

# Exploration in Deep Reinforcement Learning

**Matteo Pirotta**

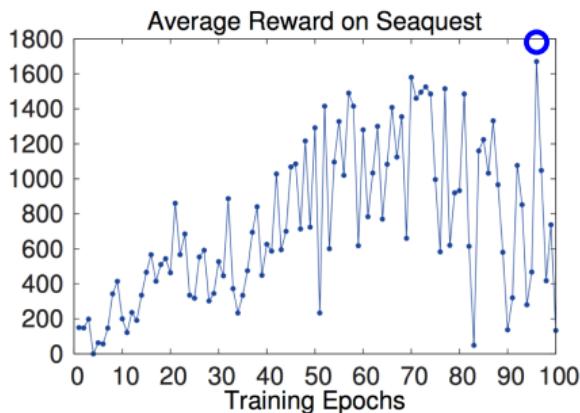
Facebook AI Research

ANITI's Reinforcement Learning Virtual School (RLVS-ANITI)

April 2, 2021

# Why Talking About Exploration-Exploitation?

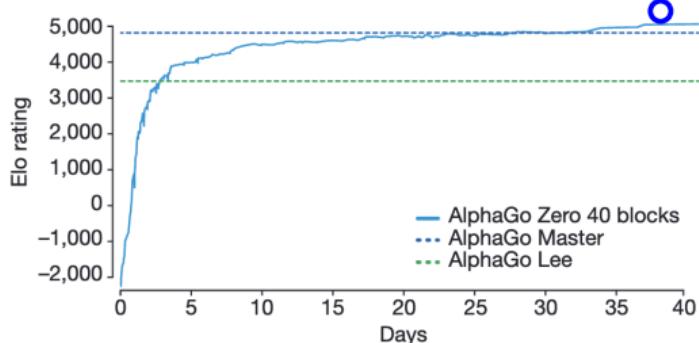
*Superhuman performance*



Mnih et al. [2015]

*10 million frames*

*Beating world champion*



Silver et al. [2016]

*4.9 million games*

Even best RL algorithms are very **sample inefficient**

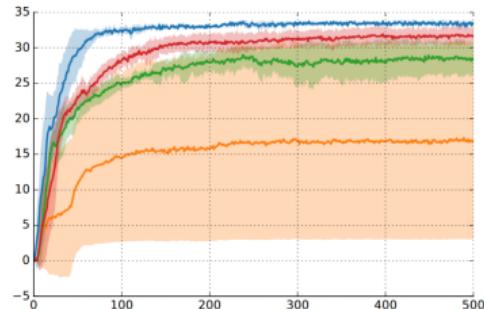
# Efficiency

- Sample efficiency
- Computational efficiency

# Why do we need exploration?

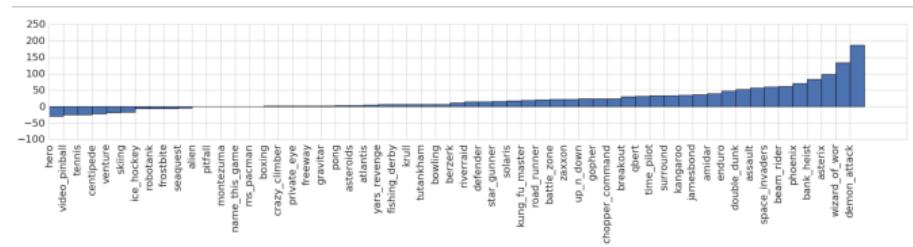
Better exploration may significantly **improve the sample efficiency**

*\*Optimism in face of uncertainty*



Tang et al. [2017]

*\*Thompson sampling*



Fortunato et al. [2018]

⚠ All these methods use function approximation (e.g., deepNN)

# Exploration in Deep RL: Outline

## 1 Introduction

- Review of Exploration Principles
- Exploration Issues in Deep RL

## 2 Exploration Bonus

## 3 Memory-Based Exploration

- Episodic Memory
- Goal-Oriented Exploration

## 4 Randomized Exploration

These slides and additional material on [my website](#) and

<https://rlgammazero.github.io/>

## 5 Conclusions

# Super-fast intro to MDPs

Only for notation

*Markov decision process* (MDP) is a tuple  $M = \langle \mathcal{S}, \mathcal{A}, r, p \rangle$

- State space  $\mathcal{S}$
- Action space  $\mathcal{A}$
- Transition function  $p(\cdot|s, a) \in \Delta(\mathcal{S})$
- Reward distribution with expectation  $r(s, a)$

*Policy*:  $\pi : \mathcal{S} \rightarrow \Delta(\mathcal{A})$

*Value functions*:

$$Q^\pi(s, a) = \mathbb{E} \left[ \sum_{t=1}^{\infty} \gamma^{t-1} r_t | s_0 = s, a_0 = a \right]$$

$$V^\pi(s) = \mathbb{E}_{a \sim \pi(s)} [Q^\pi(s, a)]$$

*Optimal policy*:  $\pi^* = \arg \max_{\pi} \{V^\pi\}$

# Online Learning Problem

---

**Input:**  $\mathcal{S}, \mathcal{A}, \pi_h, p_n$

Initialize  $Q_1(s, a) = 0$ ,  $\mathcal{D}_1 = \emptyset$

**for**  $k = 1, \dots, K$  **do** // episodes

    Define  $\pi_k$  based on  $Q_k$

**for**  $h = 1, \dots, H$  **do**

        Execute  $a_{hk} = \pi_k(s_{hk})$

        Observe  $r_{hk}$  and  $s_{h+1,k}$

**end**

    Add trajectory  $(s_{hk}, a_{hk}, r_{hk})_{h \geq 1}$  to  $\mathcal{D}_{k+1}$

    Compute  $Q_{k+1}$  from  $\mathcal{D}_{k+1}$

**end**

---

# What is Wrong with Q-learning with $\epsilon$ -greedy?

- $\epsilon$ -greedy strategy

$$a_k = \begin{cases} \arg \max_{a \in \mathcal{A}} Q_k(s_k, a) & \text{w.p. } 1 - \epsilon_k, \\ \mathcal{U}(\mathcal{A}) & \text{otherwise.} \end{cases}$$

- Q-learning update

$$Q_{k+1}(s_k, a_k) = (1 - \alpha_k)Q_k(s_k, a_k) + \alpha_k \left( r_k + \max_{a' \in \mathcal{A}} Q_{h+1,k}(s_{k+1}, a') \right)$$

$*H = 1$

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 The exploration strategy relies on **biased** estimates  $Q_k$

\* $H = 1$

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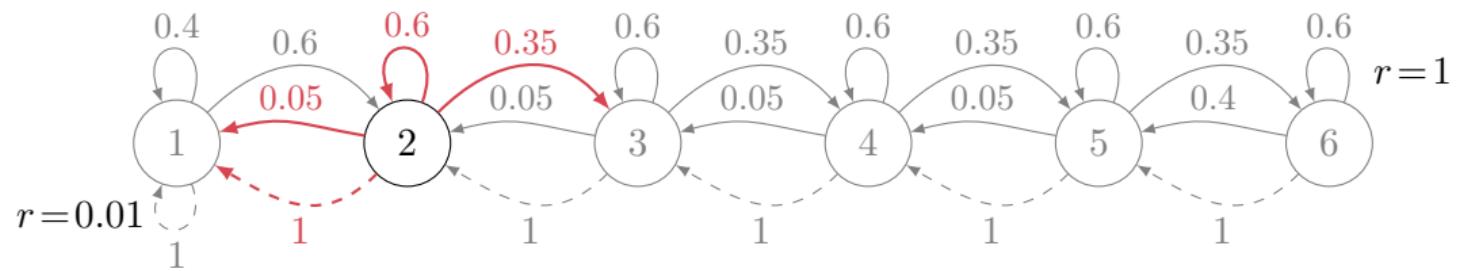
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- 👎 The exploration strategy relies on **biased** estimates  $Q_k$
- 👎 Samples are used **once**
- 👎 **Dithering effect:** exploration is not effective in covering the state space
- 👎 **Policy shift:** the policy changes at each step

$*H = 1$

# River Swim: Markov Decision Processes

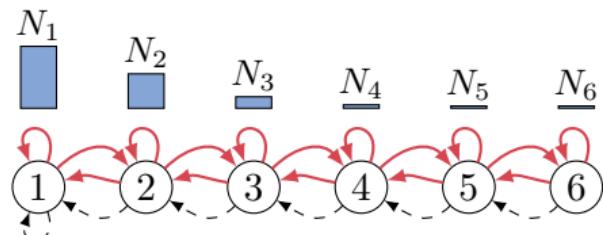
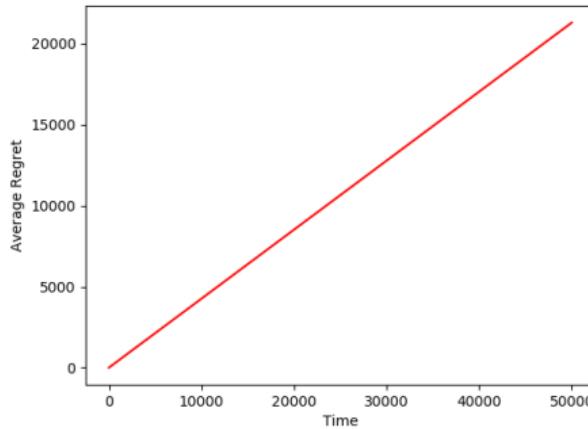
Strehl and Littman [2008]



- $\mathcal{S} = \{1, 2, 3, 4, 5, 6\}$ ,  $\mathcal{A} = \{L, R\}$
- $\pi_L(s) = L$ ,  $\pi_R(s) = R$

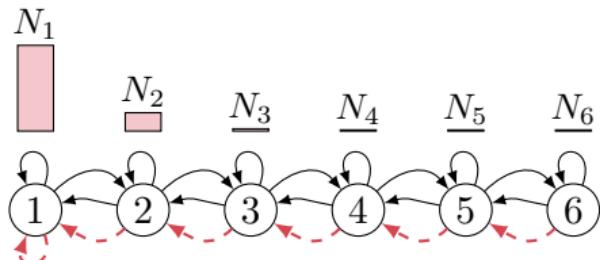
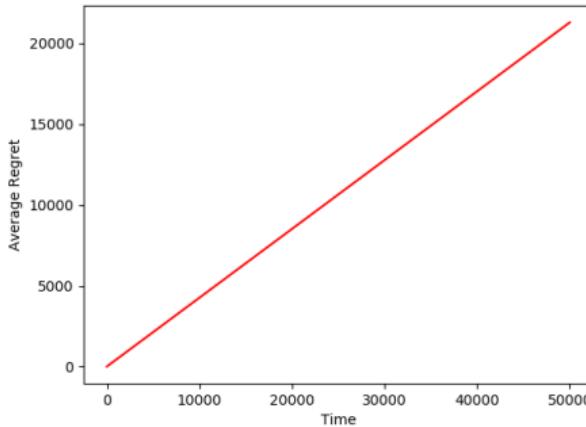
# River Swim: Q-learning w\ \epsilon-greedy Exploration

■  $\epsilon_t = 1.0$



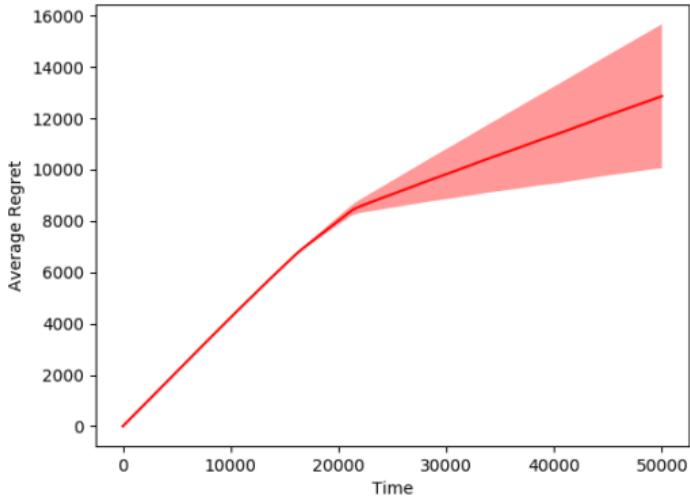
# River Swim: Q-learning w\ \epsilon-greedy Exploration

- $\epsilon_t = 1.0$
- $\epsilon_t = 0.5$



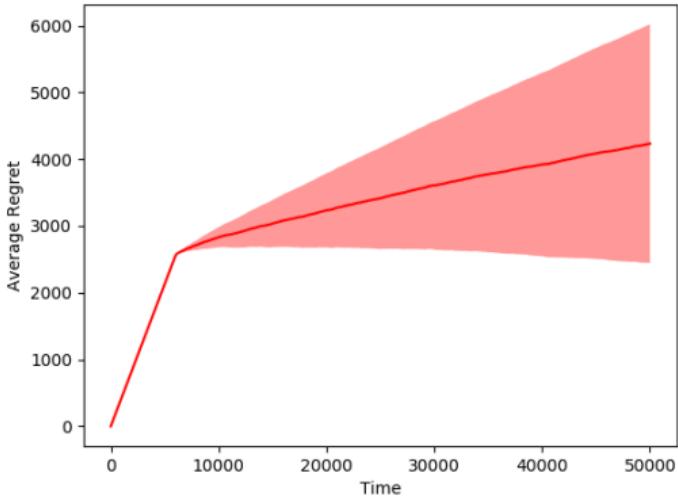
# River Swim: Q-learning w\ \epsilon-greedy Exploration

- $\epsilon_t = 1.0$
- $\epsilon_t = 0.5$
- $\epsilon_t = \frac{\epsilon_0}{(N(s_t) - 1000)^{2/3}}$



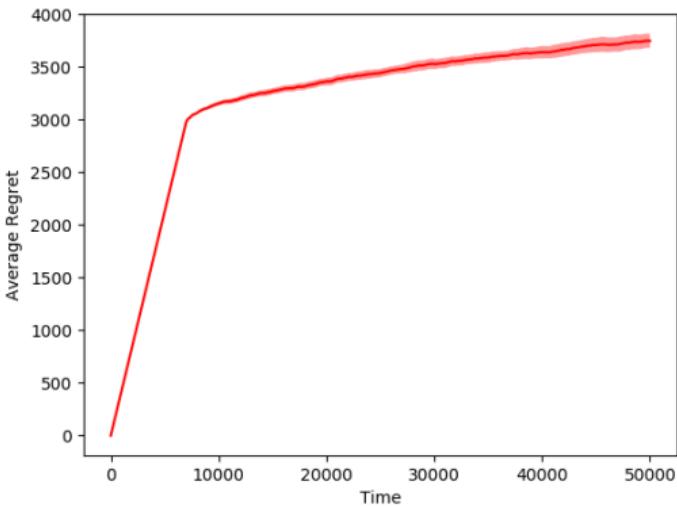
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- $\epsilon_t = \frac{\epsilon_0}{(N(s_t) - 1000)^{2/3}}$
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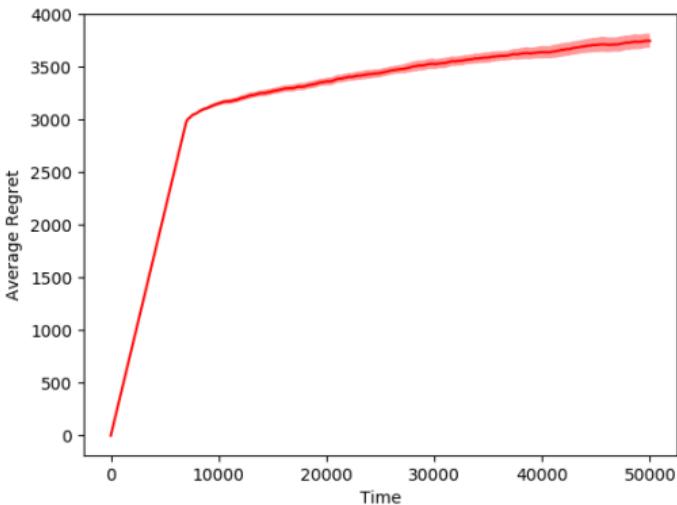
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# River Swim: Q-learning w\ \epsilon-greedy Exploration

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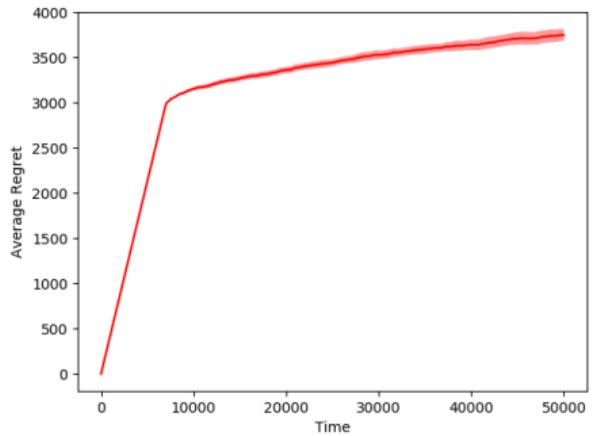


Tuning the  $\epsilon$  schedule is **difficult and problem dependent**

# River Swim: Q-learning w\ \epsilon-greedy Exploration

Main drawbacks of Q-learning with  $\epsilon$ -greedy

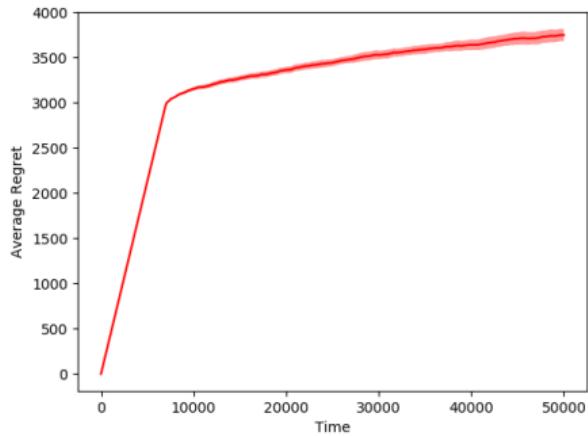
- $\epsilon$ -greedy performs *undirected* exploration
  - *Inefficient use* of samples
- 👎 **Regret:**  $\Omega\left(\min\{T, A^{H/2}\}\right)$  [Jin et al., 2018]



# River Swim: Q-learning w\ \epsilon-greedy Exploration

Main drawbacks of Q-learning with  $\epsilon$ -greedy

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  - *Inefficient use* of samples
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Uncertainty-driven exploration-exploitation

# What do we know?

In *tabular MDPs* (finite state and actions), we have several approaches for exploration

[Jaksch et al., 2010, Zhang and Ji, 2019, Fruit et al., 2018b,a, 2020, Qian et al., 2019, Wei et al., 2020, Hao et al., 2021, Gong and Wang, 2020, Abb, 2019, Azar et al., 2017, Dann et al., 2017, Zanette and Brunskill, 2018, Jin et al., 2018, Zanette and Brunskill, 2019, Zhang et al., 2020, Menard et al., 2021, Neu and Pike-Burke, 2020, Efroni et al., 2019, Cai et al., 2020, Shani et al., 2020]

and we have *efficient optimal algorithm* (i.e., matching the statistical lower-bound)

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# Exploration in Tabular MDPs

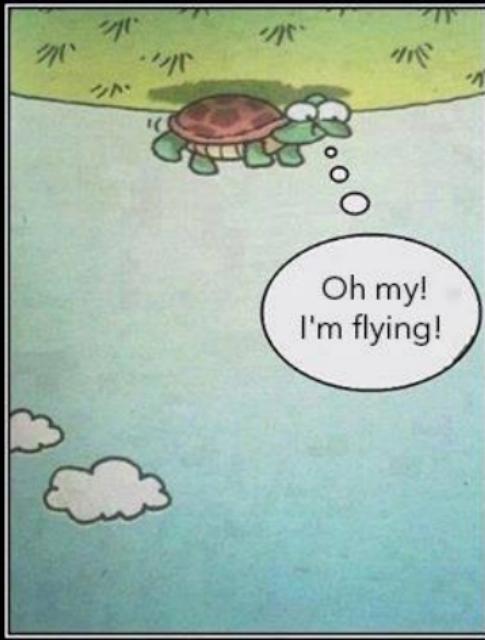
## The Four Ingredients Recipe

- 1 Build accurate estimators
- 2 Evaluate the uncertainty of the prediction
- 3 Define a mechanism to combine estimation and uncertainty
- 4 Execute the best policy

*Principles:*

- Optimism in face of uncertainty (i.e., upper-confidence bounds)
- Thompson Sampling

# The Optimism Principle: Intuition



OPTIMISM  
It's the best way to see life.

# Optimism

At each episode  $k$ , we must use an *estimate*  $Q_k$  such that

$$\forall (s, a), \quad Q_k(s, a) \geq Q^*(s, a) \quad (\text{whp})$$

to compute the policy (since we *don't know r and p*):

$$a_{hk} = \arg \max_a Q_k(s_{hk}, a)$$

$$*Q^*(s, a) = \max_a \left\{ r(s, a) + \sum_{s'} p(s'|s, a) \max_{a'} Q^*(s', a') \right\}, \text{ } p \text{ and } r \text{ are unknown}$$

# Optimism: Model Optimism and Value Optimism

## *Optimism in model space*

construct a confidence set around  $p$  and  $r$  and **jointly** optimize over models and policies

## *Optimism in value space*

construct upper confidence bounds directly on the optimal value function  $V^*$

*Both approaches lead to optimism*  $Q_k(s, a) \geq Q^*(s, a)$

# Optimism: *Model Optimism*

- Build *confidence set* around empirical transitions such that

$$D(p(\cdot|s, a), \hat{p}_k(\cdot|s, a)) \leq \beta_k^p(s, a)$$

$$|r(s, a) - \hat{r}_k(s, a)| \leq \beta_k^r(s, a)$$

and, with high probability

$$p(s, a) \in B_k^p(s, a), \quad r(s, a) \in B_k^r(s, a)$$

- Compute optimistic policy and model

$$(M_k, \pi_k) \in \arg \max_{M=(p,r) \in (B^p, B^r), \pi} \left\{ V_{1,\textcolor{red}{M}}^{\pi} \right\}$$

*Example:* [Jaksch et al., 2010]

Weissman inequality implies that  $D = \|\cdot\|_1$

and  $\beta_{hk}^p(s, a) \approx C\sqrt{S/N_k(s, a)}$

Hoeffding for reward leads to  $\beta_k^r(s, a) \approx C\sqrt{1/N_k(s, a)}$

$N_k(s, a) = \# \text{ visits to } (s, a) \text{ so far (before } k)$

$$\hat{p}_k(s'|s, a) = \frac{N_k(s, a, s')}{N_k(s, a)}$$

$$\hat{r}_k(s, a) = \frac{1}{N_k(s, a)} \sum_{t=1}^k r_t \cdot \delta_{sat}$$

# Optimism: *Value Optimism*

- Compute exploration bonus  $b_k(s, a)$

- Update estimated  $Q^*$

- *Model-based*

e.g., value iteration on  $\overline{M}_k = (\mathcal{S}, \mathcal{A}, \hat{r}_k + b_k, \hat{p}_k)$

- *Model-free*

e.g., Q-learning update

$$Q_{k+1}(s_k, a_k) = (1 - \alpha_k)Q_k(s_k, a_k) + \alpha_k \left( \hat{r}_k + b_k + \max_{a' \in \mathcal{A}} Q_{h+1, k}(s_{k+1}, a') \right)$$

*Example:* [Azar et al., 2017]

$$b_k(s, a) = C \sqrt{1/N_k(s, a)}$$

$$\begin{aligned} N_k(s, a) &= \# \text{ visits to } (s, a) \text{ so far} \\ &\text{(before } k\text{)} \end{aligned}$$

$$\hat{p}_k(s' | s, a) = \frac{N_k(s, a, s')}{N_k(s, a)}$$

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# Thompson Sampling

- Keeps track of a *belief over models or Q-values*

$$\mathbb{P}(\theta|\mathcal{D}_{k-1})$$

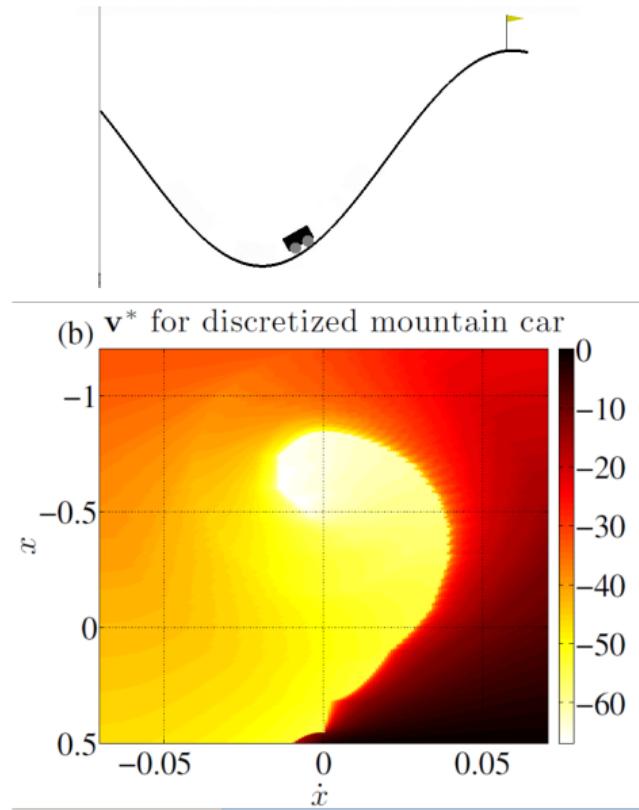
- *Samples* a plausible realization from the *posterior*

$$\theta_k \sim \mathbb{P}(\cdot|\mathcal{D})$$

- *Acts* with such realization (i.e., believes  $\theta_k$  is the true value)

*What happens if we move to general problems (i.e., non tabular)?*

# Example: Mountain Car



# Function Approximation

Theory of exploration has focused on (with several structural assumptions)

- Linear function approximation
- Kernel approximation
- General function approximation
- Neural exploration

💡 *Optimism is still a key ingredient!*

👎 *Still not very practical!*

# General Function Approximation

The agent is given a *function class*

$$\mathcal{F} : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$$

to *approximate  $Q^*$*

Idea:

- Build confidence interval  $\mathcal{B}$  of plausible  $Q^*$
- Optimistic planning, i.e., pick the best in the confidence set

⚠ *Extremely challenging without further assumptions!*  
*e.g., realizability and completeness*

*next practical algorithms!*

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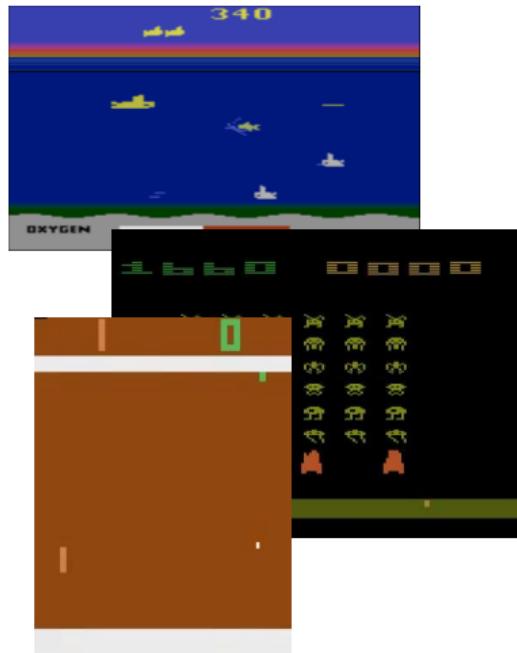
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these are easy



this is hard, *almost* impossible

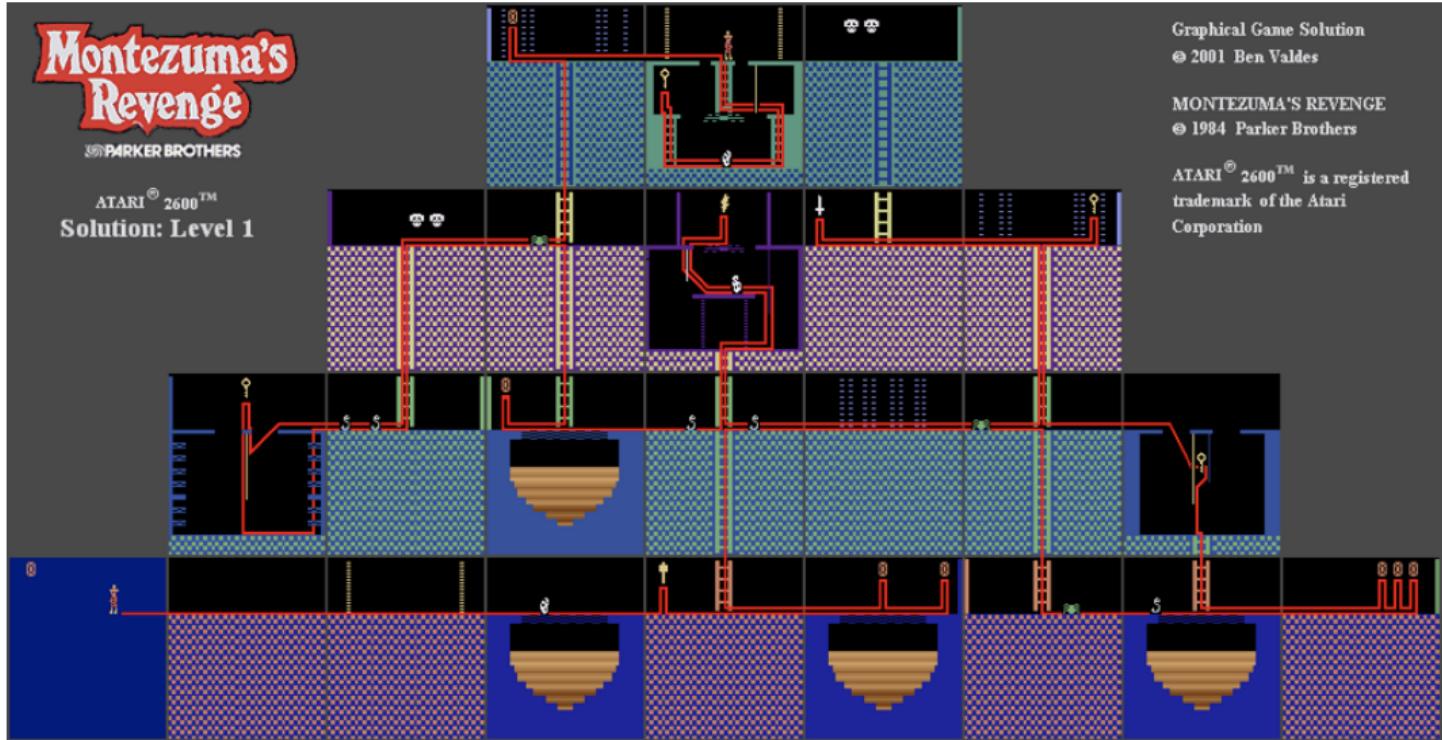


# Why?

Random exploration sometimes work!  
PONG GIF

Montezuma with random actions!  
[Link](#)

# Montezuma's Revenge: Level 1



# Exploration Issues

## 1 Discovery

Unknown State Space, Partial Observability, Sparse Reward

## 2 Controllability

Predictability, Learnability

## 3 Representation Learning

... and probably more!

# Exploration Issues

## 1 Discovery

Unknown State Space, Partial Observability, Sparse Reward

## 2 *Controllability*

Predictability, Learnability

## 3 Representation Learning

... and probably more!

# Controllability

*In front of a screen full of white noise conveying a lot of information and “novelty” and “surprise” in the traditional sense of Boltzmann and Shannon, however, it will experience highly unpredictable and fundamentally incompressible data – [Schmidhuber, 2010]*

# Controllability

*In front of a screen full of white noise conveying a lot of information and “novelty” and “surprise” in the traditional sense of Boltzmann and Shannon, however, it will experience highly unpredictable and fundamentally incompressible data – [Schmidhuber, 2010]*

- States can be interesting due to an intrinsic variability
- Agent may get trapped by these states



video1 video2

*Are these states relevant? Probably not if they are uncontrollable and/or unpredictable*

## Benchmark: Atari 57



(img for Deepmind blog)

# Equally difficult? *No*

## 1 Long-term credit assignment



Skiing



Solaris

## 2 Exploration



Montezuma's Revenge



Pitfall

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# Idea

- ① Augment the reward with an additional (vanishing) reward term

$$r_t = \underbrace{r_t^e}_{\text{extrinsic reward (standard)}} + \beta \underbrace{r_t^i}_{\text{intrinsic}}$$

- $r^e$ : *extrinsic reward* (*task reward*)
- $r^i$ : *intrinsic reward* (*exploration bonus*)

- ② Run any algorithm using the new reward  $r_t^+$

# Typical Objective

- Discover novel (or controllable) states
  - encourage the agent to discover novel information
- Improve knowledge about the environment
  - encourage the agent to perform actions to reduce uncertainty in predicting model evolution
- ...

☞ Intrinsic reward is often inspired by psychology (*intrinsic motivation*), e.g., curiosity driven exploration (*self-supervised*) when  $r_t^e = 0$

# *Arbitrary* 😊 classification

- Count-based bonus
- Prediction-based bonus
- Bonus based on Auxiliary Task

## Count-based Exploration

# Count-based Exploration

## General Scheme

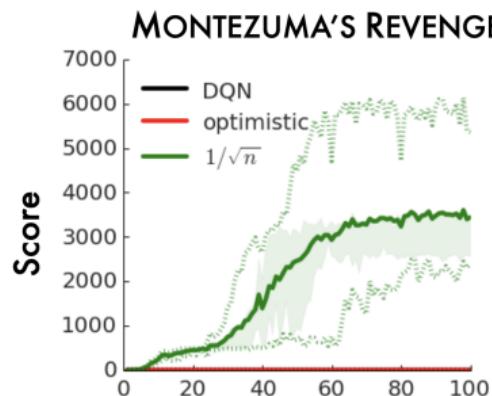
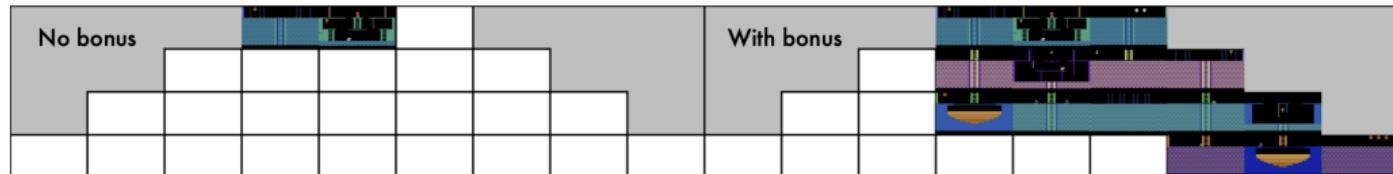
- 1 Estimate a “proxy” for the *number of visits*  $\tilde{N}(s_t)$
- 2 Add an *exploration bonus* to the rewards

$$\tilde{r}_t^+ = r_t + \beta_t \sqrt{\frac{1}{\tilde{N}(s_t)}}$$

- 3 Run *any DeepRL* algorithm on  $\mathcal{D}_t = \{(s_i, a_i, \tilde{r}_i^+, s_{i+1})\}$

  $r_t^e \approx \sqrt{1/\tilde{N}(s_t)}$  is inspired by theory (recall UCB)

# Does it work?



# Count by Density Estimation

[Bellemare et al., 2016, Ostrovski et al., 2017]

- Density estimation over a countable set  $\mathcal{X}$  (i.e., *observation space*)

$$\rho_n(x) = \rho(x|x_1, \dots, x_n) \approx \mathbb{P}[X_{n+1} = x|x_1, \dots, x_n]$$

- Recording probability

$$\rho'_n(x) = \rho(x|x_1, \dots, x_n, \textcolor{red}{x}) \approx \mathbb{P}[X_{n+2} = x|x_1, \dots, x_n, X_{n+1} = x]$$

*Pseudo count*  $\tilde{N}_n(x)$  to imitate empirical count s.t.

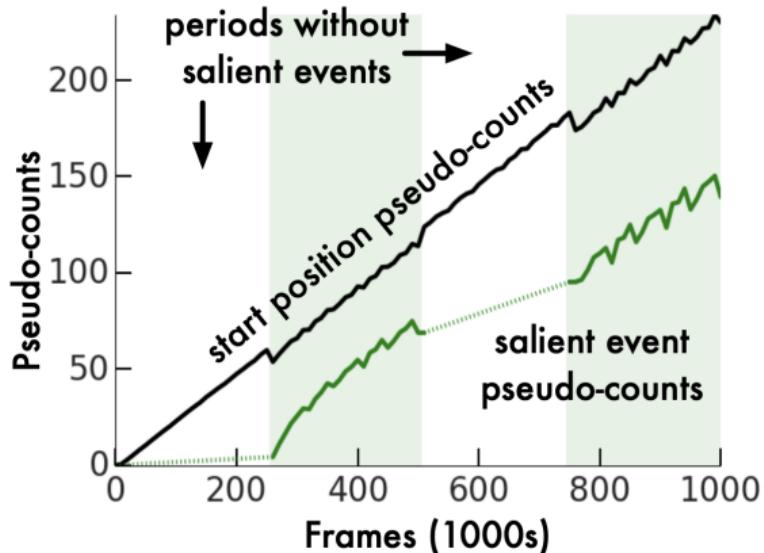
probability of  $x$  after observing a new occurrence of  $x$

$$\frac{\tilde{N}_n(x)}{\tilde{n}} = \rho_n(x) \leq \rho'_n(x) = \frac{\tilde{N}_n(x) + 1}{\tilde{n} + 1}$$

$$\implies \tilde{N}_n(x) = \frac{\rho_n(x)(1 - \rho'_n(x))}{\rho'_n(x) - \rho_n(x)} = \tilde{n}\rho_n(x)$$

# Count-based Exploration

[Bellemare et al., 2016, Ostrovski et al., 2017]



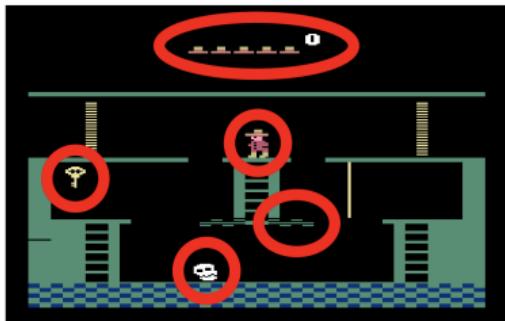
- thumb-up Any density estimation algorithm (accurate for images)  
e.g., GMM or CTS or PixelCNN

# Count-based Exploration

Bellemare et al. [2016], Ostrovski et al. [2017]

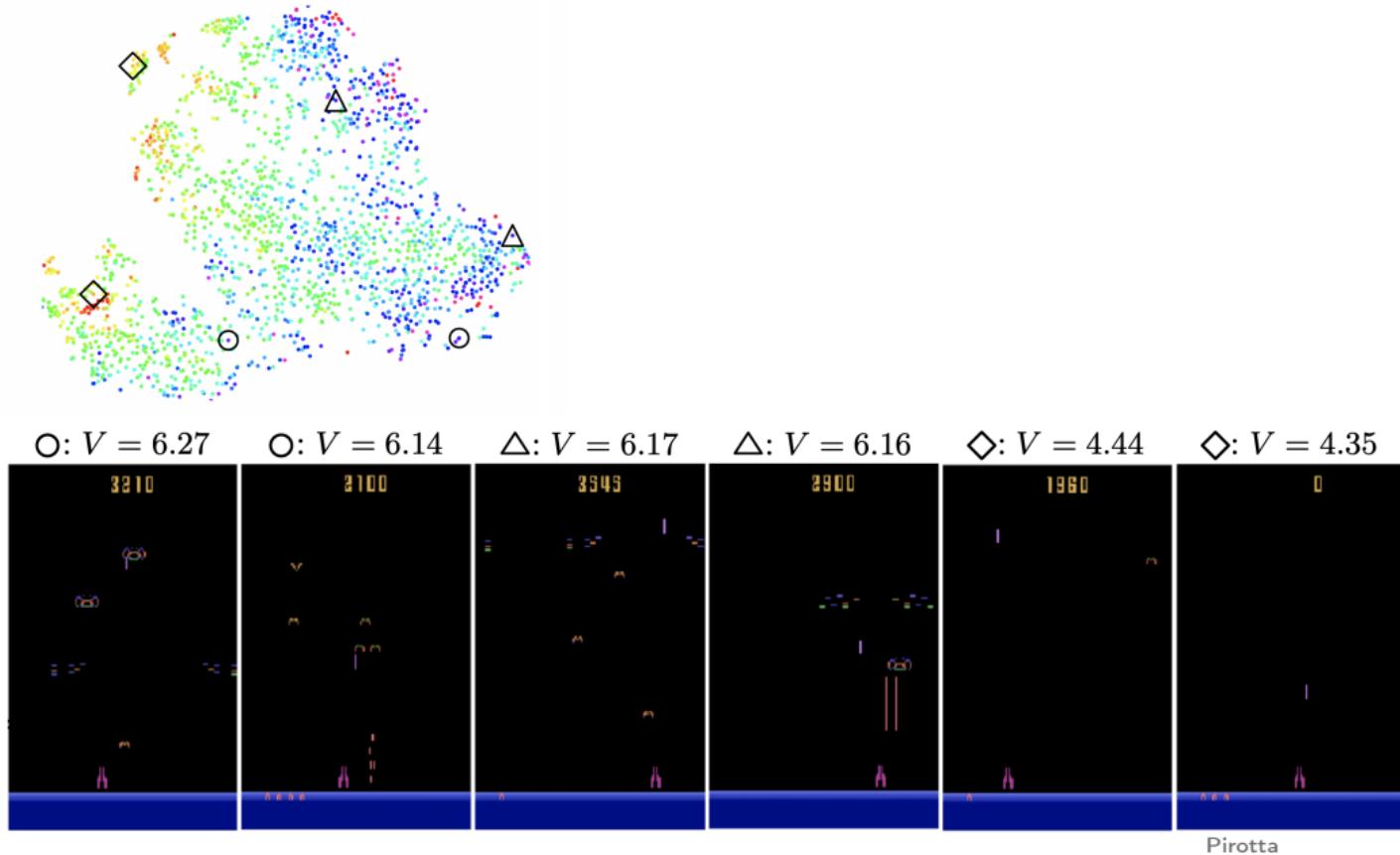
Montezuma!

# What to Count?

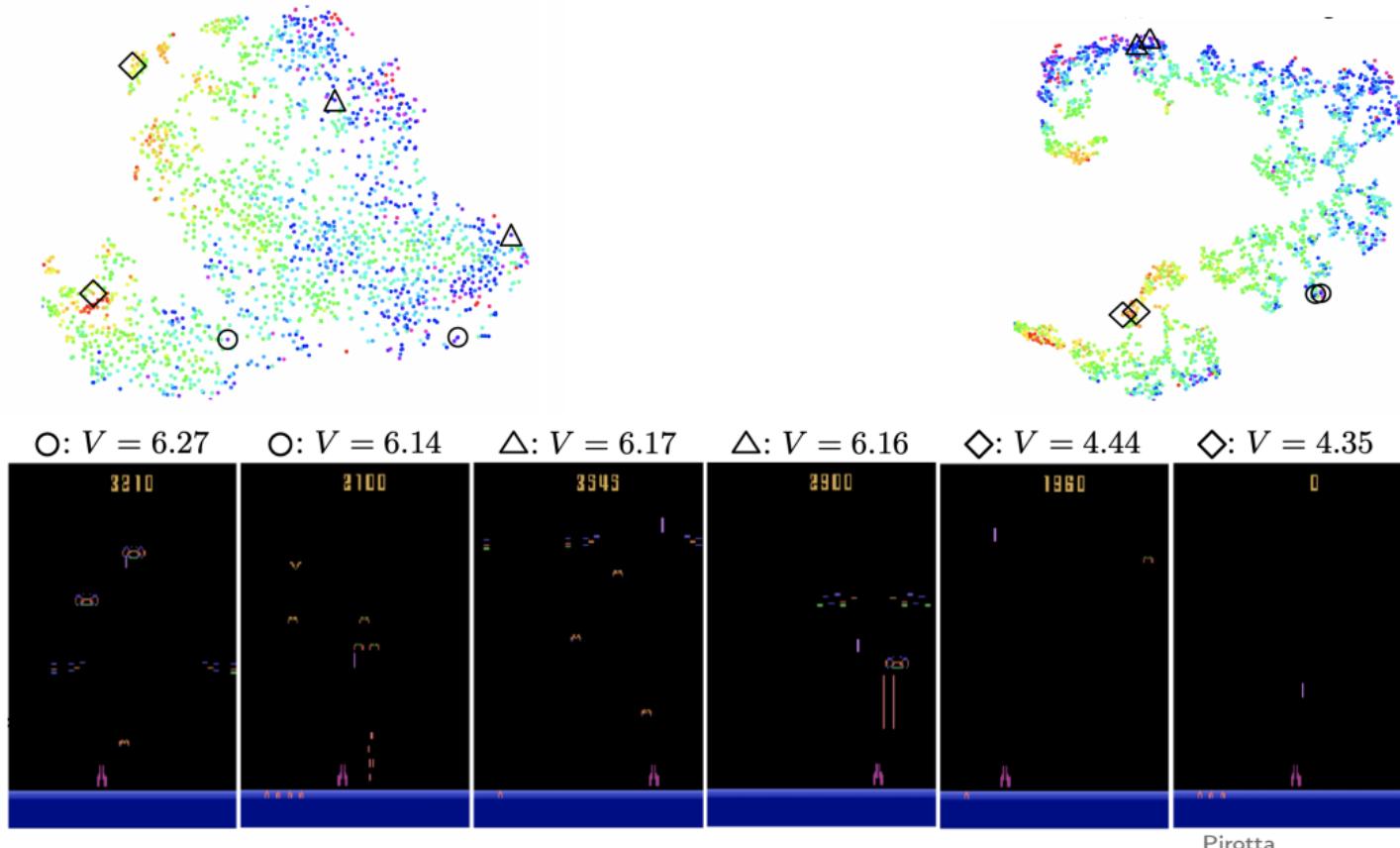


*Representation Learning? learn an embedding of state*

# What is important to learn?



# What is important to learn?



# Count-based Exploration

[Tang et al., 2017]

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**Algorithm 1:** Count-based exploration through static hashing, using SimHash

---

- 1 Define state preprocessor  $g : \mathcal{S} \rightarrow \mathbb{R}^D$
  - 2 (In case of SimHash) Initialize  $A \in \mathbb{R}^{k \times D}$  with entries drawn i.i.d. from the standard Gaussian distribution  $\mathcal{N}(0, 1)$
  - 3 Initialize a hash table with values  $n(\cdot) \equiv 0$
  - 4 **for** each iteration  $j$  **do**
  - 5     Collect a set of state-action samples  $\{(s_m, a_m)\}_{m=0}^M$  with policy  $\pi$
  - 6     Compute hash codes through any LSH method, e.g., for SimHash,  $\phi(s_m) = \text{sgn}(Ag(s_m))$
  - 7     Update the hash table counts  $\forall m : 0 \leq m \leq M$  as  $n(\phi(s_m)) \leftarrow n(\phi(s_m)) + 1$
  - 8     Update the policy  $\pi$  using rewards  $\left\{ r(s_m, a_m) + \frac{\beta}{\sqrt{n(\phi(s_m))}} \right\}_{m=0}^M$  with any RL algorithm
- 

- Use *locality-sensitive hashing* to discretize the input
  - Encode the state into a  $k$ -dim vector by random project  
small  $k$  = more hash collisions
  - Use the sign to discretize  
 $\text{small } \phi(s) \in \{-1, 1\}^k$
- *Count on discrete hashed-states*

# Count-based Exploration

[Tang et al., 2017]

---

**Algorithm 1:** Count-based exploration through static hashing, using SimHash

---

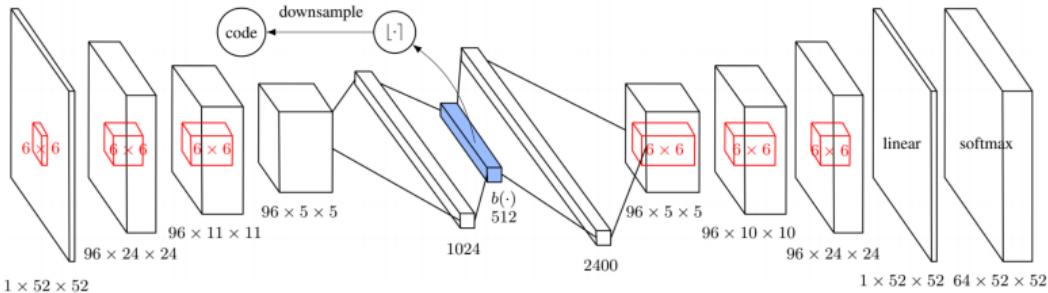
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  - Encode the state into a  $k$ -dim vector by random project  
small  $k =$  more hash collisions
  - Use the sign to discretize  
small  $\phi(s) \in \{-1, 1\}^k$
- *Count on discrete hashed-states*
- ❑ Difficult to define a good hashing function

# Count-based Exploration

[Tang et al., 2017]

Improve counts by learning a compression

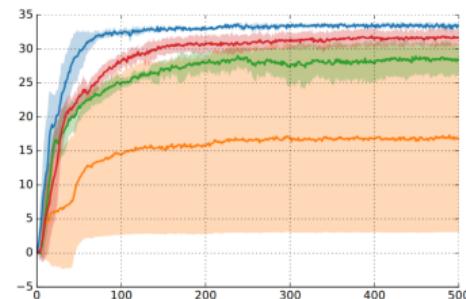


$$L(\{s_n\}_{n=1}^N) = -\frac{1}{N} \sum_{n=1}^N \left[ \log p(s_n) - \frac{\lambda}{K} \sum_{i=1}^D \min \left\{ (1 - b_i(s_n))^2, b_i(s_n)^2 \right\} \right]$$

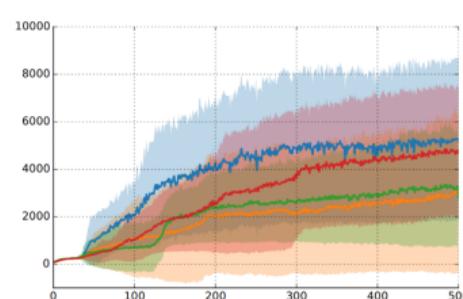
- Entropy loss for the auto-encoder
- “Binarization” loss for the “projection”
- Use all past history to update the AE
- AE should not be updated too often. **We need stable codes!**

# Count-based Exploration

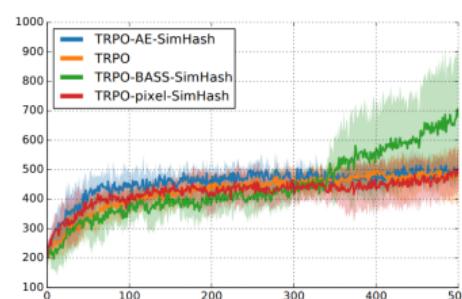
[Tang et al., 2017]



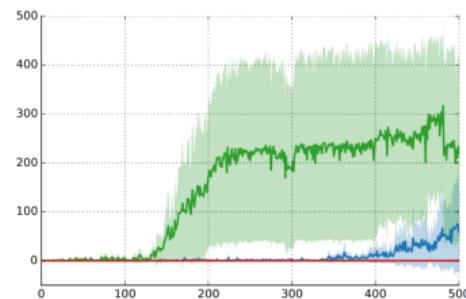
(a) Freeway



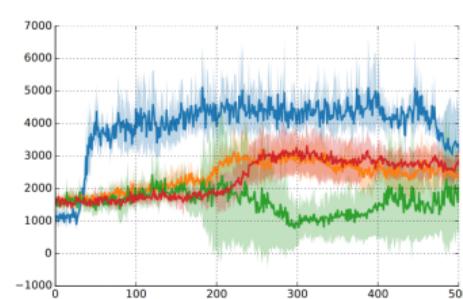
(b) Frostbite



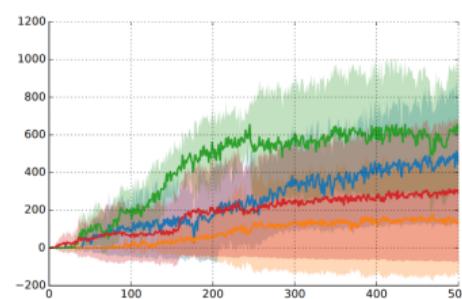
(c) Gravitar



(d) Montezuma's Revenge



(e) Solaris



(f) Venture

## Prediction-based Exploration

# Forward Dynamics Prediction

[Stadie et al., 2015]

Given an encoding  $\phi(s)$ , learn a *prediction model*

$$f : (\phi(s_t), a_t) \mapsto \phi(s_{t+1})$$

Use the prediction error

$$e_t = \|\phi(s_{t+1}) - f(\phi(s_t), a_t)\|_2^2$$

as *exploration bonus*  $r_t^i \propto e_t$

How to learn  $\phi(s)$ ?

- Pretrain the encoding (e.g., autoencoder)
- Learn it online using early samples

 *exploration and representation are intertwined!*

 *difficult to predict every possible change in the transitions*

\*the bonus is a normalized and scaled error

# Is everything relevant?

Idea: [Pathak et al., 2017]

predict only changes that depend on agent's actions, ignore the rest!

Mapping: *representation learning problem*

learn embedding  $\phi$  where only the information *relevant to the action performed by the agent* is represented (*controllability*)

# Intrinsic Curiosity Module

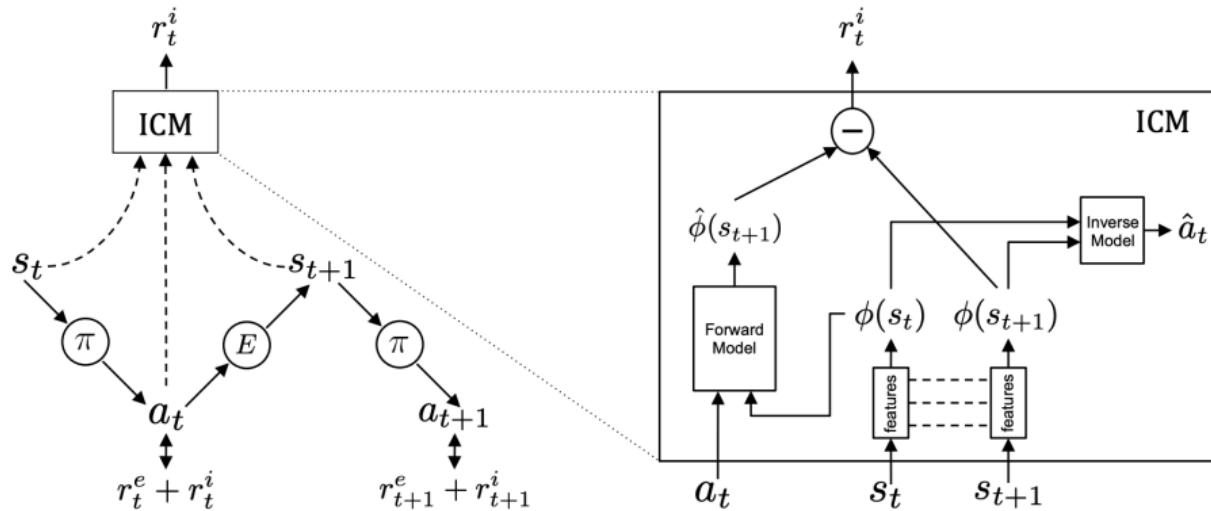
[Pathak et al., 2017]

*Inverse dynamics:*  $h : (\phi(s_t), \phi(s_{t+1})) \mapsto \hat{a}_t$

*Forward dynamics:*  $f : (\phi(s_t), a_t) \mapsto \phi(s_{t+1})$

*Intrinsic reward:*

$$r_t^i = \|\hat{\phi}(s_{t+1}) - \phi(s_{t+1})\|_2^2$$

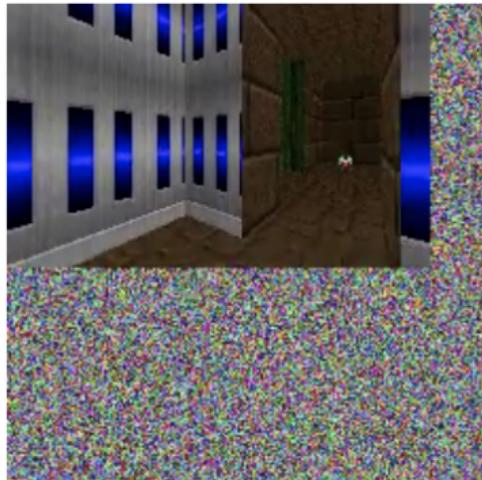


Training: end-to-end training with auxiliary losses

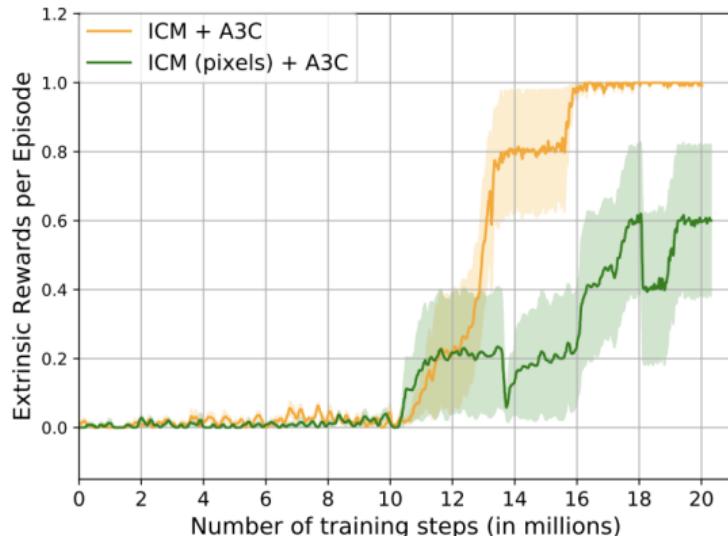
# Intrinsic Curiosity Module

[Pathak et al., 2017]

Intuition: inverse model  $h$  should be robust to uncontrollable components



(b) Input w/ noise



\*ICM (pixel) uses only forward dynamics

Inverse dynamics learning is at the base of many subsequent approaches

# Study of Curiosity Driven Exploration

[Burda et al., 2019a]

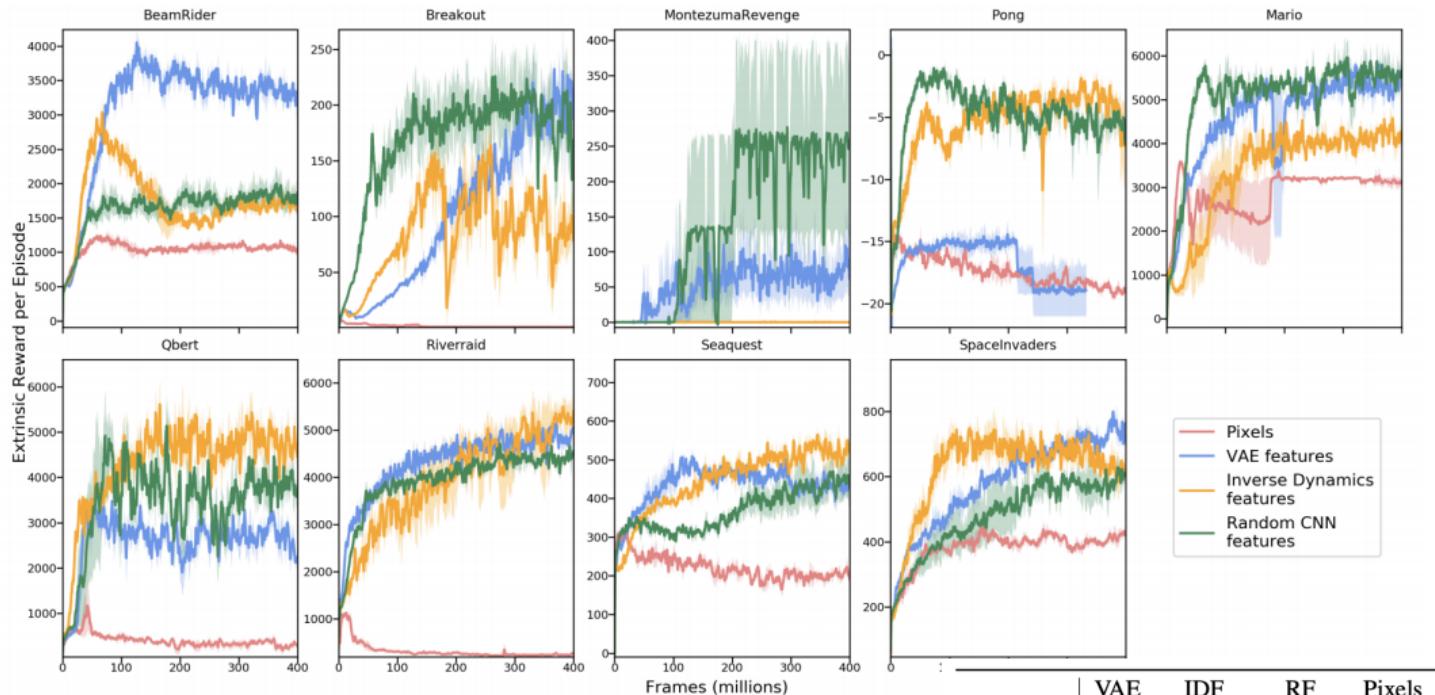
- Mostly pure exploration problems with *surprise-based reward*

$$r_t = r_t^i = \|f(s_t, a_t) - \phi(s_{t+1})\|_2^2 \approx -\log p(s_{t+1}|s_t, a_t)$$

- Authors identified 3 properties of good representations: *Compact, Sufficient, Stable*
- Compared the following methods
  - Pixel input:  $\phi(x) = x$
  - Random features (RF)
  - Variational Autoencoders (VAE): probabilistic encoder
  - Inverse dynamic features (IDF): as ICM

\*experiments done in infinite horizon setting to avoid termination leaking information

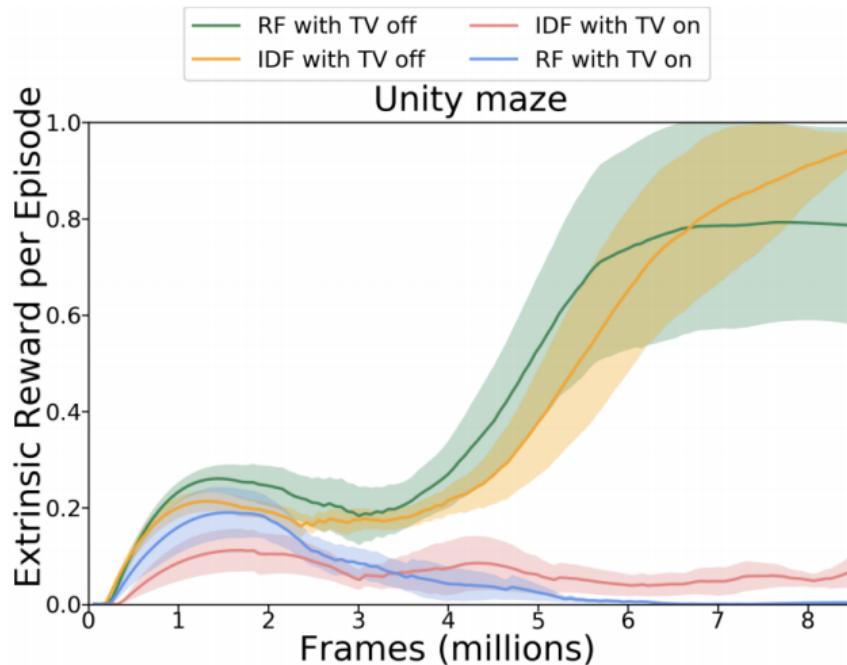
# Results



RF works quite well!

	VAE	IDF	RF	Pixels
Stable	No	No	Yes	Yes
Compact	Yes	Yes	Maybe	No
Sufficient	Yes	Maybe	Maybe	Yes

# Results: noisy TV



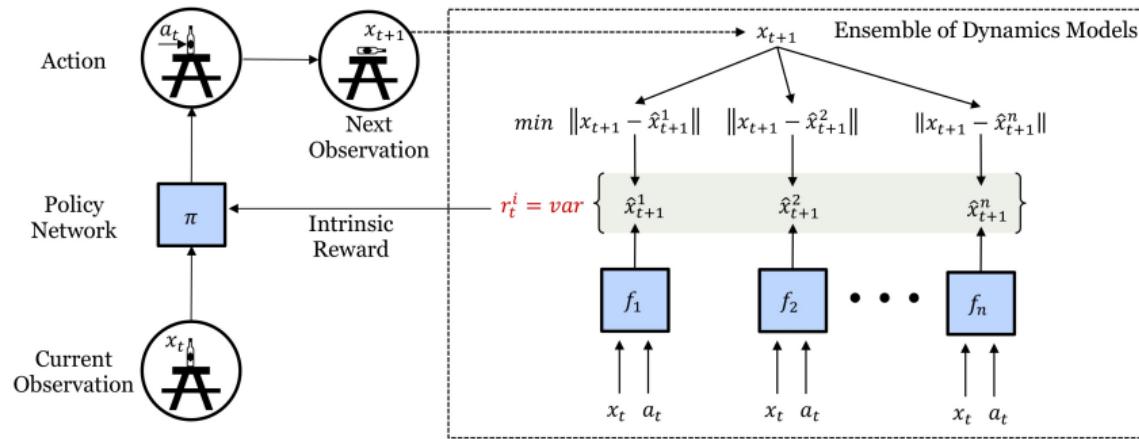
# From One Model to Many

- All the methods used a single model to predict forward or inverse dynamics
- We can also use *multiple models* and *leverage disagreement*  
high disagreement  $\implies$  low confidence  $\implies$  need more data (*exploration*)

# Self-Supervised Exploration via Disagreement

[Pathak et al., 2019]

- Ensemble method using multiple forward models ( $K$  models)



- Intrinsic reward:  $r_t^i = \mathbb{E}_k \left[ \| f_k(x_t, a_t) - \mathbb{E}_k [f_k(x_t, a_t)] \|_2^2 \right]$

- differentiable intrinsic reward
- can be paired with representation learning
- limitations of forward model learning

Auxiliary Task

# Exploration and Predictions

So far, exploration bonus was based on

- Generalized counts
- Prediction error about dynamics

but we can *use other predictions* for exploration  $\implies$  *value predictions*

# DORA

[Fox et al., 2018]

Consider two MDPs

- *Original MDP*  $M = (S, A, p, r, \gamma)$   
 $\implies$  learn  $Q_M^*(s, a)$  (*task objective*)
  
- *Cloned MDP*  $M' = (S, A, p, \textcolor{red}{0}, \gamma')$   
 $\implies$  learn  $E^*(s, a) := Q_{M'}^*(s, a) = 0$   
 (exploration)

*Exploration bonus*

$$r_t^i = \sqrt{\frac{1}{-\log E_t(s_t, a_t)}}$$

# DORA

[Fox et al., 2018]

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 (exploration)

*Exploration bonus*

$$r_t^i = \sqrt{\frac{1}{-\log E_t(s_t, a_t)}}$$

Idea:

- learn  $E^*$  online starting from  $E_0(s, a) = 1$
- The E-value should converge to 0 ( $E_k \rightarrow 0$ )
- Then,  $E_k(s, a) > 0$  represents the prediction error, i.e., uncertainty about the value of state  $(s, a)$
- $\log E$  can be seen as a *generalized count*

👉 use any preferred method to learn  $E$  with function approximation

# Random Network Distillation (RND)

- Randomly initialize two instances of the same NN (*target*  $\theta_*$  and *prediction*  $\theta_0$ )

$$f_{\theta_*} : \mathcal{S} \rightarrow \mathbb{R}; \quad f_{\theta} : \mathcal{S} \rightarrow \mathbb{R}$$

- Train the prediction network minimizing loss w.r.t. the target network

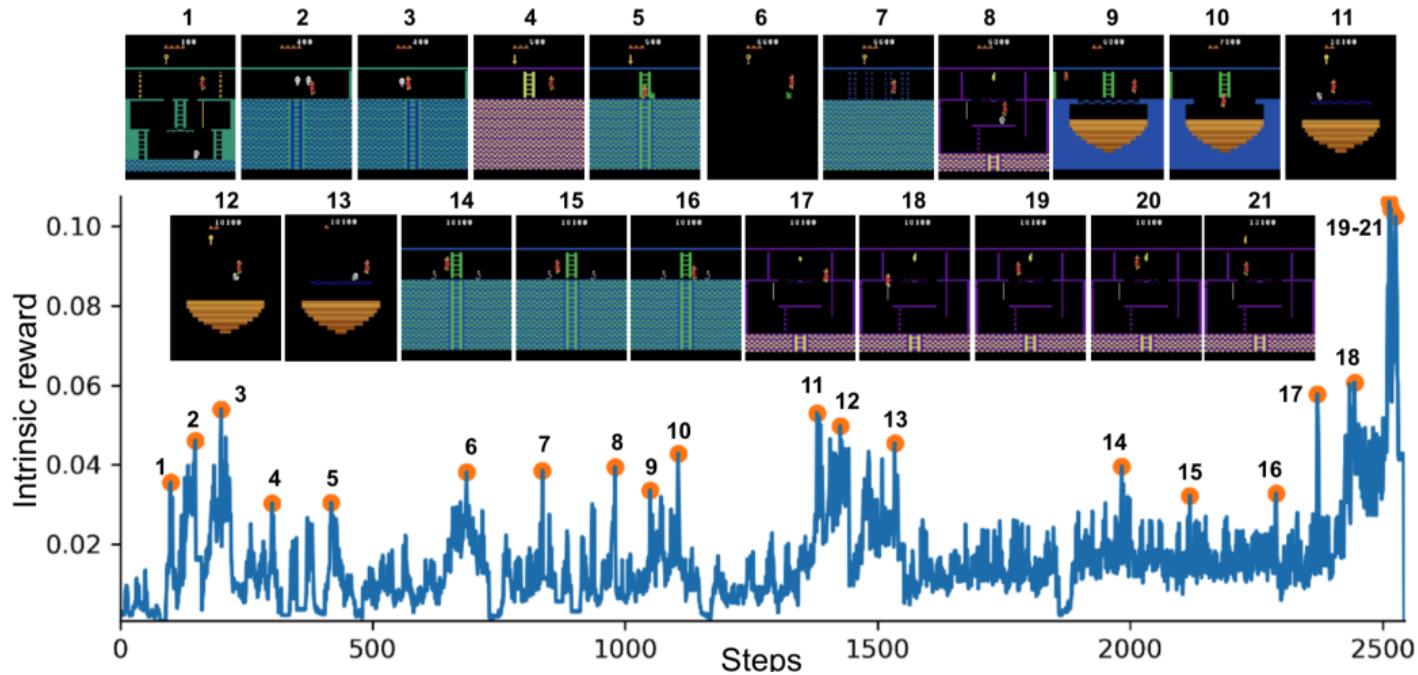
$$\theta_n = \arg \min_{\theta} \sum_{t=1}^n \left( f_{\theta}(s_t) - f_{\theta_*}(s_t) \right)^2$$

- Build “intrinsic” reward

$$r_t^i = \left| f_{\theta}(s_t) - f_{\theta_*}(s_t) \right|$$

- No model misspecification ( $f_{\theta}$  can exactly predict  $f_{\theta_*}$ )
- Influence of learning dynamics can be reduced

# Random Network Distillation (RND)



# Random Network Distillation (RND)

[Burda et al., 2019b]

## General architecture

- Separate extrinsic  $r_t^E$  and intrinsic reward  $r_t^I$
- PPO (or any other approach) with two heads to estimate  $V^I$  and  $V^E$
- Greedy policy w.r.t.  $V^I + \textcolor{red}{c}V^E$

## “Tricks”

- Rewards should be in the same range
- Use different discount factors for intrinsic and extrinsic rewards
- Non-episodic setting results in better exploration

# Random Network Distillation (RND)

[Burda et al., 2019b]

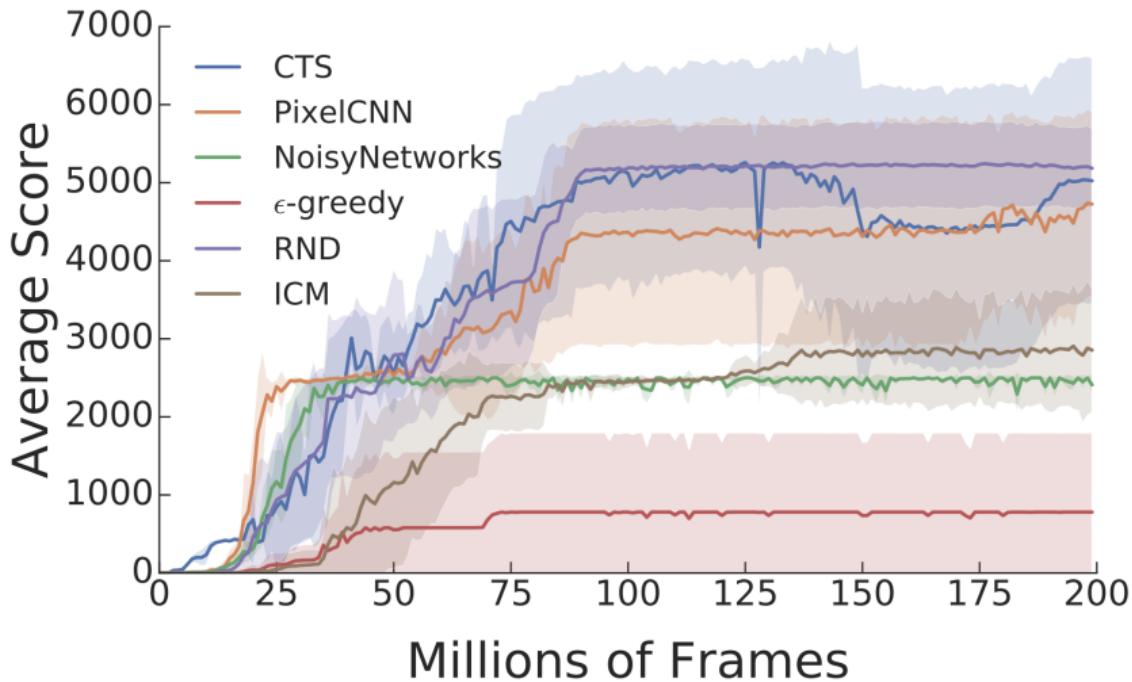
Montezuma!

finds 22 out of the 24 rooms on the first level

# Comparison

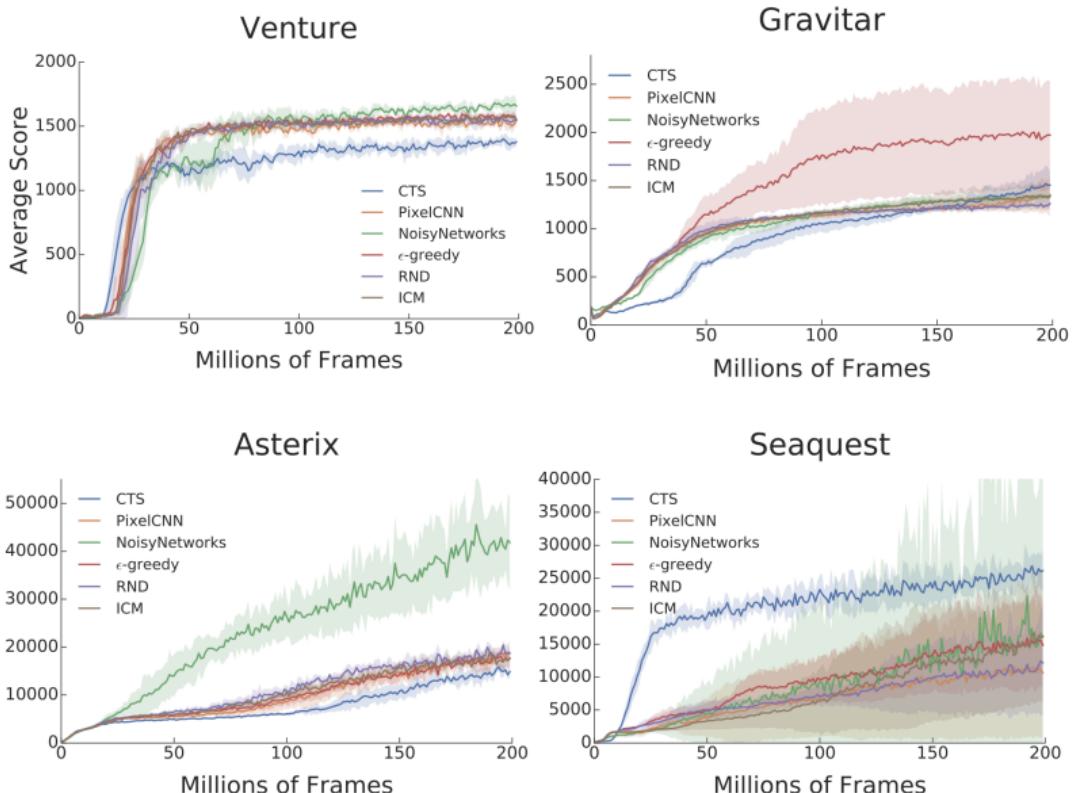
[Taïga et al., 2019]

## Montezuma's Revenge



# Comparison: not all problems require same amount of exploration

[Taïga et al., 2019]



# Exploration in Deep RL: Outline

## 1 Introduction

- Review of Exploration Principles
- Exploration Issues in Deep RL

## 2 Exploration Bonus

## 3 Memory-Based Exploration

- Episodic Memory
- Goal-Oriented Exploration

## 4 Randomized Exploration

## 5 Conclusions

# Exploration Bonus: *Issues*

- Non-stationary
- Controllability/Predictability
  - “agent finds a way to *instantly gratify itself* by exploiting actions which lead to *hardly predictable consequences*” – [Savinov et al., 2019]
- Knowledge fading
  - “after the *novelty of a state has vanished*, the agent is not encouraged to visit it again, regardless of the downstream learning opportunities it might allow” – [Badia et al., 2020b]
- Representation learning intertwined with exploration

Few of these problems are addressed through *memory* (i.e., buffer)

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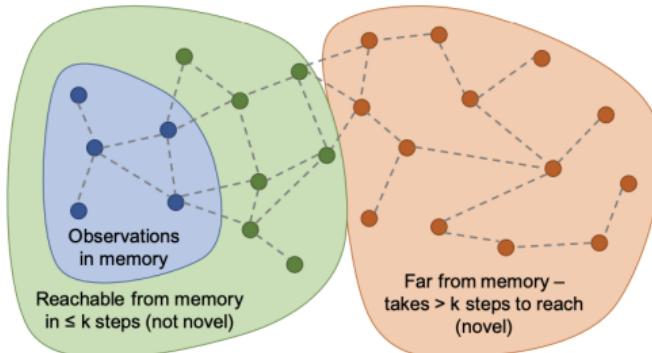
## 4 Randomized Exploration

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# Episodic Curiosity

[Savinov et al., 2019]

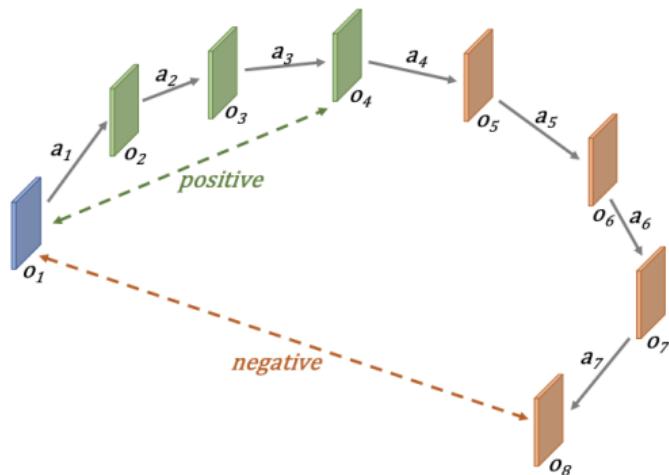
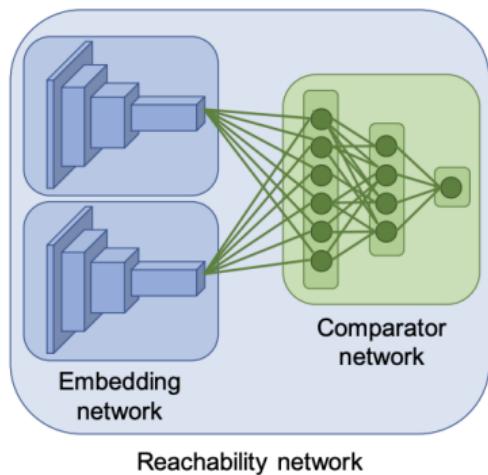
- The novelty bonus  $r_t^i$  depends on *reachability* of states  
i.e., give a reward only for those observations which take some effort to reach (*outside the known region*)
- Reachability = # steps between states



## Components:

- 1 State embedding
- 2 Comparator  
(i.e., reachability predictor)
- 3 Episodic Memory

# Episodic Curiosity: *Embedding* and *Reachability*



- Reachability is formulated as *binary classification problem*

$$C\left(\phi(s_i), \phi(s_j)\right) \mapsto [0, 1]$$

# Episodic Curiosity: *Memory*

- Stores embeddings of past observations from the *current episode*

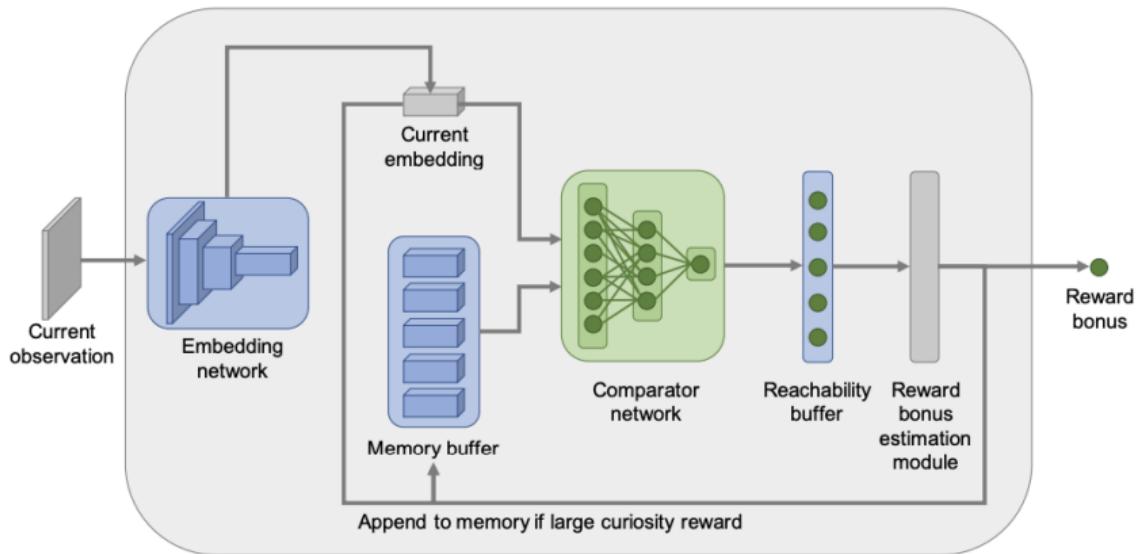
$$M = \left\{ \phi(s_t) \right\}_t$$

- *Reinitialized* at the beginning of each episode
- Limited capacity
- $\phi(s_t)$  is added to  $M$  *only if novelty (bonus) is high enough*

# Episodic Curiosity: *Bonus*

- $C(M, \phi(s_t))$  *similarity score* between the memory buffer and the current embedding (*may depend on all samples in M*)
- $\alpha$  and  $\beta$  are hyper-paramenters

$$r_t^i = \alpha(\beta - C(M, \phi(s_t)))$$



# Vanishing Novelty? *Never Give Up*

$$r_t = \underbrace{r_t^e}_{\text{extrinsic reward (standard)}} + \beta \underbrace{r_t^i}_{\text{intrinsic}}$$

Intrinsic reward should capture [Badia et al., 2020b]

1 *Long-term novelty*

reward encourages visiting states throughout training (*across episodes*)

2 *Short-term novelty*

reward encourages visiting states over a short horizon (e.g., *within an episode*)  
ignores inter-episode interactions

# Never Give Up: *intrinsic reward*

[Badia et al., 2020b]

$$r_t^i = r_t^{\text{episodic}} \cdot \min \left\{ \max \{ \alpha_t, 1 \}, L \right\}$$

per-episode novelty  
(short-term)

life-long novelty  
(long-term)

Properties:

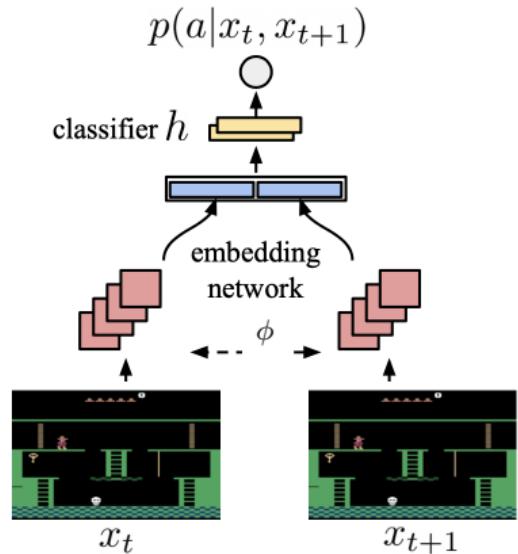
- *Rapidly discourages* revisiting states in an episode
- *Slowly discourages* revisiting frequent states across episodes

# Never Give Up: *short-term* novelty

- **Episodic memory:** to store the *controllable* states in an online fashion

$$M = \left\{ \phi(s_0), \phi(s_1), \dots, \phi(s_{t-1}) \right\}$$

- $\phi$  is an IDF (inverse dynamics features) *embedding* of the observation same as feature encoding in ICM

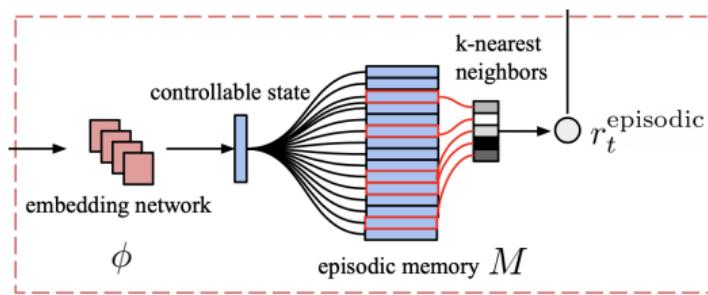


# Never Give Up (NGU): *short-term* novelty

- *Frequency-based* exploration inside the **episode**

$$r_t^{\text{episodic}} = \frac{1}{\sqrt{n(\phi(s_t))}} \approx \frac{1}{\sqrt{\sum_{\phi_i \in N_k^t} \text{Ker}(\phi(s_t), \phi_i)} + c}$$

with  $N_k^t$  being the  $k$ -nearest neighbors of  $\phi(s_t)$  in memory  $M$



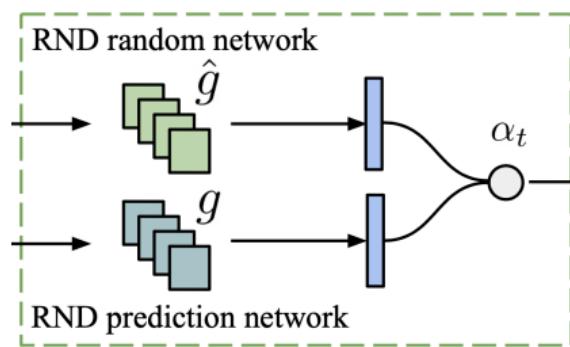
\*  $\text{Ker}(x, y) = \frac{\epsilon}{\frac{d^2(x, y)}{d_m^2} + \epsilon}$  where  $d = \ell_2$  and  $d_m$  is a running average of the squared  $\ell_2$  distance of the  $k$  nearest neighbors

# Never Give Up (NGU): *long-term* novelty

- Random Network Distillation [Burda et al., 2019b]

$$\alpha_t = 1 + \frac{\text{err}^{\text{RND}}(s_t) - \mu_e}{\sigma_e}$$

$\sigma_e$  and  $\mu_e$  are running standard deviation and mean for  $\text{err}^{\text{RND}}(s_t)$



# Never Give Up (NGU): *population training*

*Multi-task* setting: (population based, auxiliary tasks, ...)

- Learn *simultaneously* a family of problems ( $M_j$ ) by approximating  $Q(s, a; M_j)$
- ( $M_i$ ) same dynamics but *different rewards*

$$r_t^{M_j} = r_t^e + \beta_j r_t^i$$

with  $\beta_0 = 0 < \dots < \beta_{N-1} = \beta_{\max}$

- and *discount factors*  $\gamma_0 = \gamma > \dots > \gamma_{N-1}$   
in the paper  $\gamma_0 = 0.997$ , and  $\gamma_{N-1} = 0.99$

# Beyond NGU: Agent57

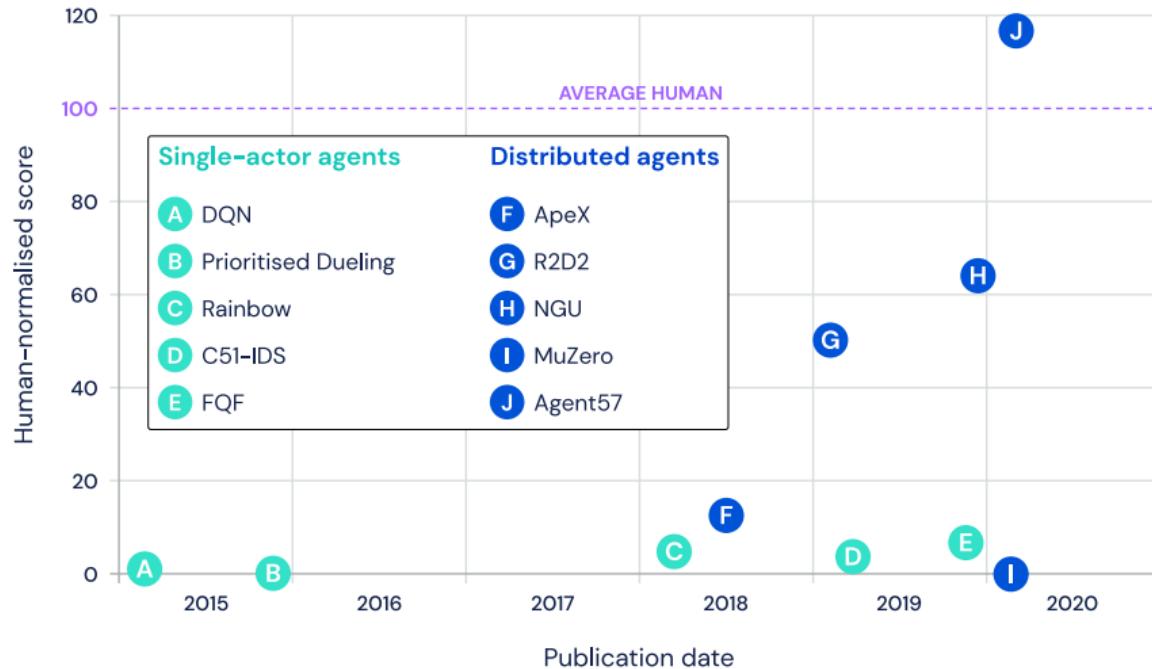
[Badia et al., 2020a]

Agent57 *builds on NGU* but uses a new

- 1 State-Action Value Function Parameterization
- 2 Adaptive Exploration over a Family of Policies (*meta controller*)

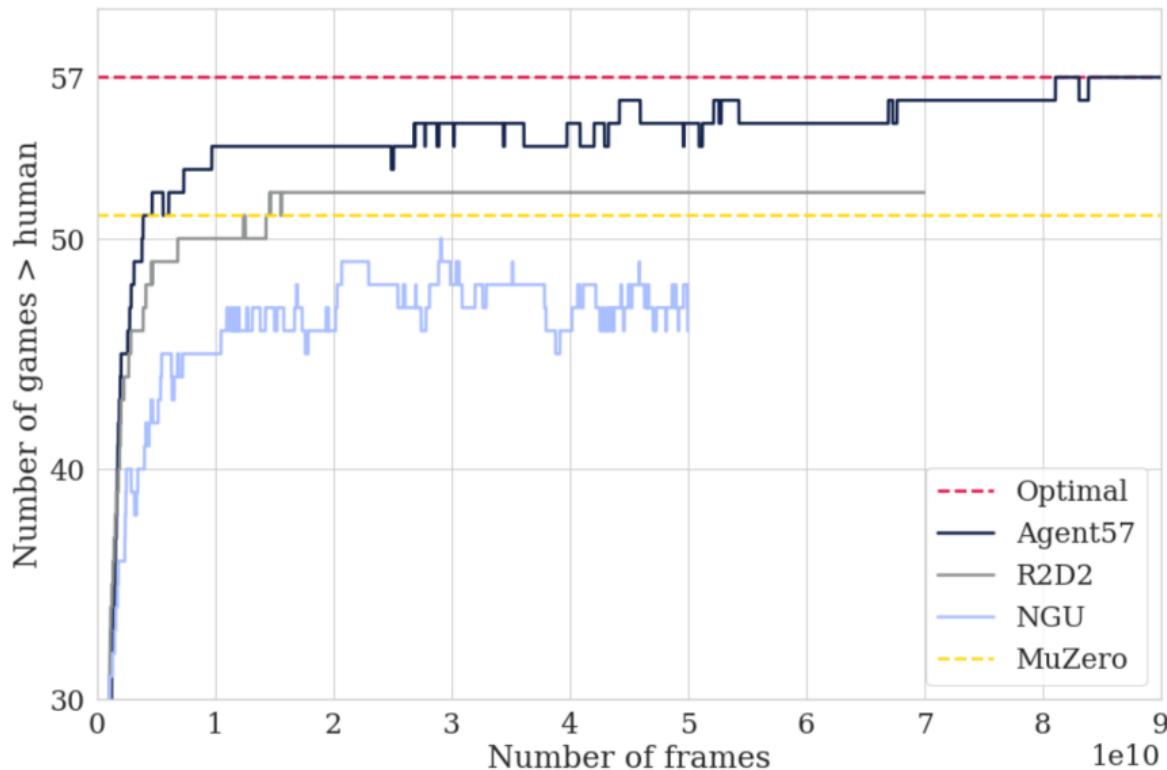
# Super-human Performance

Atari-57 5th percentile performance



"[Agent57 is the] first deep reinforcement learning agent to obtain a score that is above the human baseline on all 57 Atari 2600 games."

# Frames to human performance



# Agent57: *changes in Q*

## *Reparametrization*

$$Q(s, a, j; \theta) = \underbrace{Q(s, a, j; \theta^e)}_{\text{extrinsic}} + \beta_j \underbrace{Q(s, a, j; \theta^i)}_{\text{intrinsic}}, \quad \theta = \{\theta^e, \theta^i\}$$

- $Q^e$  and  $Q^i$  have identical architecture
- Optimized using *transformed Retrace loss* (as NGU)
  - Optimized separately based on  $r^e$  and  $r^i$  respectively
  - But same target policy  $\pi(s) = \arg \max_a Q(s, a, j; \theta)$

\* new compared to NGU. Note that [Burda et al., 2019b] used two heads for extrinsic and intrinsic value function, with a shared architecture.

# Agent57: *meta-controller*

*NGU issue:*

- all policies (i.e., models ( $M_j$ )) are trained equally, *regardless* of their contribution to the learning progress
- expected that higher  $\beta_j$  and lower  $\gamma_j$  do better in the early stages, and opposite later

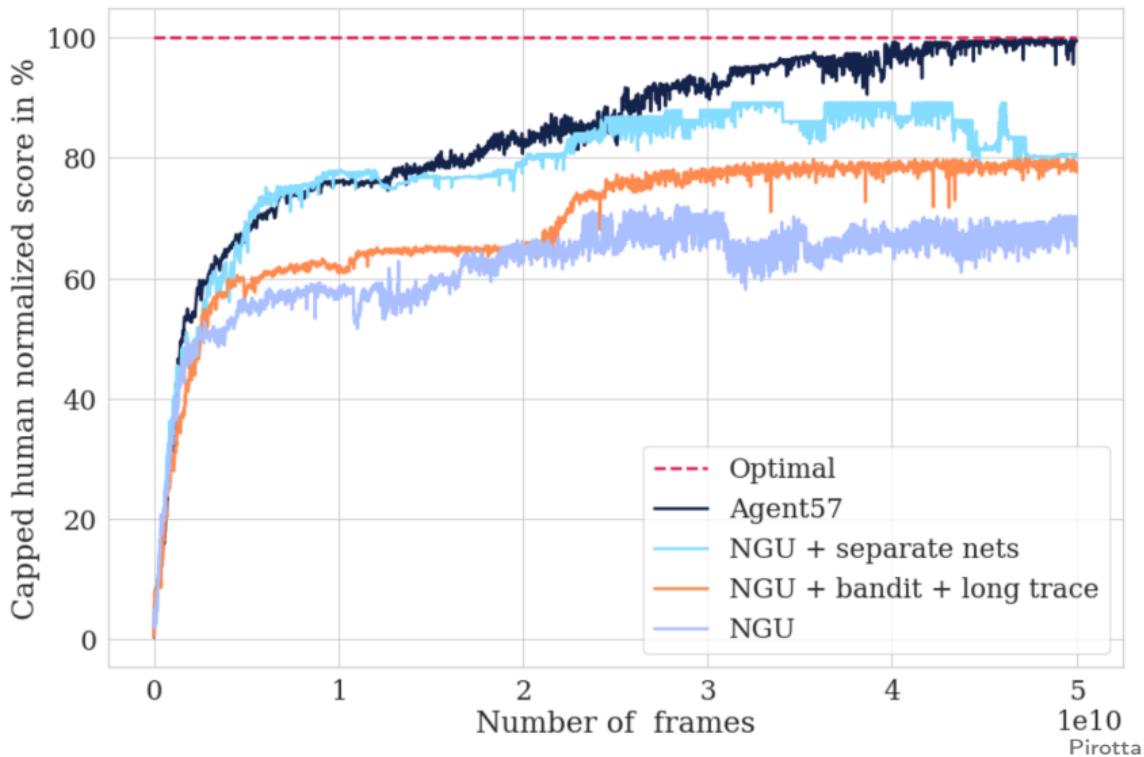
**Solution:**

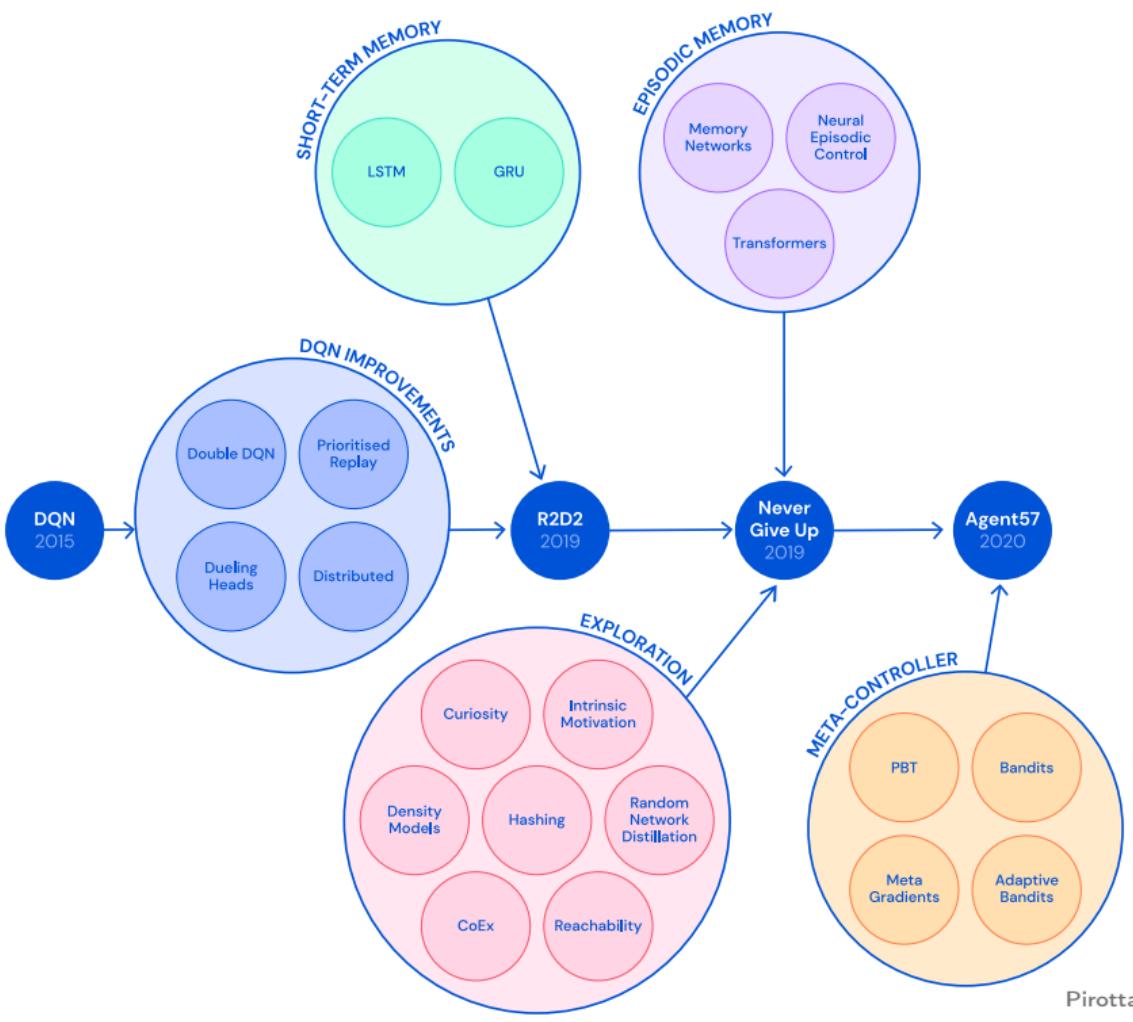
- meta-controller to prioritize what to learn  
     $\implies$  sort of automatic curriculum learning
- use *non-stationary multi-arm bandit* algorithm [e.g., sliding-window UCB]
- *non-stationary?* Agent57 is also learning the policy of each task

# Performance on 10 hard games

six hard *exploration* games, plus games that require *long-term credit assignment*.

Beam Rider, Freeway, Montezuma's Revenge, Pitfall!, Pong, Private Eye, Skiing, Solaris, Surround, and Venture





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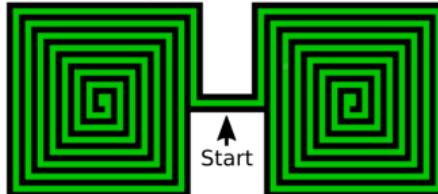
# Direct Exploration

[Ecoffet et al., 2019, 2021]

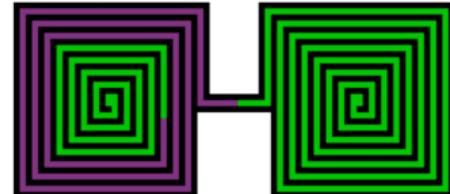
Recall a few issues of intrinsic exploration:

- Forget about promising areas they have visited
- They do not return to them for further exploration

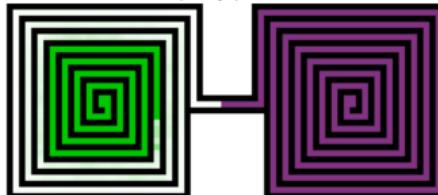
1. Intrinsic reward (green) is distributed throughout the environment



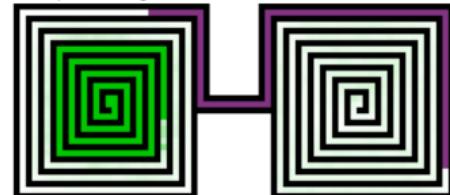
2. An IM algorithm might start by exploring (purple) a nearby area with intrinsic reward



3. By chance, it may explore another equally profitable area



4. Exploration fails to rediscover promising areas it has detached from



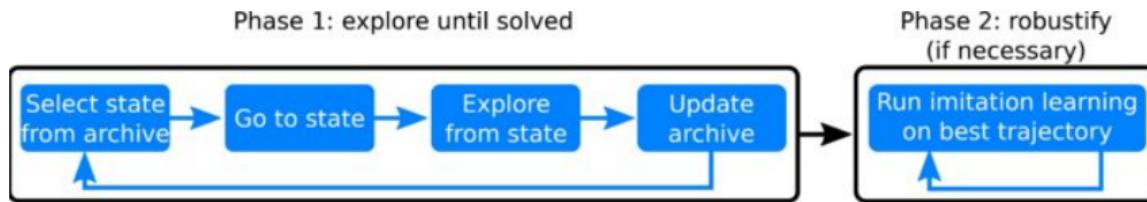
*Green* areas indicate intrinsic reward, white indicates areas where no intrinsic reward remains, and *purple* areas indicate where the algorithm is currently exploring.

💡 *It would be good to keep in memory unexplored states and target them*

# Go-Explore: *Phases*

[Ecoffet et al., 2019, 2021]

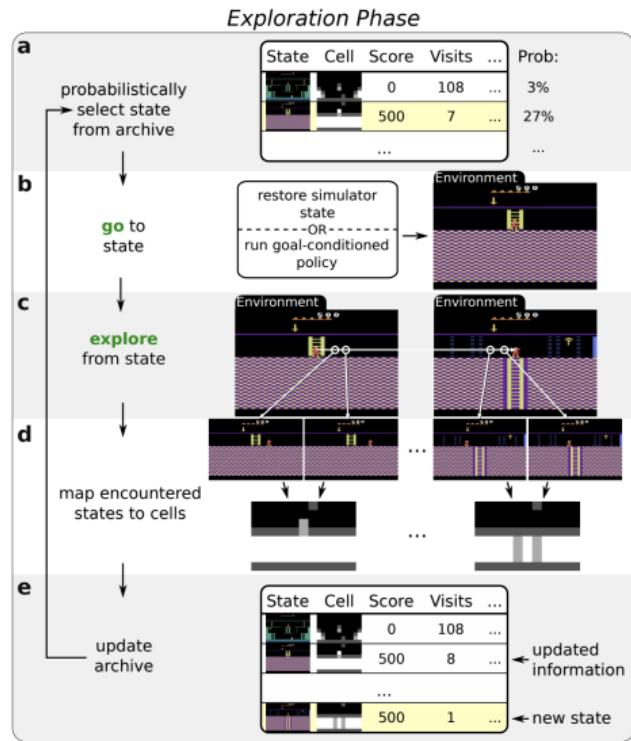
- ① Exploration
- ② Robustification



# Go-Explore: *phases* ①

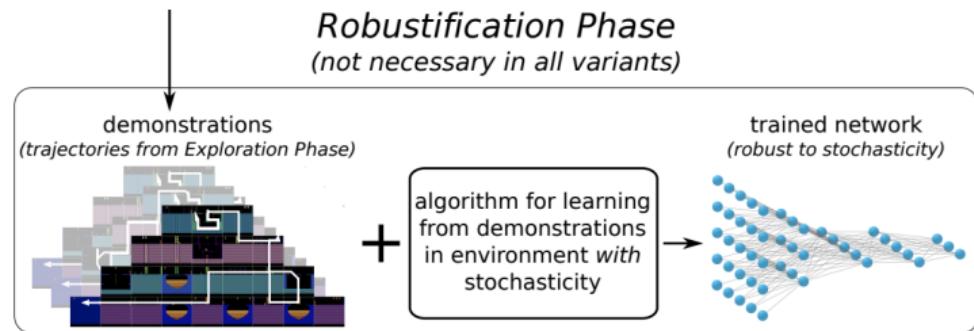
Steps:

- Select a state  $\phi(s)$  from memory  $M$   
e.g., by relevance (IM, novelty, etc.)
- Go to a state  $\phi(s)$
- Explore locally (e.g., randomly)
- Store embedding  $\phi(s')$  in  $M$



# Go-Explore: *phases ②*

- Robustification against noise
- Learning from Demonstrations (i.e., imitation learning)  
requires to store the highest-scoring trajectories



# Intuition: discover and control

- Discover states

This is done by random exploration around the targeted state

- Control states

This is obtained by the incremental approach

**⚠ Most challenging aspect is reaching the selected state in phase ①**

\* similar to theoretical approaches for autonomous exploration [e.g., Lim and Auer, 2012, Tarbouriech et al., 2020]

# Reaching a State

[Ecoffet et al., 2019, 2021]

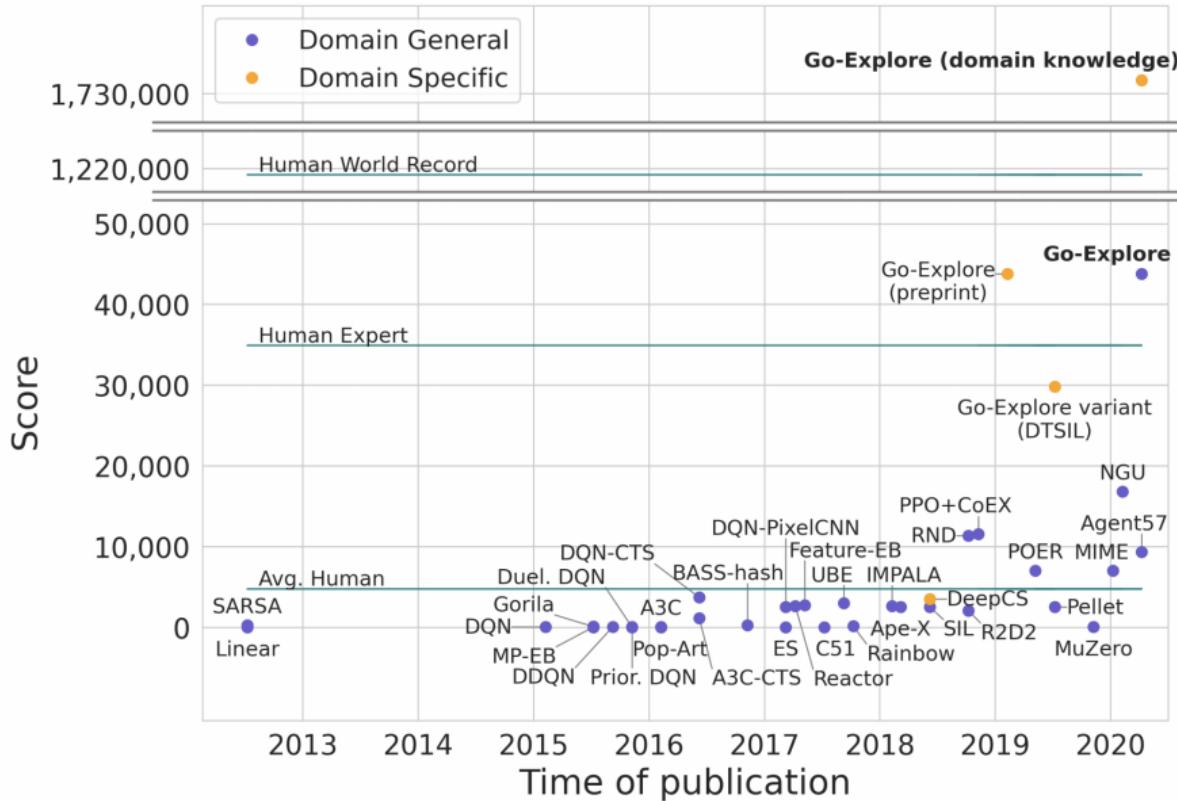
## (A) – *Resetting the simulator*

- Strong assumption
- Leverage determinism through the simulator
- Based on replaying actions

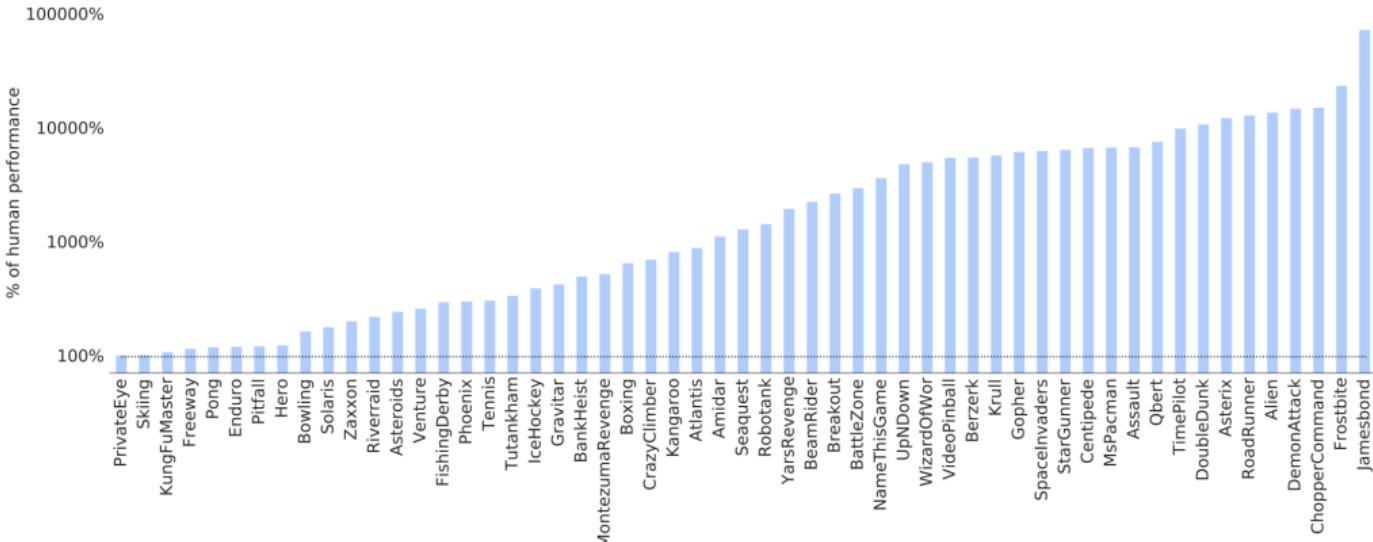
## (B) – *Goal-Oriented policy*

- Generic setting
- Learn policies aiming to reach a specific state  
learn goal-dependent quantities, e.g.,  $Q(s, a; g)$  or  $\pi(s, a; g)$
- They train  $\pi(s, a; g)$  based on the best trajectory that led to such a goal  $g$  + imitation-learning

# Results with Simulator Reset

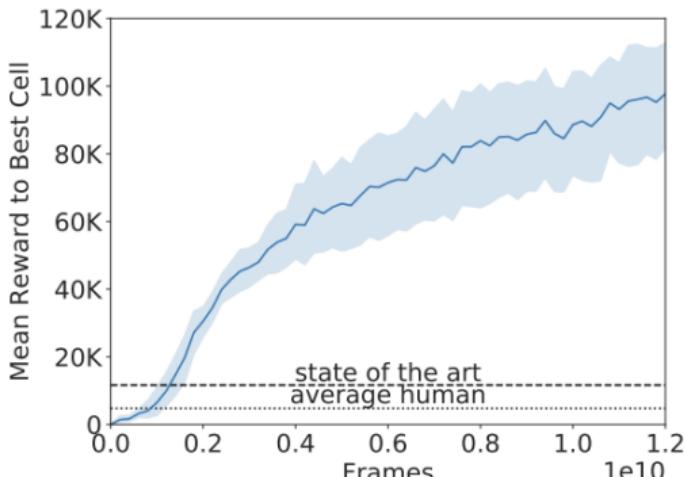


# Results with Simulator Reset - cont'd

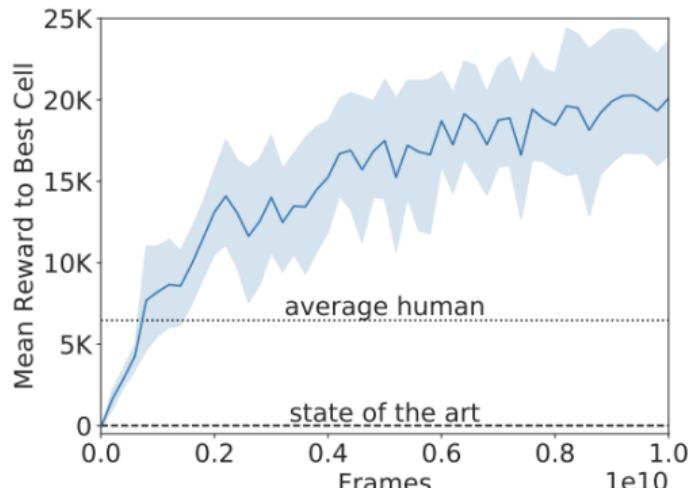


Video

# Results with Goal-Oriented Policy



(a) Montezuma's Revenge

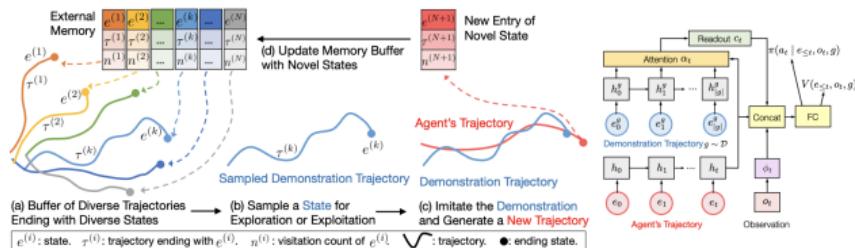


(b) Pitfall

# Other Approaches for Direct Exploration

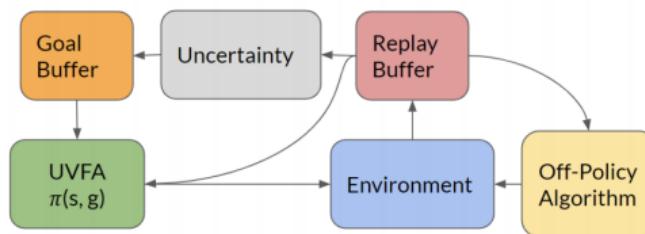
## ■ [Guo et al., 2020] (DTSIL)

keep trajectories and train a goal/trajectory oriented policy by imitation learning



## ■ [Guo and Brunskill, 2019]

learn goal-conditioned policy to directly reach highly-uncertain states



# Exploration in Deep RL: Outline

## 1 Introduction

- Review of Exploration Principles
- Exploration Issues in Deep RL

## 2 Exploration Bonus

## 3 Memory-Based Exploration

- Episodic Memory
- Goal-Oriented Exploration

## 4 Randomized Exploration

## 5 Conclusions

# Randomized Exploration

General Scheme inspired by Thompson Sampling

- 1 Estimate the parameters  $\theta$  for either policy or value function
- 2 Add randomness to the parameters  $\tilde{\theta} = \theta + \text{noise}$
- 3 Run the corresponding (greedy) policy

**Remark:** changing weights induces a consistent, and potentially very complex, state-dependent change in policy over multiple time steps

- ⇒ long-term exploration
- ⇒ no dithering

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**Remark:** changing weights induces a consistent, and potentially very complex, state-dependent change in policy over multiple time steps

- ⇒ long-term exploration
- ⇒ no dithering

⌚ The randomness needs to represent “uncertainty”

# Exploration via Randomization

- Perturb observed rewards
  - store samples  $(s, a, s', r + \text{noise})$
  - run an RL algorithm on the perturbed data
- Perturb parameters (e.g., based on posterior uncertainty)
  - leverage uncertainty on the prediction

*Randomized Value Function (RVF)* [Osband et al., 2019, 2018, Azizzadenesheli et al., 2018, Lipton et al., 2018, Touati et al., 2019, Osband et al., 2019]

# RVF: *issues*

## *Reward Perturbation*

- Minimize least-squares problem for any reward structure  
e.g., by gradient descent
- Not so easy to define the magnitude of the reward perturbation

## *Posterior Sampling*

- Posterior variance
  - easy for linear model
  - hard (almost impossible) for generic models
- A lot of approximate schemas for computing the posterior

# Posterior Distribution for Deep Neural Networks

Bayesian DQN [Azizzadenesheli et al., 2018]

- 1 Bayesian linear regression with given feature  $\phi(s) \in \mathbb{R}^d$  and given target vector for each action  $y_a$

$$\mu_a = (\Phi_a^\top \Phi_a)^{-1} \Phi_a^\top y_a \quad \Sigma_a = \Phi_a^\top \Phi_a$$

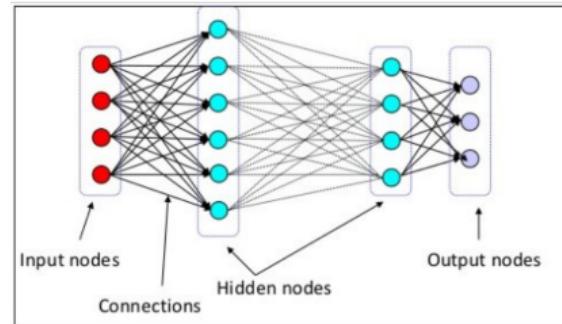
- 2 Draw a weight vector at random  $w_a \sim \mathcal{N}(\mu_a, \Sigma_a^{-1})$

- 3 Run the corresponding (greedy) policy

$$a_t = \arg \max_a Q(s_t, a) := \arg \max_a w_a^\top \phi(s_t)$$

- 4 Train  $\phi$  with standard NN to estimate  $Q$

**⚠ Same tools as in linear bandit**



# Posterior Distribution for Deep Neural Networks

## BBQ-Networks [Lipton et al., 2018]

- Uses variational inference to quantify uncertainty
- Uses independent factorized Gaussians as an approximate posterior

## MNF-DQN [Touati et al., 2019]

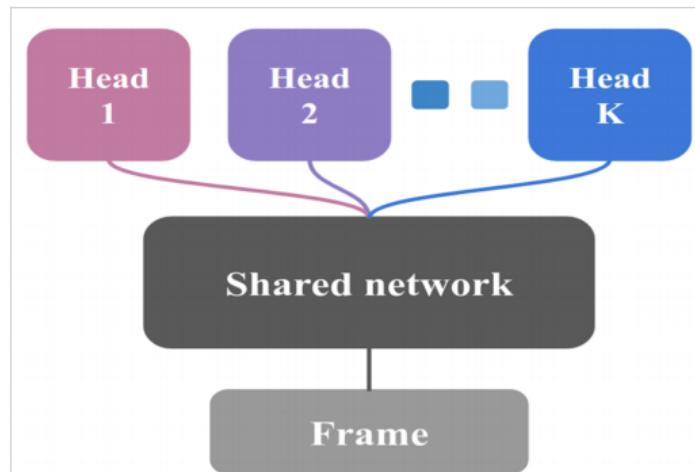
- Leverages recent advances in variational Bayesian NN
- Computationally and statistically efficient
- Uses normalizing multiplicative flows (MNF) in order to account for the uncertainty of estimates for efficient exploration

# Bootstrap DQN

[Osband et al., 2016]

DQN + bootstrapping  $\approx$  Thompson sampling

- Define multiple value functions  $Q_k$
- Update functions with different datasets
- Share part of the architecture



another way of approximating a sample from posterior

# Bootstrap DQN

[Osband et al., 2016]

## Algorithm 1 Bootstrapped DQN

- 1: **Input:** Value function networks  $Q$  with  $K$  outputs  $\{Q_k\}_{k=1}^K$ . Masking distribution  $M$ .
- 2: Let  $B$  be a replay buffer storing experience for training.
- 3: **for** each episode **do**
- 4:     Obtain initial state from environment  $s_0$
- 5:     Pick a value function to act using  $k \sim \text{Uniform}\{1, \dots, K\}$
- 6:     **for** step  $t = 1, \dots$  until end of episode **do**
- 7:         Pick an action according to  $a_t \in \arg \max_a Q_k(s_t, a)$
- 8:         Receive state  $s_{t+1}$  and reward  $r_t$  from environment, having taking action  $a_t$
- 9:         Sample bootstrap mask  $m_t \sim M$
- 10:         Add  $(s_t, a_t, r_{t+1}, s_{t+1}, m_t)$  to replay buffer  $B$
- 11:     **end for**
- 12: **end for**

- $M_t$  determines the type of bootstrapping strategy

$$g_t^k = m_t^k (y_t^Q - Q_k(s_t, a_t; \theta)) \nabla_\theta Q_k(s_t, a_t, ; \theta)$$

with target  $y_t = r_t + \max_a Q(s_{t+1}, a; \theta^-)$

# Randomized Prior Functions

[Osband et al., 2018]

*Bayesian perspective:* “generate posterior samples by training on noisy versions of the data, together with some random regularization”

## Randomized Prior + Bootstrapped DQN

- Train an ensemble of models, each on *perturbed versions of the data*
- The resulting distribution of the ensemble is used to approximate the uncertainty in the estimate

$$\mathcal{L}(\theta; \theta^-, p, \mathcal{D}) = \sum_{t \in \mathcal{D}} \left( r_t + \gamma \max_{a'} (Q_{\theta^-} + p)(s'_t, a') - (Q_\theta + p)(s_t, a_t) \right)$$

# Noisy Networks

[Fortunato et al., 2018]

- Normal NN layer  $y = wx + b$
- Double the parameters with mean and variance

$$w \rightarrow \mu^w, \sigma^w \text{ and } b \rightarrow \mu^b, \sigma^b$$

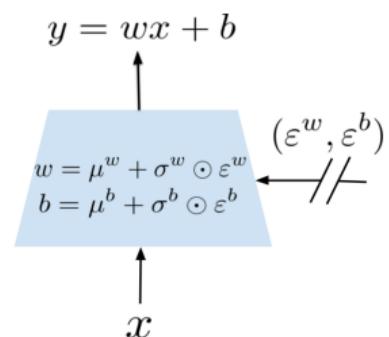
- Whenever a layer is evaluated draw  $\varepsilon^w, \varepsilon^b \sim \mathcal{D}$
- Evaluate the “random” layer as

$$y = (\mu^w + \sigma^w \odot \varepsilon^w) + \mu^b + \sigma^b \odot \varepsilon^b$$

- Let  $\zeta = (\mu^w, \sigma^w, \mu^b, \sigma^b)$ , define the expected loss

$$\bar{L}(\zeta) = \mathbb{E}_\varepsilon [L(\zeta, \varepsilon)]$$

- Gradient estimation update



# Noisy Networks: *noise models*

[Fortunato et al., 2018]

- Independent noise  $\varepsilon_{i,j}$  for each weight  $i$  at layer  $j$
- Factorized noise  $\varepsilon_{i,j} = f(\varepsilon_i)f(\varepsilon_j)$  (e.g.,  $f(x) = \text{sgn}(x)\sqrt{x}$ )
- Independent noise for target and online networks

$$y_t = r_t + \max_{a'} Q(s'_t, a'; \varepsilon', \zeta^-); \quad L_t(\zeta, \varepsilon) = (y_t - Q(s_t, a_t; \varepsilon, \zeta))^2$$

# Comparison

[Touati et al., 2019]

## Simple Chain domain

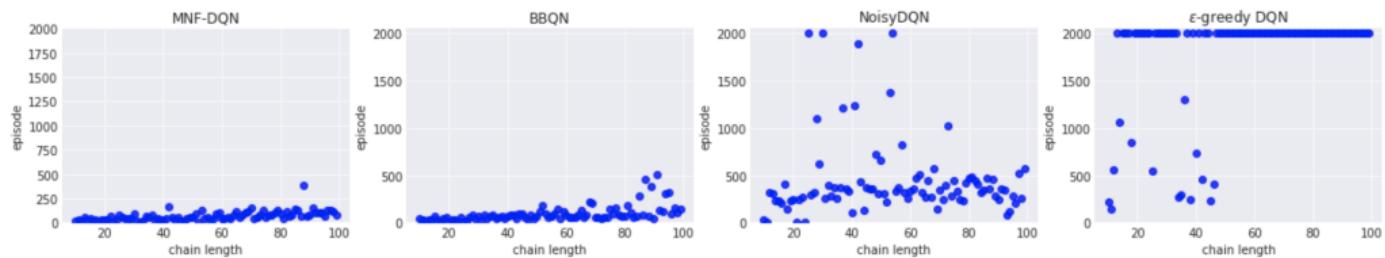
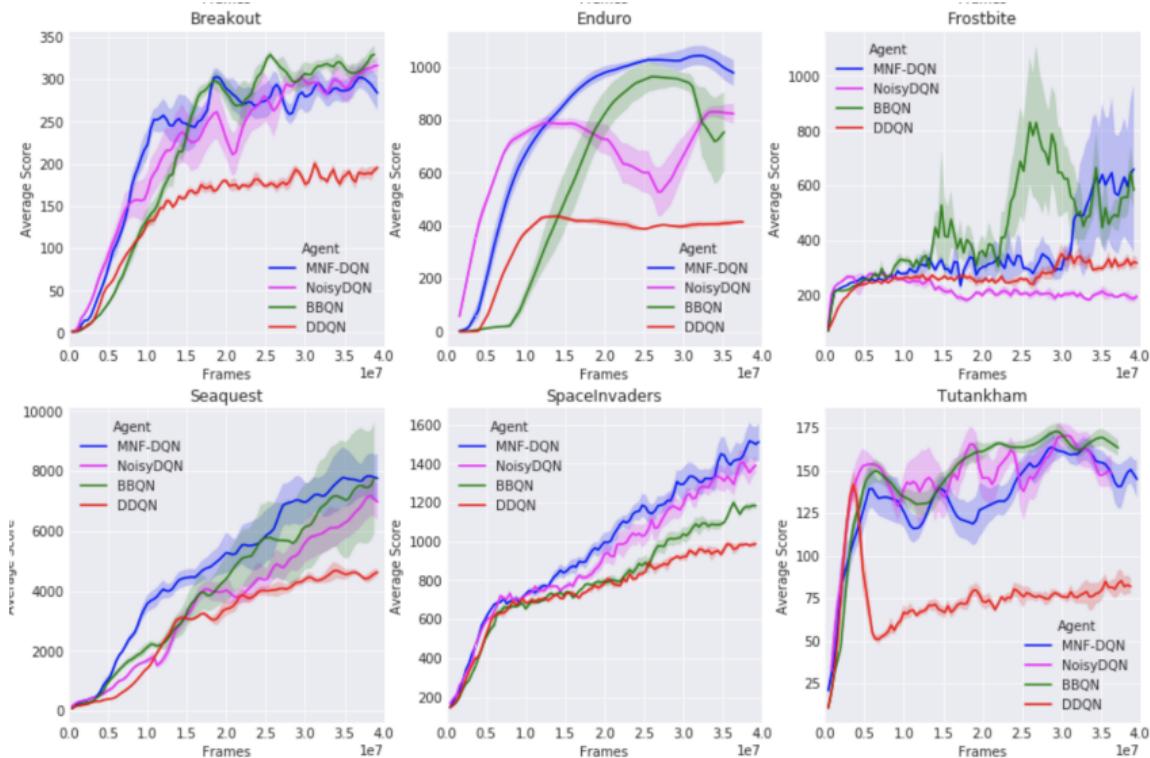


Figure 1: Median number of episodes (max 2000) required to solve the n-chain problem for (figure from left to right) MNF-DQN, BBQN, NoisyDQN and  $\epsilon$ -greedy DQN. The median is obtained over 10 runs with different seeds. We see that MNF-DQN consistently performs best across different chain lengths.

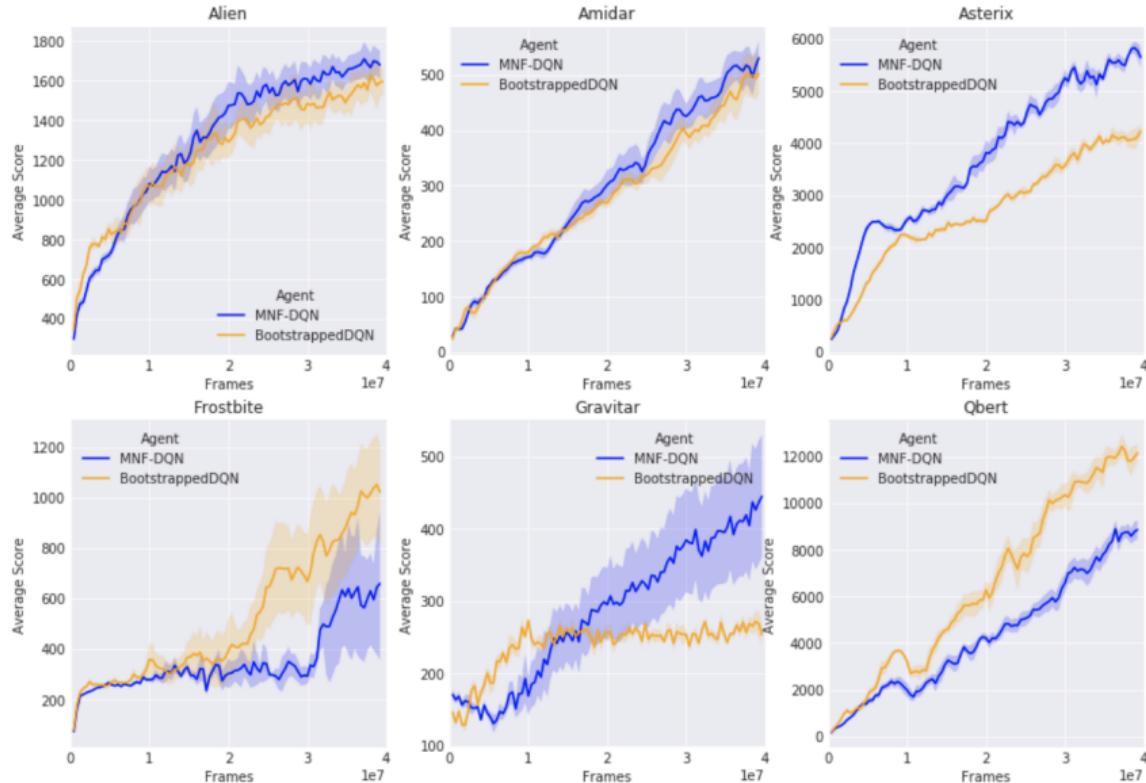
# Comparison: Atari

[Touati et al., 2019]



# Comparison: Atari

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# Exploration in Deep RL

- Several different techniques (*we have seen only a small part*)
  - No general solution
- 
- Exploration needs to account for uncertainty in the predictions
  - Should account for long-term effect

*Exploration at the level of (value/policy/model) parameters*

# What is not covered here?

- Information Gain
- Exploration via options
- Task-agnostic exploration
- Multi-task settings
- Meta learning

Thank you

# Materials

- References in these slides
- This nice blog [post](#) about exploration in DeepRL

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