Distributional analysis of sampling-based RL algorithms

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Distinguished Lecture Series
Max Planck Institute Saarbrucken
5th May 2021
1 Introduction
1 Introduction

2 Markov decision processes
Outline

1. Introduction
2. Markov decision processes
3. Distributional analysis
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2. Markov decision processes

3. Distributional analysis

4. Metrics on the space of probability distributions
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2. Markov decision processes
3. Distributional analysis
4. Metrics on the space of probability distributions
5. Algorithms are Markov chains
Basic goals in RL

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- Can we shrink it?
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- What can one observe of the behaviour?
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- What should be guaranteed?
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- What should be guaranteed?
- An equivalence relation on states so that if the equivalence classes are ’lumped’ together we cannot tell that anything has changed.
- Ideally we assume **exact** equality of real numbers.
A bit of history

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MPI, 5th May 2021 5/31
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- In the context of probability is exact equivalence reasonable?
- We say “no”. A small change in the probability distributions may result in bisimilar processes no longer being bisimilar though they may be very “close” in behaviour.
- Instead one should have a (pseudo)metric for probabilistic processes.
What are Markov decision processes?

- Markov decision processes are probabilistic versions of labelled transition systems. Labelled transition systems where the final state is governed by a probability distribution - no other indeterminacy.
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We observe the interactions and the rewards - not the internal states.
Markov decision processes: formal definition

\[(S, \mathcal{A}, \forall a \in \mathcal{A}, P^a : S \rightarrow \mathcal{D}(S), \mathcal{R} : \mathcal{A} \times S \rightarrow \mathbb{R})\]

where

\(S\) : the state space, we will take it to be a finite set.
\(\mathcal{A}\) : the actions, a finite set
\(P^a\) : the transition function; \(\mathcal{D}(S)\) denotes distributions over \(S\)
\(\mathcal{R}\) : the reward, could readily make it stochastic.
Will write \(P^a(s, C)\) for \(P^a(s)(C)\).
Bisimulation

Let $R$ be an equivalence relation. $R$ is a bisimulation if: $s R t$ if $(\forall a)$ and all equivalence classes $C$ of $R$:

- $(i)$ $R(a, s) = R(a, t)$
- $(ii)$ $P_{\text{a}}(s, C) = P_{\text{a}}(t, C)$

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- Basic pattern: immediate rewards match (initiation), stay related after the transition (induction).
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Bisimulation can be defined as the greatest fixed point of a relation transformer.
A metric-based approximate viewpoint

- Move from equality between processes to distances between processes (Jou and Smolka 1990).
A metric-based approximate viewpoint

- Move from equality between processes to distances between processes (Jou and Smolka 1990).
- Quantitative measurement of the distinction between processes.
The basic setting: metric spaces

- A pseudometric on a set $X$ is a function $d : X \times X \rightarrow \mathbb{R}^{\geq 0}$ such that
  1. $\forall x \in X$, $d(x,x) = 0$
  2. $\forall x, y \in X$, $d(x,y) = d(y,x)$
  3. $\forall x, y, z \in X$, $d(x,y) \leq d(x,z) + d(z,y)$
  4. If $d(x,y) = 0$ implies $x = y$ we say that it is a metric.

The setup: A set $M$ equipped with a metric $d$ obeying the above axioms (unlike, for example, KL-divergence which is not a metric). A metric space is complete if every Cauchy sequence has a limit point to which it converges.
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### The setup

A set $M$ equipped with a *metric* $d$ obeying the above axioms (unlike, for example, KL-divergence which is *not* a metric). A metric space is **complete** if every Cauchy sequence has a limit point to which it converges.
The grandmother of convergence arguments

If \((M, d)\) is a complete metric space and \(f : M \rightarrow M\) is a contractive function (i.e. there is a \(c \in (0, 1)\) such that for every \(x, y \in M\)
\[d(f(x), f(y)) \leq c \cdot d(x, y)\]) there is a unique \(x_0 \in M\) such that \(f(x_0) = x_0\).
Banach fixed-point theorem

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proof idea

Start anywhere and keep iterating \(f\). The sequence \(x, f(x), f(f(x)), f(f(f(x))), \ldots\) gets closer and closer because of the contractive property. Thus it has a limit (because of completeness) which is the desired fixed point.
Contractive functions and iteration

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- One has usually to do some work to show that the function of interest is contractive.
- The proof essentially says, “iterative algorithms converge.”
Bellman equations

Given an MDP $(S, A, P^a : S \rightarrow \mathcal{D}(S), \mathcal{R} : S \times A \rightarrow \mathbb{R}^{\geq 0})$
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- we define a **policy** \(\pi : S \rightarrow \mathcal{D}(A)\), a strategy for choosing an action in a state.
- The **value function** \(V^\pi : S \rightarrow \mathbb{R}\) associated with the policy \(\pi\) is given by:

\[
V^\pi(s) = \sum_{a \in A} \pi(s)(a) \left[ R(s, a) + \gamma \sum_{s' \in S} P^a(s, s') V^\pi(s') \right]
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Policy evaluation by iteration

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- The Banach fixed-point theorem says that $V_n$ converges to $V^\pi$. 
Policy iteration

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- Inductive step: evaluate $V^{\pi_n}$, then set $\pi_{n+1}$ to be equal to the greedy policy based on $V^{\pi_n}$ and repeat.
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- This converges to $\pi^*$ the optimal policy, but not by the Banach fixed point theorem.
A lattice is a partially ordered set in which every subset (even the empty set) has a least upper bound (sup) and a greatest lower bound (inf).

A monotone function from a complete lattice to itself has a least fixed point and a greatest fixed point. Actually the collection of fixed points itself is a complete lattice but that does not concern us here.
Convergence of monotone functions

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- A *monotone* function $f$ from a complete lattice $L$ to itself is a function such that for every $x, y \in L$ if $x \leq y$ then $f(x) \leq f(y)$. 

The convergence to the optimal policy follows from the monotonicity of $T_\pi$. 

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- The convergence to the optimal policy follows from the monotonicity of $T^\pi$. 


The Bellman operator for an MDP depends on details of the model.

\[ V^{n+1}(s) = (1 - \alpha)V^n(s) + \alpha(r + \gamma V^n(s')) \]

where the action \( a \) is sampled according to the policy and the reward \( r \) and next state \( s' \) are sampled from the MDP.
RL algorithms

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- Proof of convergence now involves stochastic approximation theory.
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The sequence of distributions forms a Markov chain over the space of value functions.
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Does this converge? To what limit?
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We view the algorithm as a Markov chain with the space of distributions as the state space.
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How do we reason about convergence in such a space?
Stochastic Approximation Algorithms as Markov Chains

- Algorithms like $TD(0)$ are updating random variables.
- A random variable induces a distribution so we are updating distributions.
- We view the algorithm as a Markov chain with the space of distributions as the state space.
- How do we reason about convergence in such a space?
- We need a metric on the space of probability distributions.
The basic setup

We will assume that we have an underlying metric space—the state space—and we are looking at probability distributions on top of this space.
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- I will elide all measure theory issues in this discussion, but they are there, and one cannot really work on this topic without knowing basic measure theory on metric spaces.
The total variation metric

Let $(X, d)$ be a metric space and let $P, Q$ be probability distributions defined on (the Borel sets of) $X$. 

Why I love the TV metric: easy to define, relatively easy to compute, provides all kinds of useful bounds.

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- Let \((X, d)\) be a metric space and let \(P, Q\) be probability distributions defined on (the Borel sets of) \(X\).
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- \( \kappa(P, Q) = \sup_{f \in \mathcal{F}} | \int f \, dP - \int f \, dQ | \)

But what kind of functions should we allow? Not just continuous ones. Nonexpansive or Lipschitz-1 functions:
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d(f(x), f(y)) \leq d(x, y).
\]
Such functions are always continuous but, clearly, continuous functions are not necessarily Lipschitz-1.

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It is easy to verify all the metric conditions. But this definition is only half the story.
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We can also define couplings easily between two different underlying spaces $X$ and $Y$. 
The $W$ metrics

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Kantorovich-Rubinstein duality:

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$W_p(P, Q) = \inf_{\gamma \in \mathcal{C}(P, Q)} \left[ \int_{X \times X} d(x, y)^p d\gamma \right]^{1/p}.$

Crucial point: if I find any coupling it gives an upper bound on $W_1$.

We can define a map from a metric space $\left( M, d \right)$ to the space $\left( \mathcal{P}(M), W_1 \right)$ by $x \mapsto \delta_x$. This map is an isometry.
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Bisimulation via couplings

- Recall MDP’s

\[(S, \mathcal{A}, \forall a \in \mathcal{A}, P^a : S \to \mathcal{D}(S), \mathcal{R} : \mathcal{A} \times S \to \mathbb{R})\]
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- An equivalence relation \( R \) on \( S \) is a **bisimulation** if \( sRt \) implies that \( \forall a \in \mathcal{A} \) there is a coupling \( \gamma \) of \( P^a(s) \) and \( P^a(t) \) such that the **support** of \( \gamma \) is contained in \( R \).
Markov chains on the space of functions

- In RL algorithms the update rule *usually* depends only on the current estimate and the random samples.
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It is a probabilistic mapping called a *Markov kernel*: $K : \mathbb{R}^d \times \mathcal{B} \rightarrow [0, 1]$, where $\mathcal{B}$ are the (Borel) subsets of $\mathbb{R}^d$. 

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Stochastic operators

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\mathcal{T}(V, (a_s, r_s, s'_s)_{s \in S}) = r_s \gamma V(s'_s)
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- Here \((a_s, r_s, s'_s)\) is sampled at every state \(s\).
Updates in $TD(0)$

- We will show that $TD(0)$ defines a **contractive** Markov kernel:

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Panangaden (\textsuperscript{1} University of Illinois Urbana-C}

Distributional analysis ...

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\textsuperscript{2} McGill University; \textsuperscript{3} MILA
\textsuperscript{4} DeepMind; \textsuperscript{5} GoogleBrain

MPI, 5\textsuperscript{th} May 2021 29/31
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Updates in $TD(0)$

- We will show that $TD(0)$ defines a contractive Markov kernel:
  $$W_1(K(P_1), K(P_2)) \leq (1 - \alpha + \alpha \gamma) W_1(P_1, P_2).$$

- If our coupling is given in terms of random variables $X, Y$
  $$W_1(P, Q) = \inf_{(X,Y) \in \mathcal{C}(P,Q)} \mathbb{E}[\|X - Y\|_{\infty}]$$

- Let us start with any two distributions $P, Q$ and we assume that $(X_0, Y_0)$ is the optimal coupling: $W_1(P, Q) = \mathbb{E}[\|X_0 - Y_0\|]$.

- Now we define the coupling of the next estimates by forcing them to sample the same transitions at each state: $a \sim \pi(\cdot|s), r_s \sim ...$

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- One can verify that this is a valid coupling of the updated distributions; nobody claims that this is the optimal coupling.
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However, simple inequality arguments shows that the upper bound on $W_1$ obtained with this coupling is enough to show contractivity.
The sequence of updates for $TD(0)$ converges in $W_1$ to a unique stationary distribution.
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- Deeper analysis of OPI is underway with Philip, Marc and Rosie Zhao.
Thanks!

Paper and supplement available from AISTATS 2020 website.