general which ones should be prefered

TU Graz

⁴⁶ Reward

- Let $s \in \mathcal{S}$ be the current state
- Let $a \in \mathcal{A}$ be the selected action
- Let $s' \in \mathcal{S}$ be the next state when performing a in s
- Then,
 - r(s, a) = 0 if s' is no terminal state
 - r(s, a) = +1 if s' is a success terminal state
 - r(s, a) = -1 if s' is a failure terminal state
- Reward signal is very sparse



Policy

- The **policy** π describes the behaviour of the agent
- π represents the strategy of the agent
- Using π, the agent selects an action a ∈ A for the given observation o ∈ Ω
- Formally, π can be represented as $\pi(o) = a$
- What is our policy?

\Rightarrow A good policy is what we want to learn!



Expert Policy

- If *f* ∈ *F* is not visible from *v* ⇒ *f* cannot belong to Σ' ⇒ add *c* to *C*, for *c* upon *f*, to make *f* disappear
- If such *f* exists, select corresponding node *n* ∈ N as action (expert policy)
- The action suggested by the expert policy is always optimal
- We already have the expert policy, so we do not need to learn it
- But the expert policy cannot always suggest an action
 we need another policy



ϵ -greedy Policy

- We need to explore the environment well enough to learn about the problem structure and a good policy
- We have to find a suitable balance between exploration and exploitation (= applying what has already been learned)
- Introduce a small value ϵ between 0 and 1
- With a probability of
 ϵ take a random action, otherwise take the greedy action (
 ϵ-greedy policy)
- We have defined policies, but how do we learn a good one?



Q-Learning

- **Q-Learning** is an algorithm that learns a *Q*-value for each *o*, *a* pair
- This value is used to determine the quality of a in o
- **Q-function** Q(o, a) is trained
 - \Rightarrow Optimal *Q*-function $Q^*(o, a)$
 - \Rightarrow Optimal policy $\pi^*(o) = \operatorname{argmax}_a Q^*(o, a)$
 - \Rightarrow Best *a* for given *o*
- Update Rule: $Q(O_t, A_t) \leftarrow Q(O_t, A_t) + \alpha \cdot$

 $[R_{t+1} + \gamma \max_{A} Q(O_{t+1}, A) - Q(O_t, A_t)]$



Q-Learning

- At the beginning of training, *Q*-function returns arbitrary values for all *o*, *a* pairs
- After sufficient exploration of the environment and application of the update rule ⇒ Q(o, a) becomes more meaningful
- Problem: S, A, Ω are infinite, so we cannot store and update all o, a pairs
- Solution: Generalization over several observations and actions ⇒ Q-Function approximation

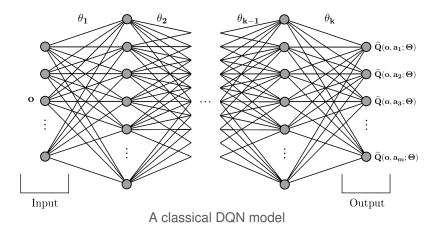


Deep Q-Learning

- Creating a function approximation $\widehat{Q}(o, a; \Theta) \approx Q(o, a)$
- *Q*(*o*, *a*; Θ) can be computed with a Deep Neural Network with model parameters Θ ⇒ Deep
 Q-Network (DQN)
- DQN approximates the Q-value for each o, a pair
- Approximations are sufficient as long as the relative quality assessments are preserved (argmax_a Q̂(o, a; Θ))



DQN





Training DQN

- Training of DQN by optimizing its parameters $\Theta = \{\theta_1, ..., \theta_k\}$
- Optimization of Θ by minimizing quadratic loss $\mathcal{L}(\Theta) = \mathbb{E}[(y - \widehat{Q}(O_t, A_t; \Theta))^2]$ with $y = R_{t+1} + \gamma \max_A \widehat{Q}(O_{t+1}, A; \Theta)$
- *L*(Θ) can be (locally) minimized using the Stochastic Gradient Descent (SGD) algorithm
- **Problem:** SGD needs *iid* data, but our data are sequentially dependent ⇒ unstable training
- Solution: Experience Replay



Experience Replay

- In each timestep *t* collect an experience $E_t = (O_t, A_t, R_{t+1}, O_{t+1})$
- E_t is stored in a **replay memory** \mathcal{M}
- During training, sample a random mini-batch b ^{iid} ∼ M and optimize ⊖ for b using SGD
- Experiences are reused in many updates ⇒ higher data efficiency
- Data in b are uncorrelated ⇒ more stable network training



Applying DQN

- When using DQN, we need to consider more issues
- (1) DQN only accepts inputs of the same size
 - Input of our DQN is *o*, or its graph *G*
 - Different G have different sizes
- (2) DQN only produces outputs of the same size
 - Output of our DQN is $\widehat{Q}(o, a_i, \Theta), \forall a_i \in \{a_1, ..., a_m\}$
 - Different *G* have different number of actions *m*

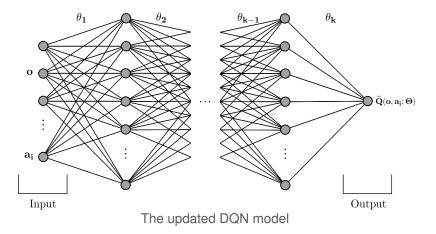


Applying DQN: Issue (2)

- This matter can be solved quite easily
- Modify DQN
 - Input: o and a single a_i
 - Output: $\widehat{Q}(o, a_i, \Theta)$
 - Compute Q-value for each a_i separately
- DQN can now be applied to different numbers of actions
- *Drawback:* Instead of a single forward pass, we now need *m* forward passes ⇒ takes more time



Updated DQN





Applying DQN: Issue (1)

- This matter is not so easy to solve
- Order of the nodes and edges in G should not matter
- Connectivity information between nodes and all features should be preserved
- Idea: Learn a fixed-sized representation of o and a, independent of the size of G
- Then, input of DQN is also of fixed size
- Solution: Graph Neural Network



Graph Neural Network

- A Graph Neural Network (GNN) processes graph-structured data
- GNN simulates an exchange of features between the nodes in the graph (message passing)
- For each node, and finally for the graph itself, a low-dimensional vector representation is learned (= Node/Graph embedding)
- Embeddings include important graph characteristics, e.g. node types, edge weights, neighbourhoods, etc.
- GNN can be seen as a Graph Embedding Network



GNN: Initial Node Embedding

- For each $n \in \mathcal{N}$ we learn a *p*-dimensional node embedding μ_n
- Initialize µ_n as follows:

 $\mu_n^{(0)} = \operatorname{relu}(\theta_1 t_n), \text{ where }$

- *t_n* is the one-hot encoded type of *n*
- $\theta_1 \in \mathbb{R}^{p \times 4}$ are trainable parameters
- relu(x) = max(0, x) is the rectified linear unit
- Initially, global node type information is collected



GNN: Message Passing

- Each n computes a message and transmits it to its neighbours
- Each n aggregates the messages of its neighbours
- Each μ_n is updated synchronously up to *T* iterations: $\mu_n^{(t)} \leftarrow F_{\theta_2}(\mu_n^{(t-1)}, \{\mu_u^{(t-1)}\}_{u \in \mathcal{N}(n)}, \{e_w\}_{e \in \mathcal{E}(n)}), \text{ where}$
 - $\mathcal{N}(n)$ are the neighbouring nodes of n
 - $\mathcal{E}(n)$ are the adjacent edges of n
 - $\{\cdot\}$ is some aggregation function (e.g. summation)
 - *F* is a neural network with θ_2 combining them



GNN: Message Passing

- Messages are propagated recursively according to the topology of G
- Only when $\mu_n^{(t)}$ has been computed for all *n*, the next iteration t + 1 starts
- The larger *T* is, the further the messages are propagated through *G*
- $\mu_n^{(T)}$ includes information of its *T*-hop neighbourhood
- Typically a small T is sufficient for a good node representation



Parameterizing $\widehat{Q}(o, a; \Theta)$

- Let $\mu_G = \sum_{n \in \mathcal{N}} \mu_n^{(T)}$ be the graph embedding of G
- Combining the GNN with our DQN, we can parametrize $\widehat{Q}(o, a; \Theta)$ with $\Theta = \{\theta_1, \theta_2, \theta_3\}$:

$$\widehat{Q}(o,a;\Theta) = H_{ heta_3}(\mu_G,\mu_n^{(T)}),$$
 where

- $\mu_{G} \in \mathbb{R}^{p}$ is a representation of o
- $\mu_n^{(T)} \in \mathbb{R}^p$ is a representation of *a*
- *H* is a neural network with θ_3 combining them
- All parameters in Θ are trainable



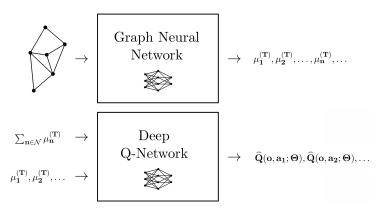
Final Model

- Our final deep reinforcement learning model has a GNN and DQN component
- GNN takes a graph and produces node embeddings of fixed size
- Aggregating all node embeddings to a graph embedding of fixed size that represents o
- DQN takes the graph embedding and one node embedding each, which represents a

• DQN produces
$$\widehat{Q}(o, a; \Theta)$$



Final Model



The final GNN-DQN model

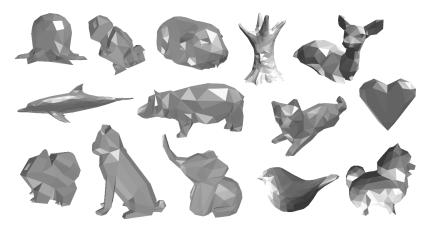


⁷ Training

- All parameters in the GNN and DQN can be learned end-to-end using reinforcement learning
- Training is done by SGD using experience replay
- In order for our model to understand the underlying problem structure, we need a lot of training data
- Initial task was to compute offset surfaces of polyhedra in R³
- Therefore, take various real world data on which our model should be trained



Training Data



Some polyhedra



Training Sample

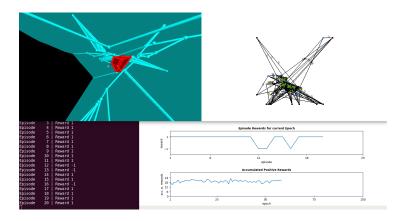
- We need many polyhedra in \mathbb{R}^3
- Each *higher-degree* vertex with its local neighbourhood is a **training sample** d
- For each d inital Σ is computed and CAP is applied
- CAP generates all experiences used in training



A training sample



Time for demo!





¹ Summary

- Σ is required for constructing a straight skeleton of a polyhedron in \mathbb{R}^3
- Σ may contain bounded facets
- CAP algorithm does not always find a suitable $\boldsymbol{\Sigma}$
- Subroutine based on reinforcement learning should learn a good policy for CAP
- Dual representation of Σ as *G* for learning model
- Q-learning with GNN and DQN
- Training requires a lot of data



² Outlook

- Clear setup of the training dataset
 - Which and how many polyhedron vertices and of what degree?
- Implementation of the Deep Q-Learning Model with the Graph Embedding Network
- Hyperparameter tuning (ε, γ, p, T, epochs, network architectures, etc.)
- Testing and evaluation
 - How well does the learning model perform on previously unseen data?