Reinforcement learning for mathematical applications

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1 Introduction

In 2020 Dylan Peifer et al[PSH20] showed how to use deep learning to improve the performance of algorithms for constructing Gröbner bases. The goal of this project was to reproduce the results of this paper, as well as attempt some other techniques.

The structure of this report is as follows: first, we'll discuss the use of reinforcement learning, a branch of deep learning used by Peifer et al. We'll cover both the conceptual framework, as well as two particular techniques: Q-learning and policy gradients. Next, a brief overview of Gröner bases, their uses, and how to compute them. The third part covers our experimental results featuring both an evaluation of existing heuristics as well as our results.

2 Gröbner bases

Since the problem we're considering is the construction of Gröbner bases, let's give a short introduction to Gröbner bases.

We fix a field k and consider the polynomial ring $R = k[x_1, \ldots, x_n]$. For a set of polynomials $F = \{f_1, \ldots, f_l\}$ we consider the ideal $I = \langle f_1, \ldots, f_l \rangle$ generated by these polynomials. Now, we wish to efficiently determine whether a given polynomial f lies in I or not. We know that R is a *unique factorization domain* so it is decidable, but giving an efficient algorithm is tricky. Instead, we extend the

generating set of the ideal in a way that doesn't change the ideal but gives us stronger properties, enabling an efficient decision algorithm.

Fix a *term order* which is a well-order relation $>$ on $\mathbb{N}^n$ such that $a > b$ implies $a + c > b + c$ for any $a, b, c \in \mathbb{N}^n$. This naturally extends to a so called *monomial order* on monomials $\{x^v = x_1^{v_1} \cdots x_n^{v_n} \mid v \in \mathbb{N}^n\}$ by comparing exponent vectors of the monomials. We'll write $>$ for both orders.

There are two common term orders: lexicographic and grevlex. Lexicographic has $a > b$ if there exists k s.t. $a_i = b_i$ for $i < k$ and $a_k > b_k$. This is the usual "alphabetix order" on tuples. Grevlex ordering is often used in implementations using Gröbner bases and has $a > b$ if $\sum_i a_i > \sum_j b_j$ or $\sum_i a_i = \sum_j b_j$ and the last non-zero entry of $a - b$ is negative.

Given a monomial order, we can define the *initial term* and the S-polynomial.

2.1 · Definition. Given a monomial order $>$, the *initial term* of a polynomial $f = \sum_v \lambda_v x^v$, denoted $in_>(f)$ is the greatest term of f with respect to $>$. We will often omit the subscript when the order is either clear from context or arbitrary.

Now, a naive division algorithm would look like this:

Algorithm 1: Division algorithm $reduce(f, F)$

Input: Polynomial f and $F = \{f_1, \ldots, f_l\}$
Output: Remainder r s.t. $f - r \in \langle F \rangle$ and $in(f_i) \nmid in(r)$ for all $f_i \in F$

1 $r \leftarrow f$
2 **while** $\exists i. in(f_i) \mid in(r)$ **do**
3 $\quad r \leftarrow r - \frac{in(r)}{in(f_i)} f_i$

This algorithm terminates since the initial term of r is strictly decreasing with respect to $>$. However, this algorithm has some problems. In particular, we do not always get that $reduce(f, F) = 0$ when f lies in the ideal generated by F, as we would expect. This is due to the choice of which polynomial to reduce with in line 3.

An example where this does not hold without a Gröbner basis is example 5.4.3 in NL .

Now, we're ready to present Gröbner bases and the theorem that makes them so important:

2.2 · Definition. A Gröbner basis for an ideal I is a set of polynomials $F = \{f_1, \ldots, f_l\} \subseteq I$ such that $in(f_i) \mid in(f)$ for all $f \in I \setminus \{0\}$.

Note that this implies $\langle F \rangle = I$.

2.3 · Theorem. *Let $G = \{f_1, \ldots, f_l\}$ be a Gröbner basis for an ideal I. Then $reduce(f, G) = 0 \iff f \in I$.*

Proof. If $reduce(f, G) = 0$ then $f = f - 0 \in I$.

If $f \in I$ and $f - r = h \in I$ then $r = f - h \in I$. But as guaranteed by the division algorithm, there is no $f_i \in G$ where $in(f_i) \mid in(r)$ even though G is a Gröbner basis. The only element in I not subject to the Gröbner basis constraint is zero, thus r must be zero. □

So, Gröbner bases are great, but how do we construct them? Do they even exist for every ideal? They do exist and we have an algorithm called Buchberger's algorithm to find them, but first, we need a construction called the S-polynomial or syzygy polynomial.

2.4 · Definition. The S-polynomial of two polynomials f and g is denoted $S(f, g) = \frac{x^w}{in(f)} f - \frac{x^w}{in(g)} g$ where $x^w = lcm(in(f), in(g))$ is a least common multiple of f and g.

The Buchberger criterion is a simple way to check if we have a Gröbner basis, and it even leads us to an algorithm for constructing Gröbner bases.

2.5 · Theorem. *Let $F = \{f_1, \ldots, f_l\}$ be a set of polynomials and let $I = \langle F \rangle$ be the ideal generated by F. If $reduce(S(f_i, f_j), F) = 0$ for all $f_i, f_j \in F$ then F is a Gröbner basis for I.*

Proof. See appendix. □

We can now present the Buchberger algorithm:

Algorithm 2: Buchbergers algorithm

Input: A set of polynomials $F = \{f_1, \ldots, f_l\}$
Output: A Gröbner basis G of the ideal $I = \langle F \rangle$

```
1 G ← F
2 P ← {(f_i, f_j) | 1 ≤ i < j ≤ l}
3 while |P| > 0 do
4     (g, h) ← select(P)
5     P ← P \ {(g, h)}
6     r ← reduce(S(g, h), G)
7     if r ≠ 0 then
8         P ← update(P, G, r)
9         G ← G ∪ {r}
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Notice that the algorithm uses 2 routines we haven't defined: *select* and *update*. The simplest implementations are select(P) = P_1 taking the first pair in P and update(P, G, r) = $P \cup \{(f, r) \mid f \in G\}$. We'll see better and more refined implementations later.

Buchberger's algorithm adds remainders of syzygy polynomials until they all reduce to 0. Keeping theorem 2.5 in mind, it is clear that G will be a Gröbner basis when the algorithm terminates.

To produce a faster version of Buchberger's algorithm, these two routines are good places to start. During *update* we can eliminate a large number of pairs using simpler criteria than theorem 2.5. We'll discuss a better version in section 2.1.

The problem of selecting the next pair of polynomials is not easy and it turns out to have serious consequences. Simply switching from taking the first pair to taking the last one, i.e. treating P as a stack instead of a queue, can reduce the number of polynomial additions by almost 50%.

There are several standard selection strategies:

Random	Pick a random pair uniformly.
First	Pick the lexicographically smallest pair, where the order of polynomials is given by their order in G.
Queue	Treat P as a queue and select the pair that was added first.
Stack	Treat P as a stack and select the pair that was most recently added.
Degree	Pick the pair (f, g) with the smallest total degree of $lcm(in(f), in(g))$.
Normal	Pick the pair (f, g) where $lcm(in(f), in(g))$ is smallest in the used monomial order.
Sugar	Pick the pair (f, g) with the smallest *sugar degree* which is the degree $S(f, g)$ would have had if the polynomials had been homogenized.
TrueDegree	Introduced in [PSH20], pick the pair (f, g) whose S-polynomial has the lowest degree.

2.1 A better *update*

In the Buchberger algorithm, a pair (f, g) will be removed if reduce$(S(f, g), G) = 0$. However, this is a computationally expensive test. Fortunately, there are some easier tests that can eliminate a large number of pairs. I'll describe the tests described in Gebauer & Möller.

2.1.1 Operational description

Gebauer & Möller reduction is performed as part of the procedure update(P, G, r). First, in the pair set P we remove every pair (f, g) where $in(r)|\text{lcm}(in(f), in(g))$ and $\text{lcm}(in(f), in(r)) \neq \text{lcm}(in(f), in(g)) \neq \text{lcm}(in(g), in(r))$.

Next, consider the set $P' = \{(f, r) \mid f \in G\}$. These are all the pairs we should naively add to P. Partition P' into equivalence classes using the equivalence realation $(f, r) \sim (g, r) \iff \text{lcm}(in(f), in(r)) = \text{lcm}(in(g), in(r))$. Remove every equivalence class containing no element (f, r) satisfying $\text{lcm}(in(f), in(r)) = in(f)in(r)$ and take a representative from each remaining equivalence class. Let P'' be this set of representatives and let $P \cup P''$ be the result of update(P, G, r).

2.1.2 Justification and proof

Simply put, Gebaur& Möller reduction consists of reducing a Gröbner basis. Once a Gröbner basis is constructed, we may throw away any redundant element. This process is described above and the proof that this maintains the Gröbner basis property can be found in [Lau03] section 5.8.

For the setup we need to extend the concept of Gröbner bases to free modules over a polynomial ring. R be a multinomial ring in n variables over a field k and $e_1, \ldots, e_m$ be the canonical basis of R^m. Since every element of R^m is a k-linear combination of elements of the form $x^v e_i$, $v \in \mathbb{N}^n$, we call these $x^v e_i$ for monomials. Now, the definition of Gröbner bases require two more parts: a monomial order and a divisability test. Monomial orders work the same way, they're a total order satisfying

$$x^{v_1} e_i < x^{v_2} e_j \implies x^{v_1+v} e_i < x^{v_2+v} e_j$$

for all $v \in \mathbb{N}^n$. We say that $x^{v_1} e_i$ divides $x^{v_2} e_j$ iff $i = j$ and x^{v_1} divides x^{v_2}. Now, the definition of a Gröbner basis is the same, and we will repeat it here: a Gröbner basis for a submodule $M \subset R^m$ is a set of elements $F = \{m_1, \ldots, m_t\} \subset M$ such that $in(m_i)$ divides $in(m)$ for all $m \in M \setminus \{0\}$.

Now, consider the ideal of monomials $I = \langle x^{v_1}, \ldots, x^{v_m} \rangle \subset R$ and the natural surjection $p : R^m \to I$ sending e_i to x^{v_i}. Now, let K be the kernel of p and notice that the syzygies in I are a basis of K.

Example. If $I = \langle x, y, z \rangle$ then K will have a basis consisting of the syzygies $\{xe_2 - ye_1, xe_3 - xe_1, ye_3 - ze_2\}$. □

More generally, the elements

$$S_{ij} = x^{\text{lcm}(v_i, v_j) - v_j} e_j - x^{\text{lcm}(v_i, v_j) - v_i} e_i,\ 1 \leq i < j \leq m$$

are basis elements of K. However, this basis is usually not minimal. Now, we need two propositions, the first due to Schreyer.

2.6 · Theorem. *There exists a monomial order called the Schreyer order such that set $\{S_{ij} \mid 1 \leq i < j \leq m\}$ is a Gröbner basis for K over this order.*

The second is proposition 2.9.9 from [CLO98].

2.7 · Theorem. *Let $G = \{g_1, \ldots, g_m\}$ be a basis for an ideal I. Then G is a Gröbner basis for I iff for every basis element of the syzygies of G $S = \sum_{i=1}^{m} x^{u_i} e_i$ we have $\sum_{i=1}^{m} x^{u_i} g_i \to_G 0$.*

Now, this is a refinement of the Buchberger S-criterion. It is therefore enough to reduce the S-pairs corresponding to any Gröbner basis of the syzygies. In particular, we may take the basis $\{S_{ij} \mid 1 \leq i < j \leq m\}$ and reduce it to a minimal Gröbner basis before reducing mod G and adding to G.

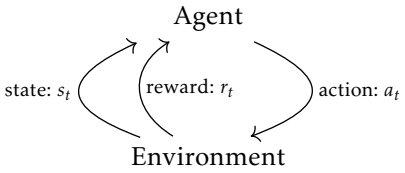
3 Abstract framework of deep learning

We would like to use modern advances in machine learning to learn a better selection strategy for Buchberger's algorithm. However, to do so we need some machinery. Since we need to use the *select*-function multiple times, we need to use a branch of machine learning called *reinforcement learning*.

3.1 Reinforcement-learning and Markov Decision Processes

Constructing Gobner bases can be seen as an interaction between an agent and an environment: we pick a pair to reduce, perform polynomial reduction, add some new pairs to the set of pairs and go again. We want to do the least amount of work when we're done. This interaction can be modeled using Markov decision processes.

A Markov decision process (MPD for short) is an interaction between an environment and an agent. At timestep $t = 0, 1, 2, \ldots$ the agent recieves a *state*, S_t and selects an *action*, a_t. The agent then recives a *reward*, r_{t+1} and a new state s_{t+1} and the process repeats.



This gives rise to a *trajectory* which looks like this:

$$\tau = s_0, a_0, r_1, s_1, a_1, r_2, s_2, a_2, \ldots$$

We'll sometimes denote $\tau_p = s_p, a_p, r_{p+1}, s_{p+1}, \ldots$.

Formally, this can be described in terms of the following definition:

3.1 · Definition. *Environment and policy*

- Fix two non-empty, finite sets S and $R \subset \mathbb{R}$ and a family of non-empty finite sets A_s for all $s \in S$. We call S the *state-space*, A_s an *action-space* and R the *reward space*. Then an *environment* is a probability distribution

  $$p(s', r \mid s, a) = P(s_{t+1} = s', r_{t+1} = r \mid s_t = s, a_t = a)$$

  for all $s, s' \in S$, $r \in R$ and $a \in A(s)$.
- Given an environment, an *policy* is a propability distribution $\pi(a \mid s)$ of taking an action a given a state s.

An important property of a MPD is that the probability of s_t depends only on s_{t-1} and a_{t-1}, not all of the earlier states and actions. Do also note, that we can derive marginal probabilities from the $p - function$, for example the probability of reaching a certain state

$$p(s' \mid s, a) = P(s_{t+1} = s' \mid s_t = s, a_t = a) = \sum_{r \in R} p(s', r \mid s, a).$$

Now, an agent can interact with an environment by choosing actions and revieving rewards. Such an interation leads to a trajectory $\tau = s_0, a_0, r_1, s_1, a_1, r_2, s_2, a_2, \ldots$. We're interested in minimizing the total reward of the trajectory or the *return*

$$G(\tau) := \sum_{t=1}^{\infty} \gamma^t r_t$$

where $0 < \gamma < 1$ is put in place to ensure convergence of the infinite series. However, if the rewards are eventually always zero, we may choose $\gamma = 1$. Usually a value around 0.99 is chosen for γ.

3.2 Pair selection as a Markov Decision Process

The problem of pair selection is modeled as a Markov Decision Process. During a run of Buchberger's algorithm the *select* subroutine is implemented by the agent. At timestep t, the agent sees the state P_t which is the current set of polynomial pairs. The agent must then choose a pair $a_t \in P_t$ which is fed back into Buchberger's algorithm as the result of *select*. The environment then updates by removing p from P, reducing the corresponding and S-polynomial, and updating G and P.

The reward r_t given for the action a_t is -1 times the number of polynomial additions performed when reducing a_t. This metric is chosen since it is the most expensive computation and it serves as a proxy for total computation.

This loops until a complete Gröbner basis is constructed at timestep T, yielding the trajectory $\tau = (P_0, a_0, r_0, \ldots, P_T, a_T, r_T)$. The goal of the agent is to maximize the exprected return $\mathbb{E}[\sum_{t=1}^{T} r_t]$ which is minimizing the number of polynomial additions.

It is not immediately obvious that the state-space is finite. However, the running time of Buchberger's algorithm has been shown to be worst-case $d^{2^{n+\mathcal{O}(1)}}$ where n is the number of variables and d is the maximum total degree of any generator. This means the set P of polynomial pairs can at most grow that large. Since at any step there is a finite number of actions and the algorithm terminates after a bounded number of actions, the number of possible states is finite. It's very large but finite.

4 Learning strategies

The abstract framework of Markov Decision Processes is a rather simple idea. And indeed, that is not where the magic of reinforcement learning is. Reinforcement learning solves the challenge of credit assignment. We have sampled some trajectories, some leading to a high reward and some to a lower reward. How do we know what actions were responsible for the high rewards? How should we update the agent to increase future rewards? In this section, we'll describe two approaches: value estimation and policy gradients as well as some standard "tricks" that are used to improve performance.

4.1 Value-estimation and Q-learning

Most classical reinforcement learning is about estimating value functions – how good a state or action is. For example, we can define the *value* of a state s given

an agent π to be

$$v_\pi(s) = \mathbb{E}\Big[G(\tau_p) \mid s_p = s, \pi\Big] = \mathbb{E}\left[\sum_{k=p}^{T} \gamma^k r_k \mid s_p = s, \pi\right].$$

Here we sample the actions a_t from the probability distribution given by π.

The value-function can be expressed recursively:

$$\begin{aligned} v_\pi(s) &= \mathbb{E}[G(\tau_p) \mid s_p = s, \pi] && (1)\\ &= \mathbb{E}\left[\sum_{k=p}^{T} \gamma^k r_k \mid s_p = s, \pi\right] && (2)\\ &= \mathbb{E}\Big[r_p + \gamma G(\tau_{p+1}), \mid s_p = s, \pi\Big] && (3) \end{aligned}$$

Now, we can further use the law of total probality twice to get

$$\begin{aligned} v_\pi(s) &= \mathbb{E}[r_p + \gamma G(\tau_{p+1}) \mid s_p = s] && (4)\\ &= \sum_a \pi(a \mid s)\mathbb{E}[r_p + \gamma G(\tau_{p+1}) \mid s_p = s] && (5)\\ &= \sum_a \pi(a \mid s) \sum_{s',r} p(s', r \mid s, a)\mathbb{E}[r + \gamma G(\tau_{p+1}) \mid s_{p+1} = s'] && (6)\\ &= \sum_a \pi(a \mid s) \sum_{s',r} p(s', r \mid s, a)(r + \gamma \mathbb{E}[G(\tau_{p+1}) \mid s_{p+1} = s']) && (7)\\ &= \sum_a \pi(a \mid s) \sum_{s',r} p(s', r \mid s, a)(r + \gamma v_\pi(s')) && (8) \end{aligned}$$

And this actually gives us a way to learn. By starting with a random policy π_0 we can sample some trajectories, giving us values for r, a and s. Then the above is a number of linear equations that can be solved to find $v_{\pi_0}(s)$ for every s. Based on this value function we can devise a new strategy π_1 which chooses the action leading to the most valuable state. Repeating this process, called policy iteration in the literature, should provide better and better agents. It does work, but it has some serious limitations. An obvious one is in the face of non-deterministic environments: how do we know which state each action will lead to? That requires a good model of the environment to answer, which we may not have.

One solution to the problem above is to shift our focus slightly to consider the value of *actions* instead of states. We can define an *action-value* function, denoted

$$q_\pi(s, a) = \mathbb{E}[G(\tau_p) \mid s_p = s, a_p = a, \pi].$$

Using these we can define the *optimal* value functions:

4.1 · Definition.

$$v_*(s) = \max_\pi v_\pi(s)$$

is called the *optimal value function* and

$$q_*(s,a) = \max_\pi q_\pi(s,a)$$

is called the *optimal action-value function*

These two functions can be expressed in terms of each other:

$$\begin{aligned} v_*(s) &= \max_\pi v_\pi(s) \\ &= \max_\pi \mathbb{E}[G(\tau_p \mid s_p = s, \pi)] \\ &= \max_\pi \sum_a \pi(a \mid s)\, \mathbb{E}[G(\tau_p) \mid s_p = s, a_p = a, \pi] \\ &= \max_\pi \sum_a \pi(a \mid s)\, q_\pi(s,a) \\ &= \max_a q_*(s,a) \end{aligned}$$

and similarly we can get

$$q_*(s,a) = R(s,a) + v_*(s').$$

These of course also satisfies the recursive relations from before:

$$\begin{aligned} v_*(s) &= \max_a q_*(s,a) \\ &= \max_a \mathbb{E}[G(\tau_p) \mid s_p = s, a_p = a, \pi_*] \\ &= \max_a \mathbb{E}[r_p + \gamma v_*(s_{p+1}) \mid s_p = a, a_p = a, \pi_*] \\ &= \max_a \sum_{s',r} p(s' \mid s,a)(r + \gamma v_*(s')) \end{aligned}$$

which is called the Bellman equation for v_*. The Bellman equation for q_* is

$$q_*(s,a) = \sum_{s',r} p(s', r \mid s, a)(r + \gamma \max_{a'} q_*(s', a')).$$

These equations inspires the learning equation

$$Q(s_p, a_p) = (1-\alpha)Q(s_p, a_p) + \alpha(r_{p+1} + \gamma \max_a Q(s_{p+1}, a))$$

Here, α is called the learning rate. This is a slight variation of policy iteration, but whereas policy iteration worked on the state-value function, this equation

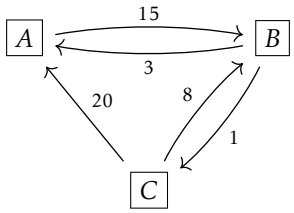


Figure 1: A simple graph-based environment

applies to the action-value function as well. It can be shown that under light assumptions this learning method converges to the optimal q-function, for a full exposition see [WD92].

Example. Consider the graph in figure 1. If the agent initially takes each possible action with equal probability, we might observe the trajectory $\tau = (A, B, C, A, B, A, B, C, B, C)$. With learning rate $\alpha = 0.5$ and decay $\gamma = 1$ we get the following updates:

s	s'	r	Update		
A	B	15	$Q(A,B) = \frac{1}{2}0 + \frac{1}{2}(15+0)$	=	7.50
B	C	1	$Q(B,C) = \frac{1}{2}0 + \frac{1}{2}(1+0)$	=	0.50
C	A	5	$Q(C,A) = \frac{1}{2}0 + \frac{1}{2}(20+7.5)$	=	13.70
A	B	15	$Q(A,B) = \frac{1}{2}7.5 + \frac{1}{2}(15+0.5)$	=	11.40
B	A	3	$Q(B,A) = \frac{1}{2}0 + \frac{1}{2}(3+11.4)$	=	7.20
A	B	15	$Q(A,B) = \frac{1}{2}11.4 + \frac{1}{2}(15+7.2)$	=	16.80
B	C	1	$Q(B,C) = \frac{1}{2}0.5 + \frac{1}{2}(1+13.7)$	=	5.70
C	B	8	$Q(C,B) = \frac{1}{2}0 + \frac{1}{2}(8+7.2)$	=	11.20
B	C	1	$Q(B,C) = \frac{1}{2}5.7 + \frac{1}{2}(1+13.7)$	=	10.10

Yielding the final values

$$
\begin{aligned}
Q(A,B) &= 16.80 \\
Q(B,A) &= 7.20 \\
Q(B,C) &= 10.10 \\
Q(C,A) &= 13.70 \\
Q(C,B) &= 11.20
\end{aligned}
$$

As we see, the agent has already learned the non-obvious but optimal tour $A \to B \to C \to A \to ...$ since the large reward from going $C \to A$ is propagated backwards in line 7. □

4.2 Deep Q-learning

The method described above is called tabular learning, as it stores every state-action mapping in a table. This becomes infeasible as the state- and action-space grows. Deep Q-learning attempts to approximate the Q-function with a single neural network. The change is simple, instead of directly updating $Q(s,a)$ as above we compute the loss

$$loss = (Q(s_p, a_p) - R(s_p, a_p) + \max_a Q(s_{p+1}, a))$$

and use backpropagation to compute the gradient of that loss function. Then we can use gradient descent to minimize the loss.

Deep Q-learning got its first big success with the program TD-gammon by Gerald Tesauro in 1992. TD-Gammon learned to play backgammon just below the level of expert humans using Q-learning. The remarkable thing is that not only did it train only by playing against itself, but it had no hardcoded heuristics to guide it. It got a score when the game was over and no other feedback during the game.

4.2.1 Experience replay

Even though TD-Gammon was a huge success, it took a long time before similar results were seen in other games. It wasn't before 2013 that DeepMind succeeded in learning several classic Atari games using Q-learning. Their secret ingredient was *experience replay*.

Normal Q-learning is a temporal-difference learning method, which means it only learns from the timestep it just took. Experience replay keeps track of previous experiences and uses them when doing an update. To do this, we keep a trajectory of the currect episode, sample some random times from it and perform gradient descent on every remembered timestep simultaneously. Specifically, for a random sample $D = \{t_i\} \subset \mathbb{N}$ of timesteps, we compute the vector

$$G_t = \begin{cases} r_t + max_a Q(s_{t+1}, a) & \text{if } s_t \text{ is non-terminal} \\ r_t & \text{if } s_t \text{ is terminal} \end{cases}$$

for every $t \in D$ and let our loss-function be the euclidean distance from G to the vector $H_t = Q(s_t, a_t)$ for $t \in D$.

While there is no proven reason why this should aid learning, DeepMind provides three reasons: First, it utilizes the data more efficiently by using each timestep in several parameter updates which ought to speed up the learning. Second, rewards are often correlated between consecutive steps. For example, if we're trying to balance a pole, the pole is not suddenly out of balance. Thus, rewards will have a positive correlation with previous rewards. Taking samples breaks up these correlations, which reduces the variance between updates. Third, they theorize that, since the policy updates with the estimated Q-function, there could some feedback loops between the agent and the samples leading to oscillations and potentially divergence. Using experience replay could smooth out these feedbacks and break any feedback loops.

Whatever the reason, experience replay has turned out to be a very important part of successful Q-learning.

4.3 Policy gradient

Value estimation and Q-learning had the nice property that there was in some sense a concrete function we learned, the value associated with something. Policy gradient is different and exploits the backpropagation algorithm. The idea is that instead of trying to approximate something that we know, compute an error function between our current agent and some observed data, we can just specify that some behaviour was good and have the neural network optimize towards doing that again.

That was vague, so let's do some math. We have an agent with some parameters θ and a reward function $G(\tau)$ taking a trajectory τ and giving us a total reward for that trajectory. Since we want to optimize $E[G(\tau) \mid \theta]$ we can do that by taking the gradient wrt. *theta* i.e. $\nabla_\theta E[G(\tau) \mid \theta]$. This expression is difficult to compute, so let's do some rearranging:

$$
\begin{aligned}
\nabla_\theta E[G(\tau) \mid \theta] &= \nabla_\theta \sum_t P(t \mid \theta) G(\tau) \\
&= \sum_t G(\tau) \nabla_\theta P(t \mid \theta) \\
&= \sum_t G(\tau) P(t \mid \theta) \frac{\nabla_\theta P(t \mid \theta)}{P(t \mid \theta)} \\
&= \sum_t G(\tau) P(t \mid \theta) \nabla_\theta \log P(t \mid \theta) \quad \text{since } \frac{\nabla_\theta x}{x} = \nabla_\theta \log x. \\
&= E[G(\tau) \nabla_\theta \log P(t \mid \theta)]
\end{aligned}
\tag{9}
$$

Now we're in good shape. Since log is a monotonically growing function we now get, that if $G(\tau) > 0$ we can increase $E[G(\tau) \mid \theta]$ by increasing $P(t \mid \theta)$, at least locally. Similarly, if $G(\tau) < 0$, decreasing $P(T \mid \theta)$ will increase $E[G(\tau) \mid \theta]$.

Remark. The above derivation can be done more generally than we've done in 9. By assuming an arbitrary, not necessarily discrete, probability distribution of states, we could replace the sum with an integral for a more general derivation.□

Right, so how do we increase the probability of a trajectory? Intuitively, we just increase the probability of the actions the trajectory consists of, and this turns out to be sufficient. Since each action is taken independently of previous actions, we have

$$P(t \mid \theta) = P(s_0) \prod_{i=0}^{T-1} \pi_\theta(a_i \mid s_i) P(s_{i+1}, r_i \mid s_i, a_i).$$

Taking the logarithm and gradient on both sides, we get that

$$\nabla_\theta \log P(t \mid \theta) = \nabla_\theta \sum_{i=0}^{T-1} \log \pi_\theta(a_i \mid s_i)$$

and thus, by taking this together with 9 that

$$\nabla_\theta E[G(\tau) \mid \theta] = E\left[G(\tau) \nabla_\theta \sum_{i=0}^{T-1} \log \pi_\theta(a_i \mid s_i) \right]$$

and this finally gives us a good way to update our neural network: simply increase $\pi_\theta(a_i \mid s_i)$ by following the gradient of the neural network.

Now, this is great if we have direct access to a gradient descent optimizer. However, most modern machine learning frameworks are fixed to the model of minimizing an error function. The solution is very simple; to maximize $G(\tau) \sum_i \log \pi_\theta(s_i \mid s_i)$ we can minimize $-G(\tau) \sum_i \log \pi_\theta(a_i \mid s_i)$. Thus our loss could be just that.

Policy gradient methods have turned out to generally perform better than deep q-learning. They are however very difficult to work with and will often fail to converge. That is, when they do work, they outperform Q-learning methods, but getting them to work can be tricky. The next section discusses one common problem and some possible solutions.

4.3.1 Normalization & baseline

There are many challenges when doing policy gradient learning in practice. One is that rewards are often very high variance and not balanced. For example,

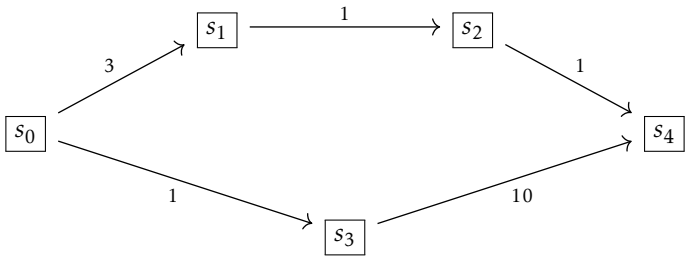


Figure 2: Example of a situation in which normalization of rewards is a bad idea.

if we only care about achieving a goal without the possibility of failure, every reward will be positive so every action will be encouraged. The reason things still work in this situation is that actions leading to higher rewards will lead to steeper gradients and be "encouraged more". In this case, we can get better performance by normalizing rewards by subtracting the mean and dividing by the standard deviation.

This method, however, is not always a good idea. Consider for example the graph in figure 2 with two possible reward trajectories: $r_1 = (1, 10)$ and $r_2 = (3, 1, 1)$. Normalized, these become $r_1' = (-0.99, 0.99)$ while $r_2' = (1.41, -0.7, -0.7)$, hence we encourage the second trajectory. This method works if we can take actions independently of previous actions but in other cases it might not. It gets better if we maintain a running average over previous trajectories, but it can still fail.

Another way of normalizing is by comparing to a baseline. We could train a value estimator alongside our policy gradient network and use the predictions from this network to normalize the observed rewards. That is, if we observe a trajectory $\tau = (s_0, a_0, r_0, s_1, a_1, r_1, \dots)$ and we have network approximating $r_p' = \mathbb{E}[r_p \mid s_p]$ we can normalize to get $\tau' = (s_0, a_0, r_0 - r_0', \dots)$. If the approximation is good, this would reduce the variance and balance rewards around zero.

Baseline normalization is what's usually used when using policy gradient methods in practice. It's simple to add if you already have some experience with neural networks and it's much more robust than naive normalization.

4.4 Advantage estimation

An alternative to normalization is *advantage estimation*. Here, we compute a *value function*[1] of each state and normalize using the value difference. Specifically, given a trajectory $\tau = (\overrightarrow{s}_t, \overrightarrow{a}_t, \overrightarrow{r}_t)$ we compute values $v_t = V(s_t)$ and new rewards $r'_t = r_t + (v_{t+1} - v_t)$. The idea is that if we get a good state, where many actions yields a high reward, we want to rescale those rewards to ensure we still pick the best and not just any of the good ones.

If we're trying to balance a pole then the advantage might be the absolute angle of the pole from vertical. When computing Gröbner bases, Dylan Peifer used two different value functions, one is the number of pairs left to reduce and the other is the total number of polynomial additions it would take to complete Buchberger's algorithm if we were using the degree strategy instead of the agent.

A variation on advantage estimation is *generalized* advantage estimation introduced in [Sch+18]. Here, we modify the computation of the return, instead of

$$G(\tau) = \sum_{t=0}^{\infty} \gamma^t r_t$$

we compute

$$G(\tau, \lambda) = (1-\lambda) \sum_{n=1}^{\infty} \lambda^{n-1} \sum_{t=0}^{n-1} \gamma^t r_t$$

Here $0 \leq \lambda \leq 1$ is a hyperparameter, controlling a trade-off between variance and bias. With $\lambda = 0$ this is the usual (unbaised) return function. Increasing λ towards 1 lowers the variance of the returns but gives a greater bias.

5 Experimental setup

Following the work of Dylan Peifer [PSH20] we use a neural network to learn pair selection in Buchberger's algorithm. After the agent selects a pair, we reduce the corresponding S-polynomial and give the agent a reward, which is -1 times the number of polynomial additions used in the reduction step. This is following the setup of [PSH20].

Also in line with [PSH20] we focus on binomial ideals (ideals generated by polynomials with exactly 2 non-constant terms) to simplify the task of representing a polynomial to a network. It is guaranteed that a Groebner basis

[1] This value function is not the same as the one in section 4.1. The clash in naming is unfortunate, but this is the terminology used in literature, so I will follow it.

n-d-s	Random	First	Queue	Stack	Degree	Normal	TrueDegree
3-10-4	349.9	286.5	295.2	1001.1	216.1	239.2	191.7
3-10-10	429.1	366.7	413.1	680.1	355.6	357.9	300.0

Table 1: Performance of standard selection strategies on 500 Gröbner bases

for an ideal generated by binomials will consist of binomials. This enables us to encode a pair of binomials in known space.

A special case of binomial ideals are *lattice ideals* which are generated by binomials in which each variable appears in only one of the terms. These have applications in optimization and integer programming, for example https://arxiv.org/pdf/math/0508287.pdf. Thus, binomial ideals are still useful, although it would interesting to explore how to represent polynomials with an arbitrary number of terms to a neural network.

5.1 Generating random ideals

To produce training data we generate a set of random binomials for each episode of the training. We parameterize the space of possible binomial ideals by three numbers: the number of variables in the polynomial ring n, the maximum total degree of any binomial d, and the number of generating polynomials s.

We generate exponent vectors as follows: sample a random integer $1 \leq r \leq d$ uniformly and then sample a vectors from $\{\mathbb{N}^n \mid \sum_i v_i \leq r\}$ uniformly. This scheme is chosen as it distributes total degree uniformly. If we had sampled from $\{\mathbb{N}^n \mid \sum_i v_i \leq d\}$ we would get more binomials of high total degree.

For the coefficients we take the coefficient field to be $\mathbb{Z}/32003\mathbb{Z}$ and take coefficients uniformly from $\mathbb{Z}/32002\mathbb{Z}^*$.

5.2 Evaulation of existing selection strategies

Let's take a look at how existing strategies perform, see table 1. The baseline ought to be picking a random pair. The easiest strategy to implement is an agent simply saying 1 every time since 1 is always an allowed action. This would be the queue strategy. This performs surprisingly well despite being very simple. It makes intuitive sense: The first added pairs are the pairs of the generating set. Especially when the generating set is small is it very likely that none of these are redundant, so it makes sense to consider dem. Compare this to the "opposite"

strategy: always picking the most recently added pair. This performs extremely badly with few generators, but less badly with more generators since then some generators ought to be redundant. Notice, that queue and stack can't be learned by the neural network. Since the network scores each pair independently it can't know which was added first.

Degree and Normal strategies both outperform the queue strategy and degree outperforms normal but more so with few generators. However, TrueDegree, which was introduced in [PSH20], outperforms every other strategy. TrueDegree was found as an approximation of the strategy learned by their neural network.

5.3 Important implementation details

	Random			Degree		
s (ER)	Additions	Selections	(ms)	Additions	Selections	(ms)
4 (ER)	344.0	86.7	(3.37)	219.4	58.4	(5.72)
10 (ER)	431.3	109.1	(4.28)	327.8	77.6	(11.54)
4 (R)	1525.8	287.0	(11.31)	731.6	147.8	(81.53)
10 (R)	1976.8	367.9	(13.35)	1354.3	224.7	(117.99)
4 (E)	226.9	83.6	(2.33)	141.1	54.6	(5.39)
10 (E)	258.7	106.1	(3.01)	194.2	79.1	(10.68)
4 ( )	664.5	243.5	(4.91)	392.9	132.6	(59.13)
10 ( )	987.5	390.9	(7.81)	594.3	213.9	(118.8)

Table 2: Performance of two selection strategies on different settings. E=Full Gebauer&Möller pair eleminiation, R=Reduce every term instead of the leading. n=3, d=10

Using the setup for evaluating the neural network, we can compare some common optimizations. The results can be seen in table 2

5.3.1 Pair elimination

Pair elimination as in Gebaur-Möller reduction has long been known to drastically improve performance. We confirm that here, the lowest numbers are achieved using pair elimination.

5.3.2 Fully reducing polynomials

The division algorithm presented in Algorithm 1 only reduces the leading term of the polynomial. However, it makes sense to reduce every term, such that no leading term in the set of polynomials divides any term of the reduced polynomial. This gives smaller polynomials (lower total degree) which should increase the chance that it divides a later polynomial. With this reasoning, it has generally been accepted as a good idea, but it might not be so clear-cut.

We see that while fully reducing the polynomials doesn't change the number of required selections much, it adds a lot of polynomial additions, which are expensive. It seems (at least in our implementation) that the number of additions correlates much better with execution time than the number of selections. This should be noted as a difference between our implementation and the one found in [PSH20] as they fully reduce polynomials and we do not.

5.4 Network architecture

A challenge when applying neural networks to this problem is the uneven size of the input. The agent needs to select a pair from an arbitrarily large list of pairs. To solve this, we try employing Q-learning and policy gradient networks. Instead of having the network select a pair, we try to score each pair and select the one with the highest score. This removes the need to encode the entire state.

For the Q-network we try to learn the function

$$Q_\pi(\langle f, g\rangle) = \mathbb{E}[G(\tau_p) \mid \langle f, g\rangle \in s_p, \pi].$$

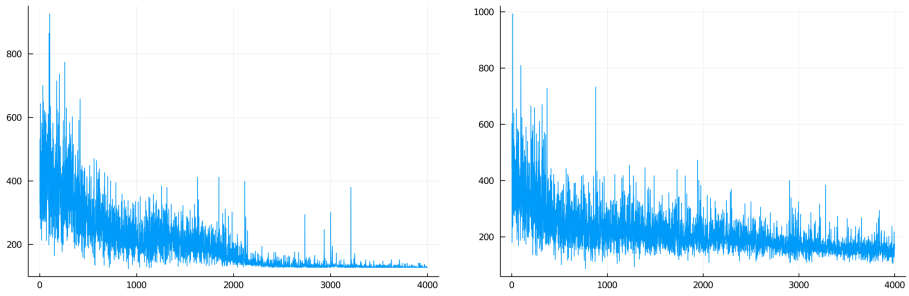
i.e. the expected number of polynomial reductions after choosing this pair.

For the policy gradient network, there is no particular function we try to learn. However, the two networks have one thing in common: since they only "see" one pair of polynomials at a time, they are very limited. They cannot exploit knowledge of what the Gröbner basis currently looks like and they cannot explicitly compare polynomials.

This means the networks don't directly learn pair selection. Instead, they learn an embedding of polynomial pairs into $\mathbb{R}$.

The encoding of a binomial pair follows the encoding given by Dylan Peifer, sending a polynomial pair $\langle c_1 x^{a_1} + c_2 x^{a_2}, c_1' x^{a_1'} + c_2' c^{a_2'}\rangle$ to the vector $[a_1 \mid a_2 \mid a_1' \mid a_2']$.

Example. Consider the situation with $n = 3$ variables and an ideal generated by $F = \{4xyz + x^2z, 19z + x^2y^5z^3, x + y\}$. This gives the pairs $P = \{(1,2),(1,3),(2,3)\}$.



(a) 3 layers trained on a single ideal.

(b) 2 layers trained on a single ideal.

Figure 3: Comparison of model sizes when training on a single ideal.

Considering each pair as a row-vector, we can represent this as the following $|P| \times 4n$ matrix:

$$\left[\begin{array}{cccccc|cccccc} 1 & 2 & 3 & 2 & 0 & 1 & 0 & 0 & 1 & 2 & 5 & 3 \\ 1 & 2 & 3 & 2 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 2 & 5 & 3 & 1 & 0 & 0 & 0 & 1 & 0 \end{array}\right]$$

□

The architecture of the neural network is given below:

$$\boxed{1 \times 4n} \xrightarrow{relu \circ (A_{64,4n} + b_{64})} \boxed{1 \times 64} \xrightarrow{(A_{1,64} + b)} \boxed{1 \times 1}$$

Here, $A_{64,4n}$ is a matrix of size $64 \times 4n$ and b_{64} is a vector of length 64. The same network architecture is used for the baseline network.

5.5 Network perfomance

After debugging many issues, we started to see results. To calibrate the shape and size of the network we trained it on a single ideal with 3 variables, maximum degree of 10 and 4 generators. Using three layers here resulted in it overfitting, which means rote learning the optimal sequence. While this may seem like a success at first glance, it's really not, since the network has learned by rote instead of an actual strategy. We can see a comparison to using two layers in figure 3

Going up the full training set, we trained the model on dynamically generated ideals. The performance turned out to match the degree strategy but did not exceed it significantly. We theorize this is because we did not implement GAE but instead went with baseline normalization. The results can be seen in table 3

Strategy	Random	Degree	Agent
Score	398.7	219.6	206.4

Table 3: Evaluation of the final model trained on random ideals generated by 4 polynomials of degree less than 10 over three variables. Result is average of 1000 random ideals.

The model was trained on 24000 ideals using an ADAM optimizer with a learning rate of 10^{-4}. We tried finetuning the model by running it for another 8000 iterations with learning rate 10^{-5} but this did not improve performance. The training process can be seen in figure 4

Figure 4: Convergence of the neural network. The graph shows a running average of polynomial additions for each network update with window size 1000.

6 Technological choices and demo

We chose to write the code for this experiment in Julia using the Flux framework for deep learning and building the ReinforcementLearning.jl project as a skeleton for reinforcement learning.

Writing the program in julia had two advantages: we could keep all the

code in a single language and we improved running time significantly over the implementation by [PSH20].

Taking a look at https://github.com/dylanpeifer/deepgroebner we see that ~ 25% of the project is written in C++. This is an implementation of the Buchberger algorithm and code supporting that and it's necessary to keep the code fast. However, a TensorFlow model is built in Python and they must use Python code to bridge between TensorFlow and the custom Buchberger code, even though both are written in C++. This incurs a cost, both on the programmer who needs to learn two languages, and on the runtime. Converting between Python and C++ is not free and since this exchange needs to happen at each selection, taking approximately 100 selections to produce a Gröbner basis, this cross-over happens about 8.000.000 times during a training run.

By keeping everything in Julia, which is a very fast language, we only need to learn a single language, and we prevent the overhead. In practice, this means that we can train the same models as they did in similar timeframes but on an Intel i5 CPU instead of a c5n.xlarge AWS instance even with an naive implementation.

7 Hitchhikers guide to the code

The code for this project can be found at https://github.com/0708andreas/Deepgroebner.jl and is mainly structured into three files.

(1) groebner.jl holds general code for working with multinomials and computing Gröbner bases. This is the code you could also find in an advanced computer algebra system.

(2) GroebnerEnv.jl holds the code for the environment for the agent to interact with.

(3) model.jl holds the setup code to create a new agent and train it.

7.1 groebner.jl

We start by defining a structure to hold a single term. A term is represented as a coefficient and an exponent vector:

```
1 struct term{N}
2     l :: GFElem{Int64}    # coefficient
```

```
    a :: NTuple{N, Int64} # exponent
end
```

Then a multinomial is simply a list of terms. This lets us express several constructions very consicely, for example multiplication:

```
(*)(t :: term, r :: term) = term(t.l * r.l, t.a .+ r.a)
(*)(t :: term, f ) = Ref(t) .* f
```

Especially computing the S-polynomial is almost a direct translation of the mathematical definition.

```
S(f, g) = let gamma = lcm(LT(f), LT(g))
    minus((gamma/LT(f))*f, (gamma/LT(g))*g)
end
```

This file also houses the multinomial division algorithm (here called mdiv instead of reduce as reduce has another meaning in Julia), a full implementation of Buchberger's algorithm, code to perform Gebauer&Möller reduction and a simple implementation of Buchberger's S-criterion:

```
function is_groebner_basis(G)
    return all([mdiv(S(G[i], G[j]), G) == [] for i in 1:length(G) for j in
    ↪  i:length(G)])
end
```

7.2 GroebnerEnv.jl

In GroebnerEnv.jl we find the GroebnerEnv structure. It is a subtype of an AbstractEnv, which is defined in the package ReinforcementLearning.jl. We make good use of this package to provide the structure of reinforcement learning.

The GroebnerEnv structure holds a parameters field containing the number of variables in the multinomials, the maximum degree of binomials and how many generators to use for each ideal. It also holds the not-yet-finished Gröbner basis G, the list of pairs to reduce P as well as the reward given for the last action, whether we've completed the Gröbner basis or not, how many selections we've performed and a random number generator.

```
mutable struct GroebnerEnv{N, R<:AbstractRNG} <: AbstractEnv
    params::GroebnerEnvParams
    G::Array{Array{term{N}, 1}, 1}
    P::Vector{NTuple{2, Array{term{N}, 1}}}
    reward::Int
    done::Bool
    t::Int
    rng::R
end
```

The interaction with the environment is as follows: the environment is initialized with a call to RLBase.reset!(env). Then the result of RLBase.state(env) is given to the agent, which picks a number a between 1 and length(P). Then we call env(a) which selects the a'th pair, reduces it, adds the result to the Gröbner basis, adds new pairs to P and updates env.reward. This process is repeated until env.done is set to true.

This file also holds a function `eval_model` which is used to evaluate the agents performance.

7.3 model.jl

The model.jl file holds the code for both a Q-learner and a policy gradient learner. If we focus on the policy gradient learner, since that's one we got to work, it's a structure holdning an approximator (a neural network) and baseline network as well as the decay factor γ and some other parameters.

The function for interacting with rhe environment looks like this:

```
function (pi::VPGPolicy)(env::AbstractEnv)
    to_dev(x) = send_to_device(device(pi.approximator), x)

    logits = env > state > to_dev |> pi.approximator

    dist = softmax(logits; dims=2)
    w = Weights(dropdims(dist; dims=1))
    action = sample(pi.rng, 1:length(w), w)

    action
end
```

It applies the approximator to `state(env)`, takes softmax on the resulting vector and uses that as a probability distribution from which to sample the action.

Next, we have an update function, which updates the agent after each episode. Condensed, the looks like this.

```
function RLBase.update!(
    pi::VPGPolicy,
    traj::ElasticSARTTrajectory,
    env::AbstractEnv,
    ::PostEpisodeStage,
)
    states = traj[:state]
    actions = traj[:action] |> Array # need to convert ElasticArray to Array, or code will fail on gpu
    gains = traj[:reward] > x -> discount_rewards(x, pi.gamma)

    for idx in Iterators.partition(shuffle(1:length(traj[:terminal])), pi.batch_size)
        S = select_last_dim(states, idx)
        A = actions[idx]
        G = gains[idx] > x -> Flux.unsqueeze(x, 1)

        gs = gradient(Flux.params(pi.baseline)) do # update baseline
            d = gains[idx] .- [maximum(pi.baseline(s)) for s in S]
            loss = mean(d .^ 2) # MSE
            Zygote.ignore() do
                pi.baseline\_loss = loss
            end
            loss
        end
        RLBase.update!(pi.baseline, gs)

        gs = gradient(Flux.params(model)) do
            log\_prob = [logsoftmax(model(s); dims=2) for s in S]
            log\_prob\_a = [log\_prob[i][A[i]] for i in 1:length(A)]
            loss = -mean(log\_prob\_a .* d)

            Zygote.ignore() do
                pi.loss = loss
            end
            loss
        end
        RLBase.update!(model, gs)
    end
```

```
end
```

The code uses julias broadcast operators, so `a .* b` is the entry-wise product of two vectors a and b. Similarly `d .^ 2` squares each entry of the vector d.

Finally, we set up the experiment:

```
function pg_experiment(  params :: GroebnerEnvParams,
                         episodes :: Int,
                         learn_rate = 10^-3,
                         gamma = 0.99f0,
                         seed = 123;
                         env = nothing)

    rng = StableRNG(seed)

    n = params.nvars
    d = params.maxdeg
    s = params.npols

    if env == nothing
        env = rand_env(params)
    end

    agent = Agent(
        policy = VPGPolicy(
            approximator = NeuralNetworkApproximator(
                model = Chain(
                    Dense(n*4, 128, relu; initW = glorot\_uniform(rng)),
                    Dense(128, 128, relu; initW = glorot\_uniform(rng)),
                    Dense(128, 1; initW = glorot\_uniform(rng))
                ),
                optimizer = ADAM(learn_rate),

            ) > cpu,
            baseline = NeuralNetworkApproximator(
                model = Chain(
                    Dense(n*4, 128, relu; initW = glorot_uniform(rng)),
                    Dense(128, 128, relu; initW = glorot_uniform(rng)),
                    Dense(128, 1; initW = glorot_uniform(rng)),
                ),
                optimizer = ADAM(learn_rate),
            ) > cpu,
            gamma = gamma,
            rng = rng,
```

```
        ),
        trajectory = ElasticSARTTrajectory(state = Vector{Array{Int, 2}} =>
        ↪  (),
                                           reward = Int => ()),
    )

    stop\_condition = StopAfterEpisode(episodes)

    total\_reward\_per\_episode = TotalRewardPerEpisode()
    time\_per\_step = TimePerStep()
    hook = ComposedHook(
        total\_reward\_per\_episode,
        time\_per\_step,
    )

    description = "# Make Gröbner bases with Policy Gradients"

    Experiment(agent, env, stop\_condition, hook, description)
end
```

and this experiment can be run in an interactive shell like this:

```
using Deepgroebner
params = GroebnerEnvParams(3, 10, 4, nothing)
e = pg_experiment(params, 120_000, 10^-4)
run(e)

eval_model(m_pg.env, strat_rand)
eval_model(m_pg.env, strat_degree)
eval_model(m_pg.env, m_pg.policy)
```

which also uses the `eval_model` function to compare the trained model against two standard strategies.

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