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7. Conclusions
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- A plethora of algorithms and techniques, but the cost depends on the size of the state space.
- Can we *learn* representations of the state space that accelerate the learning process?
Behavioural equivalence is fundamental

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- What should be guaranteed?
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- Ideally we assume exact equality of real numbers.
Cantor and the back-and-forth argument
A bit of history

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What are Markov decision processes?

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- There is a *reward* associated with each transition.
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.

There is a reward associated with each transition.

We observe the interactions and the rewards - not the internal states.
Markov decision processes: formal definition

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

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 \(S\)

\(R\): the reward, could readily make it stochastic.

Will write \(P^a(s, C)\) for \(P^a(s)(C)\).
Policies

MDP

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**Policy**

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The goal is **choose** the best policy. *We* do not know it in advance; *we* must **learn** it.
Bellman equations

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- 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)[R(s, a) + \gamma \sum_{s' \in S} P^a(s, s') V^\pi(s')]
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Given an MDP \((S, A, P^a : S \rightarrow \mathcal{D}(S), \mathcal{R} : S \times A \rightarrow \mathbb{R}^\geq 0)\), 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:

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T^\pi(V^\pi) = V^\pi.
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Given a policy $\pi$ we have the associated Bellman operator $T^\pi$ on the space of value functions.
Policy evaluation by iteration

- Given a policy $\pi$ we have the associated Bellman operator $T^\pi$ on the space of value functions.
- If $V^\pi$ is the value function we write $V_n$ for its $n$th iterate:
  \[ V_{n+1} = T^\pi(V_n). \]
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- If $V^\pi$ is the value function we write $V_n$ for its $n$th iterate:
  $$V_{n+1} = T^\pi(V_n).$$
- The Banach fixed-point theorem says that $V_n$ converges to $V^\pi$. 
Policy iteration

- Start with some policy $\pi_0$ and compute $V^{\pi_0}$
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- Start with some policy $\pi_0$ and compute $V^{\pi_0}$
- 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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- 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.
- This converges to $\pi^*$ the optimal policy, but not by the Banach fixed point theorem.
For large state spaces, learning value functions $S \times A \rightarrow \mathbb{R}$ is not feasible. Representation learning means learning such a $\phi$.

The elements of $M$ are the “features” that are chosen. They can be based on any kind of knowledge or experience about the task at hand.
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Representation learning means learning such a $\phi$. 

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**Panangaden**

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**Representation learning**

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Bisimulation

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

1. $R(a, s) = R(a, t)$
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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.
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 basic setting: metric spaces

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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.
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- We will then look at ways to define a metric on the space of probability distributions.
- It should be, somehow, related to the metric of the underlying space.
- 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 Kantorovitch metric

- What is the observable aspect of a probability distribution?

\[ \kappa(P, Q) = \sup_{f \in \phi} \left| \int f \, dP - \int f \, dQ \right| \]

But what kind of functions should we allow? Not just continuous ones. Nonexpansive or Lipschitz-1 functions:

\[ d(f(x), f(y)) \leq d(x, y) \]

Such functions are always continuous but, clearly, continuous functions are not necessarily Lipschitz-1.

\[ \kappa(P, Q) = \sup_{f \in \text{Lip}^1} \left| \int f \, dP - \int f \, dQ \right| \]

It is easy to verify all the metric conditions. But this definition is only half the story.
What is the observable aspect of a probability distribution?
- Expectation values.
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- It is easy to verify all the metric conditions.

- But this definition is only half the story.
How to relate two distributions? Think of a distribution as a pile of sand.
Couplings

- How to relate two distributions? Think of a distribution as a pile of sand.
- We need to move some sand around to make the pile $P$ look like $Q$. 

There are many different ways to do it. Each way is a "transport plan." A coupling of two distributions $P$, $Q$ defined on $X$ is a joint distribution $\gamma$ on $X \times X$ such that the marginals of $\gamma$ are $P$ and $Q$.

There is always the independent coupling: $\gamma(A \times B) = P(A)Q(B)$.

But there are many others: the convex combinations of couplings are couplings.

We write $C(P,Q)$ for the set of couplings of $P$ and $Q$.

We can also define a coupling to be a pair of random variables $R$, $S$ with distributions $P$, $Q$ respectively.

We can also define couplings easily between two different underlying spaces $X$ and $Y$. 

Couplings

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Panangaden

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Representation learning

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- If we measure the cost by a metric $d$ we get

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\text{cost} = \int_{X \times X} d(x, y) \, d\gamma
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We define a metric:

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W_1(P, Q) = \inf_{\gamma \in \mathcal{C}(P, Q)} \int_{X \times X} d(x, y) \, d\gamma.
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Kantorovich-Rubinstein duality:

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

We can define a map from a metric space $(M, d)$ to the space $(\mathbb{P}(M), W_1)$ by $x \mapsto \delta_x$. This map is an isometry.
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Recall MDP’s

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

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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** $\omega$ of $P^a(s)$ and $P^a(t)$ such that the **support** of $\omega$ is contained in $R$. 

Computing the bisimulation metric

Let $\mathcal{M}$ be the space of $1$-bounded pseudometrics over $S$, ordered by $d_1 \leq d_2$ if $\forall x, y; d_2(x, y) \leq d_1(x, y)$. 

This is a complete lattice.

We define $T_K : \mathcal{M} \to \mathcal{M}$ by:

$$T_K(d)(x, y) = \max \left[ |R(x, a) - R(y, a)| + \gamma Wd(P_a(x), P_a(y)) \right]$$

This is a monotone function on $\mathcal{M}$.

We can find the bisimulation as the fixed point of $T_K$ by iteration:

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An important bound proved by Ferns et al.

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Too high in practice!
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Unfortunately it is not easy to obtain these samples and in particular most methods used give biased samples.
Non-optimal policies

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- We often need $V^\pi$ for non-optimal policies and the bismulation metric does not help us bound it.
The MICo distance

- MICo: matching under independent couplings.

Do not try to find the optimal coupling use a simple known coupling, the independent coupling. We define a new update $T_{MICo}$:

$$ T_{MICo} : S \times S - \rightarrow S \times S $$

instead of $T_K$.

We define $r_\pi(x) := \mathbb{E}_{a \sim \pi(s)}[R(x, a)]$ and $P_\pi(x) = \sum_a \pi(x)(a) P(a|x)$. $(T_{MICo}(x, y) = |r_\pi(x) - r_\pi(y)| + \gamma \mathbb{E}_{x' \sim P_\pi(x), y' \sim P_\pi(y)}[U(x', y')]$. If we use the $L_\infty$ norm, $T_{MICo}$ is a contraction so we have a fixed point by Banach's fixed point theorem. Call the fixed point $U_\pi$.

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- $|V^\pi(x) - V^\pi(y)| \leq U^{\pi}(x, y)$. 

A new type of distance

Diffuse metric

1. \[ d(x, y) \geq 0 \]
2. \[ d(x, y) = d(y, x) \]
3. \[ d(x, y) \leq d(x, z) + d(z, y) \]
4. Do not require \[ d(x, x) = 0 \]

Panangaden (1 Google Brain, Montreal 2 McGill University 3 Montreal Institute of Learning Algorithms (Mila) 4 DeepMind, London)
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What is MICO?

Similar to, but not the same as, partial metrics (Matthews) or weak partial pseudometrics (Heckmann). They require stronger conditions than our triangle and they can then extract a real metric and something like a “norm”. Our examples violate their conditions.
What is MICo?

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MICo distance is a diffuse metric.
Nearly all machine learning algorithms are optimization algorithms.

For details read https://psc-g.github.io/posts/research/rl/mico/
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One often introduces extra terms into the objective function that push the solution in a desired direction.
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We defined a loss term based on the fixed point of the MICo update operator.
MICo loss

- Nearly all machine learning algorithms are optimization algorithms.
- One often introduces extra terms into the objective function that push the solution in a desired direction.
- We defined a loss term based on the fixed point of the MICo update operator.
- We assume a value-based agent learning as estimate based on two function approximators $\psi, \phi$ with their own sets of parameters.
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We defined a loss term based on the fixed point of the MICo update operator.
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We then define a loss term based on the MICo distance.
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For details read [https://psc-g.github.io/posts/research/rl/mico/](https://psc-g.github.io/posts/research/rl/mico/)
Experimental setup

\[ \mathcal{L}_{TD}(\psi(\phi(x))) \]

\[ \mathcal{L}_{MICo}(\phi(x), \phi(y)) \]

\[ \mathcal{L}_{TD}(\psi(\phi(y))) \]

\[ \psi(\phi(x)) \]

\[ \psi(\phi(y)) \]

\[ \phi(x) \]

\[ \phi(y) \]
Experiments

- Added the MICo loss term to a variety of existing agents: all those available in the Dopamine Library; 5 in all.
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- Added the MICO loss term to a variety of existing agents: all those available in the Dopamine Library; 5 in all.
- Hyperparameters settings were taken from the Library.
- The learning algorithms tried to learn good strategies for Atari games. We tried each agent with and without the MICO loss term on 60 different Atari games.
Results for Rainbow

*Human normalized Rainbow + MICO improvement over Rainbow (30.73 avg. improvement, 41/60 games improved)*

![Improvement Graph](image-url)
Results for DQN

Human normalized DQN + MiCo improvement over DQN (26.51 avg. improvement, 41/60 games improved)
Conclusions

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- Variations of the concept of metric seem to be important.
- Connections to Reproducing Kernel Hilbert Space theory is being explored.