CertRL : **Formalizing Convergence Proofs of Value and Policy Iteration in Coq**

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Introduction - Reinforcement Learning

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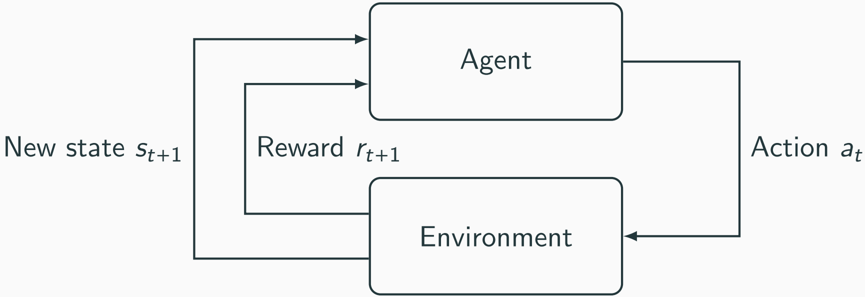
These successes motivate the use of reinforcement learning in safety-critical and correctness-critical settings.

Reinforcement Learning Theory



Reinforcement Learning Theory

This generates a *trajectory* of states, actions and (expected) rewards.

$$
\begin{aligned}
& s_0 \;\; a_0 \;\; s_1 \;\; a_1 \;\; s_2 \;\; a_2 \;\; \ldots && (1)\\
& \qquad\quad\; r_1 \qquad\quad r_2 \qquad\quad \ldots && (2)
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A *policy* π is a map from *states* to *actions*. The *long-term value* of π is defined as the discounted sum of rewards. For $0 \leq \gamma < 1$:

$$r_0 + \gamma r_1 + \gamma^2 r_2 + \gamma^3 r_3 \ldots \qquad (3)$$

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Goal: Find a policy mapping states to actions that maximizes the agent's long-term reward.

Example

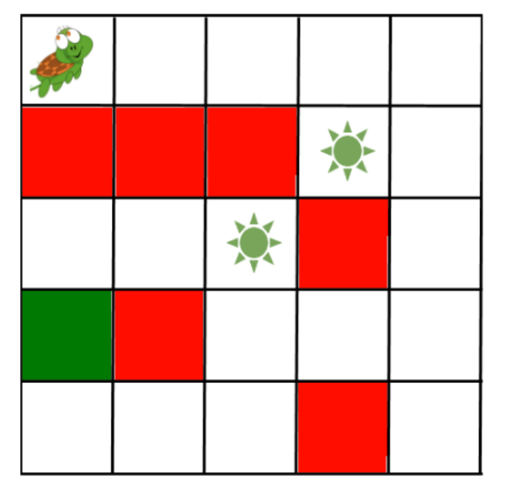

Figure 1: Turtle in a Gridworld ✿

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The primary correctness property for reinforcement learning algorithms is *convergence*: in the limit, a reinforcement learning algorithm should converge to a policy that optimizes for the long-term value.

CertRL contains a Coq formalization of *Value iteration* and *Policy iteration*. [1]

- These are canonical RL algorithms, often taught as the first reinforcement learning methods in machine learning courses.
- Their convergence proofs contain the main ingredients of a typical convergence argument for an RL algorithm.
- Their convergence is usually assumed implicitly in implementations.
- These algorithms are at the core of the *dynamic programming* paradigm.

[1] Formalization is available at https://github.com/IBM/FormalML

Markov Decision Processes ✿

```
Record MDP := mkMDP {
    (** State and action spaces. *)
    state : Type;
    act : forall s: state, Type;

    (** The state and action spaces are finite. *)
    fs :> Finite (state) ;
    fa :> forall s, Finite (act s);

    (** The state space and the fibered action spaces are
        nonempty. *)
    ne : NonEmpty (state) ;
    na : forall s, NonEmpty (act s);
```

Markov Decision Processes – continued

```
    (** Probabilistic transition structure. t(s,a,s') is the
        probability that the next state is s’
        given that you take action a in state s.
        One can also consider it to be an act-indexed
        collection of Kleisli arrows of Pmf. *)
    t : forall s : state, (act s -> Pmf state);

    (** Reward when you move to s' from s by taking action a. *)
    reward : forall s : state, (act s -> state -> R)
}
```

The set of time steps may be finite or infinite. That is, the MDP may be *finite-horizon* or *infinite-horizon*.

Markov Decision Processes - Policies

A *decision rule* ✿ is a mapping from states to actions.

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Definition dec_rule (M : MDP) := forall s : M.(state), (M.(act)) s.
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A policy of the form:

$$\pi, \pi, \pi, \ldots$$

is called a *stationary policy*.

MDP Transition Structure

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Is there an alternative to formalizing matrices and matrix multiplication?

Giry Monad

Key idea: Kleisli composition of the Giry monad recovers the Chapman-Kolmogorov formula.

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We first define the type of discrete probability measures ✿ on a type as

```
Record Pmf (A : Type) := mkPmf {
  outcomes : list (nonnegreal * A);
  sum1 : list_fst_sum outcomes = R1
}.
```

Giry Monad

We then define two basic operations:

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where $\delta_a(x) = 1$ if $a = x$ and 0 otherwise. These operations satisfy the "monad laws" making $(P, \mathrm{bind}, \mathrm{ret})$ into a monad called the Giry monad.

Kleisli Composition

Given $f : A \to P(B)$ and $g : B \to P(C)$, Kleisli composition puts f and g together to give a map $(f \rightarrowtail\!\!\!\rightarrow g) : A \to P(C)$.

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\begin{aligned}
f \rightarrowtail\!\!\!\!\rightarrow g &:= \lambda x : A, \text{bind } (f\ x)\ g && (4)\\
&= \lambda x : A, \left(\lambda c : C, \sum_{b:B} g(b)(c) * f(x)(b) \right) && (5)\\
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which is exactly the Chapman-Kolmogorov formula. So $(f \rightarrowtail g)\ x\ c$ gives the total probability of transitioning from x to c through an intermediate state in B.

Kleisli Iterates in an MDP

For a fixed decision rule π, we get a Kleisli arrow $T_\pi : S \to P(S)$ defined as $T_\pi(s) := T(s)(\pi(s))$.

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$$T_\pi^k(s_0) := (\mathrm{ret}\ s_0 \rightarrowtail\!\!\!\!\rightarrow \underbrace{T_\pi \rightarrowtail\!\!\!\!\rightarrow \ldots \rightarrowtail\!\!\!\!\rightarrow T_\pi}_{k\ \text{times}}) : P(S) \tag{7}$$

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Since this is a probability measure, we can find the expected reward at the k-th step as:

$$r_k^\pi(s) := \mathbb{E}_{T_\pi^k(s)}[r(s,\pi(s))] = \sum_{s' \in S} \left[r(s,\pi(s),s') T_\pi^k(s)(s') \right] ✿ \tag{8}$$

Long-Term Value

Let $\gamma \in \mathbb{R}, 0 \leq \gamma < 1$ be a *discount factor*, and $\pi = (\pi, \pi, \dots)$ be a stationary policy. Then, the long-term value $V_\pi : S \to \mathbb{R}$ is given by

$$V_\pi(s) = \sum_{k=0}^{\infty} \gamma^k r_k^\pi(s) \text{ ✿} \tag{9}$$

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We can prove that the long-term value satisfies the Bellman equation:

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Note that the Bellman equation says that V_π is the fixed point of the operator

$$\mathrm{B}_\pi : (S \to \mathbb{R}) \to (S \to \mathbb{R}) \tag{11}$$

$$W \mapsto r(s, \pi(s)) + \gamma \mathbb{E}_{T(s,\pi(s))} W \tag{12}$$

Optimal Long-Term Value

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This suggests that V_* also satisfies a similar Bellman equation:

$$V_*(s) = \max_{a \in A(s)} \left\{ r(s,a) + \gamma \mathbb{E}_{T(s,a)} [V_*] \right\}$$

So, V_* is the fixed point of the operator

$$\begin{aligned} \hat{\mathrm{B}} :& (S \to \mathbb{R}) \to (S \to \mathbb{R}) \\ & W \mapsto \lambda s, \max_{a \in A(s)} \left(r(s,a) + \gamma \mathbb{E}_{T(s,a)}[W] \right) \end{aligned}$$ ✿

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- The optimal policy π_* can be computed once we know V_*.
- The Banach Fixed Point theorem says that the function iterates of a contractive map converge to its fixed point.
- This gives us a recipe to compute V_* and hence also the optimal policy.

Value Iteration

Value iteration proceeds by:

1. Initialize a value function $V_0 : S \to \mathbb{R}$.
2. Define $V_{n+1} = \hat{\mathrm{B}} V_n$ for $n \geq 0$. At each stage, the following policy (greedy policy) is computed

$$\pi_n(s) \in \operatorname{argmax}_{a \in A(s)} \left(r(s, a) + \gamma \mathbb{E}_{T(s,a)}[V_n] \right)$$

Value Iteration – Pseudocode

Data:

Markov decision process (S, A, T, r)

Initial value function $V_0 = 0$

Threshold $\theta > 0$

Discount factor $0 \leq \gamma < 1$

Result: V^*, the value function for an optimal policy.

```
for n from 0 to ∞ do
    for each s ∈ S do
        V_{n+1}[s] = max_a ( r(s, a) + γ E_{T(s,a)}[V_n] )
    end
    if ∀s |V_{n+1}[s] − V_n| < θ then
        return V_{n+1}
    end
end
```

Policy Iteration

Policy iteration is a similar iterative algorithm that benefits from a more definite stopping condition. Define the *Q function* to be:

$$Q_\pi(s, a) := r(s, a) + \gamma \mathbb{E}_{T(s,a)}[V_\pi].$$

The policy iteration algorithm proceeds in the following steps:

1. Initialize the policy to π_0.
2. Policy evaluation: For $n \geq 0$, given π_n, compute V_{π_n}.
3. Policy improvement: From V_{π_n}, compute the greedy policy:

$$\pi_{n+1}(s) \in \operatorname{argmax}_{a \in A(s)} \left[Q_{\pi_n}(s, a) \right]$$

4. Check if $V_{\pi_n} = V_{\pi_{n+1}}$. If yes, stop.
5. If not, repeat (2) and (3).

Contraction Coinduction

The convergence proofs rely on the classical Banach fixed point theorem:

Theorem (Banach fixed point theorem on subsets ✿)

Let (X, d) *be a complete metric space and* ϕ *a closed nonempty subset of* X. *Let* $F : X \to X$ *be a contraction and assume that* F *preserves* ϕ. *Then* F *has a unique fixed point in* ϕ; *i.e., a point* $x^* \in X$ *such that* $\phi(x^*)$ *and* $F(x^*) = x^*$. *The fixed point of* F *is given by* $x^* = \lim_{n\to\infty} F^{(n)}(x_0)$ *where* $F^{(n)}$ *stands for the n-th iterate of the function* F.

Contraction Coinduction

We can restate this as:

$$\frac{\phi : X \to \mathsf{Prop} \quad \phi \text{ closed} \quad \exists x_0, \phi(x_0) \quad \phi(u) \to \phi(F(u))}{\phi(\mathsf{fix}\ F\ x_0)} \text{ ✿}$$

This is called Kozen's *metric coinduction*.

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This is called Kozen's *metric coinduction*.

- This proof rule helps to streamline and simplify proofs of theorems about streams and stochastic processes.
- It allows us to automatically infer that a given (closed) property holds in the limit whenever it holds *ab initio*.
- Low level $\epsilon - \delta$ arguments – typically needed to show that a given property holds of the limit – are now neatly subsumed by a single proof rule, allowing reasoning at a higher level of abstraction.

Contraction Coinduction

Our convergence proofs use a specialized version of metric coinduction called *contraction coinduction* (following Feys, Hansen and Moss) to reason about order statements concerning fixed points of contractive maps.

Theorem (Contraction coinduction)

Let X be a non-empty, partially ordered, complete metric space in which the sets $\{x | x \leq y\}$ and $\{x | x \geq z\}$ are closed for all $y, z \in X$. If $F : X \to X$ is a contraction and is order-preserving, then:

- $\forall x, F(x) \leq x \Rightarrow x^* \leq x$ *and*
- $\forall x, x \leq F(x) \Rightarrow x \leq x^*$

where x^* is the fixed point of F.

Proofs by Contraction Coinduction

Theorem 15 (Proposition 1 of [FHM18] ✿). *The greedy policy is the policy whose long-term value is the fixed point of $\hat{\mathbf{B}}$:*

$$V_{\sigma_*} = \hat{V}$$

Proof.

(1) $V_{\sigma_*} \leq \hat{V}$ follows by Theorem 14.
(2) Now have to show $\hat{V} \leq V_{\sigma_*}$. Note that we have V_{σ_*} is the fixed point of B_{σ_*} by Theorem 11.
(3) We can now apply contraction coinduction with $F = \mathbf{B}_{\sigma_*}$.
(4) The hypotheses are satisfied since by Theorem 11, the $\mathbf{B}_{\sigma_*}$ is a contraction and it is a monotone operator.
(5) The only hypothesis left to show is $\hat{V} \leq \mathbf{B}_{\sigma_*}\hat{V}$.
(6) But in fact, we have $\mathbf{B}_{\sigma_*}(\hat{V}) = \hat{V}$ by the definition of σ_*.

□

(a) English proof adapted from [FHM18].

```
Lemma exists_fixpt_policy
: forall init,
  let V'  := fixpt (bellman_max_op) in
  let pi' := greedy init in
  ltv gamma pi' = V' init.
Proof.
intros init V' pi';
eapply Rfct_le_antisym; split.
  – eapply ltv_Rfct_le_fixpt.
  – rewrite (ltv_bellman_op_fixpt _ init).
     apply contraction_coinduction_Rfct_ge'.
    + apply is_contraction_bellman_op.
    + apply bellman_op_monotone_ge.
    + unfold V', pi'.
      now rewrite greedy_argmax_is_max.
Qed.
```

(b) Coq proof ✿

Proofs by Contraction Coinduction

The idea behind the proof of the policy improvement theorem is easy to understand. Starting from (4.7), we keep expanding the q_π side with (4.6) and reapplying (4.7) until we get $v_{\pi'}(s)$:

$$
\begin{aligned}
v_\pi(s) &\le q_\pi(s, \pi'(s)) \\
&= \mathbb{E}[R_{t+1} + \gamma v_\pi(S_{t+1}) \mid S_t = s, A_t = \pi'(a)] && \text{(by (4.6))} \\
&= \mathbb{E}_{\pi'}[R_{t+1} + \gamma v_\pi(S_{t+1}) \mid S_t = s] \\
&\le \mathbb{E}_{\pi'}[R_{t+1} + \gamma q_\pi(S_{t+1}, \pi'(S_{t+1})) \mid S_t = s] \\
&= \mathbb{E}_{\pi'}[R_{t+1} + \gamma \mathbb{E}_{\pi'}[R_{t+2} + \gamma v_\pi(S_{t+2})] \mid S_t = s] \\
&= \mathbb{E}_{\pi'}\big[R_{t+1} + \gamma R_{t+2} + \gamma^2 v_\pi(S_{t+2}) \bigm| S_t = s\big] \\
&\le \mathbb{E}_{\pi'}\big[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \gamma^3 v_\pi(S_{t+3}) \bigm| S_t = s\big] \\
&\ \ \vdots \\
&\le \mathbb{E}_{\pi'}\big[R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} + \gamma^3 R_{t+4} + \cdots \bigm| S_t = s\big] \\
&= v_{\pi'}(s).
\end{aligned}
$$

Conclusions & Future Work

- Proved convergence of classical value and policy iteration algorithms in Coq.
- Also computed optimal value functions (for a possibly non-stationary policy) for a finite horizon MDP.
- Used the Giry monad and contraction coinduction to streamline and simplify proofs.
- Stochastic Approximation algorithms for model-free RL algorithms such as Q-learning etc.