Computer Engineering Department

# Exploration in RL

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Courtesy: Most of slides are adopted from CS 285, UC Berkeley.

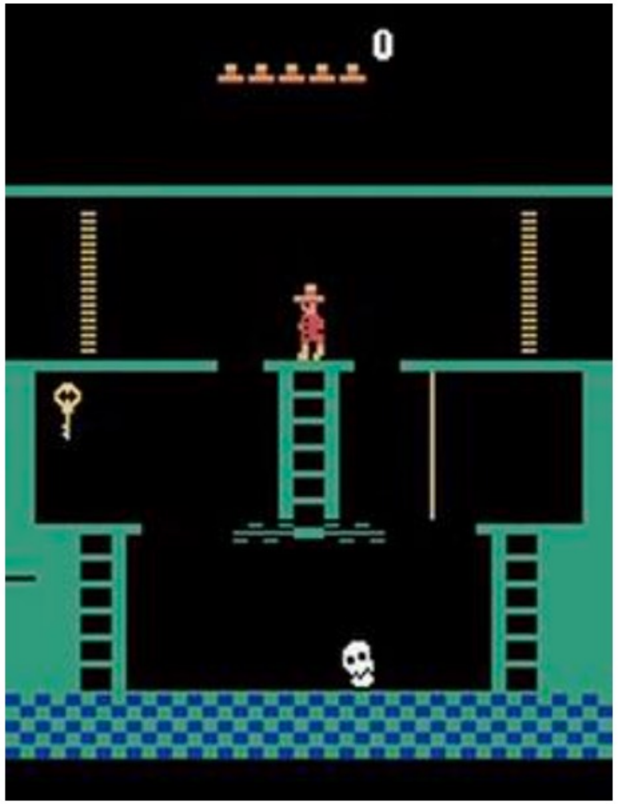
# What's the problem?

this is easy (mostly)


Why?

this is impossible

# Montezuma's revenge




- Getting key = reward
- Opening door = reward
- Getting killed by skull = nothing (is it good? bad?)
- Finishing the game only weakly correlates with rewarding events
- We know what to do because we understand what these sprites mean!

# Why exploration can be difficult?

- **Temporally extended** tasks like Montezuma's revenge become increasingly difficult based on
  - How extended the task is
  - How little you know about the rules
- Lets' assume a complex task
  - Consisting of multiple sub-task, each is a prerequisite for the next sub-task.
  - Each should be solved in a sequence to get a high reward
  - Epsilon greedy does not obviously help:
  - Suppose you mastered up to the $k^{th}$ sub-task.
  - You have to exploit up to the $k^{th}$ task and then explore onwards.
  - Now the chance to only explore in the sub-task (k+1) is $(1-\varepsilon)^{O(k)}\varepsilon^{O(1)}$.
  - For eps = 0.1, k = 5, this is ~ 6%. For eps = 0.5, this is ~ 3%.

# Exploration and exploitation

- Two potential definitions of exploration problem:
  - How can an agent **discover** **high-reward strategies** that require a temporally **extended sequence of complex behaviors** that, **individually, are not rewarding**?
  - How can an agent decide whether to **attempt new behaviors** (to discover ones with higher reward) or **continue to do the best thing it knows so far**?

# Optimal Exploration?

- Bayesian model of the environment. (POMDP with belief state)
- Optimize the expected reward under all uncertainties.
- Requires knowledge of state dynamic distribution class, the prior, and maintaining the belief state.
- Here we seek simpler solutions which could be extended to more complex scenarios.
- Compare the regret in such models against the Bayes' optimal approach.

$$\mathrm{Reg}(T) = TE[r(a^\star)] - \sum_{t=1}^{T} r(a_t)$$

expected reward of best action
(the best we can hope for in expectation)

actual reward of action
actually taken

# Bandits

assume $r(a_i) \sim p_{\theta_i}(r_i)$

e.g., $p(r_i = 1) = \theta_i$ and $p(r_i = 0) = 1 - \theta_i$

$\theta_i \sim p(\theta)$, but otherwise unknown

this defines a POMDP with $\mathbf{s} = [\theta_1, \ldots, \theta_n]$

belief state is $\hat{p}(\theta_1, \ldots, \theta_n)$

- solving the POMDP yields the optimal exploration strategy
- but that's overkill: belief state is huge!
- we can do very well with much simpler strategies

how do we measure goodness of exploration algorithm?

regret: difference from optimal policy at time step $T$: $\text{Reg}(T) = TE[r(a^\star)] - \sum_{t=1}^{T} r(a_t)$

expected reward of best action (the best we can hope for in expectation)

actual reward of action actually taken

# Optimistic exploration

keep track of average reward $\hat{\mu}_a$ for each action $a$

exploitation: pick $a = \arg\max \hat{\mu}_a$

optimistic estimate: $a = \arg\max \hat{\mu}_a + C\underline{\sigma_a}$

some sort of variance estimate

**intuition: try each arm until you are *sure* it's not great**

example (Auer et al. Finite-time analysis of the multiarmed bandit problem):

$$a = \arg\max \hat{\mu}_a + \sqrt{\frac{2 \ln T}{N(a)}}$$

number of times we picked this action

$\mathrm{Reg}(T)$ is $O(\log T)$, provably as good as any algorithm

# Probability matching/posterior sampling

assume $r(a_i) \sim p_{\theta_i}(r_i)$

this defines a POMDP with $\mathbf{s} = [\theta_1, \ldots, \theta_n]$

belief state is $\underline{\hat{p}(\theta_1, \ldots, \theta_n)}$

this is a *model* of our bandit

idea: sample $\theta_1, \ldots, \theta_n \sim \hat{p}(\theta_1, \ldots, \theta_n)$

pretend the model $\theta_1, \ldots, \theta_n$ is correct

take the optimal action

update the model

- This is called posterior sampling or Thompson sampling
- Harder to analyze theoretically
- Can work very well empirically
- See: Chapelle & Li, "An Empirical Evaluation of Thompson Sampling."

# Information gain

## Bayesian experimental design:

say we want to determine some latent variable $z$ (e.g., $z$ might be the optimal action, or its value)

which action do we take?

let $\mathcal{H}(\hat{p}(z))$ be the current entropy of our $z$ estimate

let $\mathcal{H}(\hat{p}(z)|y)$ be the entropy of our $z$ estimate after observation $y$ (e.g., $y$ might be $r(a)$)

the lower the entropy, the more precisely we know $z$

$$\mathrm{IG}(z, y) = E_y[\mathcal{H}(\hat{p}(z)) - \mathcal{H}(\hat{p}(z)|y)]$$

typically depends on action, so we have $\mathrm{IG}(z, y|a)$

# Information gain example

$$\mathrm{IG}(z, y|a) = E_y[\mathcal{H}(\hat{p}(z)) - \mathcal{H}(\hat{p}(z)|y)|a]$$

how much we learn about $z$ from action $a$, given current beliefs

Example bandit algorithm:
Russo & Van Roy "Learning to Optimize via Information-Directed Sampling"

$y = r_a$, $z = \theta_a$ (parameters of model $p(r_a)$)

$g(a) = \mathrm{IG}(\theta_a, r_a|a)$ – information gain of $a$

$\Delta(a) = E[r(a^\star) - r(a)]$ – expected suboptimality of $a$

choose $a$ according to $\arg\min_a \frac{\Delta(a)^2}{g(a)}$

don't take actions that you're sure are suboptimal

don't bother taking actions if you won't learn anything

# General themes

UCB:

$$a = \arg\max \hat{\mu}_a + \sqrt{\frac{2 \ln T}{N(a)}}$$

Thompson sampling:

$$\theta_1, \dots, \theta_n \sim \hat{p}(\theta_1, \dots, \theta_n)$$

$$a = \arg\max_a E_{\theta_a}[r(a)]$$

Info gain:

$$\mathrm{IG}(z, y|a)$$

- Most exploration strategies require some kind of uncertainty estimation (even if it’s naïve)
- Usually assumes some value to new information
  - Assume unknown = good (optimism)
  - Assume sample = truth
  - Assume information gain = good

# Optimistic exploration in RL

UCB: $$a = \arg\max \hat{\mu}_a + \underbrace{\sqrt{\frac{2 \ln T}{N(a)}}}_{\text{"exploration bonus"}}$$

lots of functions work, so long as they decrease with $N(a)$

can we use this idea with MDPs?

count-based exploration: use $N(\mathbf{s}, \mathbf{a})$ or $N(\mathbf{s})$ to add *exploration bonus*

use $r^+(\mathbf{s}, \mathbf{a}) = r(\mathbf{s}, \mathbf{a}) + \mathcal{B}(N(\mathbf{s}))$

bonus that decreases with $N(\mathbf{s})$

use $r^+(\mathbf{s}, \mathbf{a})$ instead of $r(\mathbf{s}, \mathbf{a})$ with any model-free algorithm

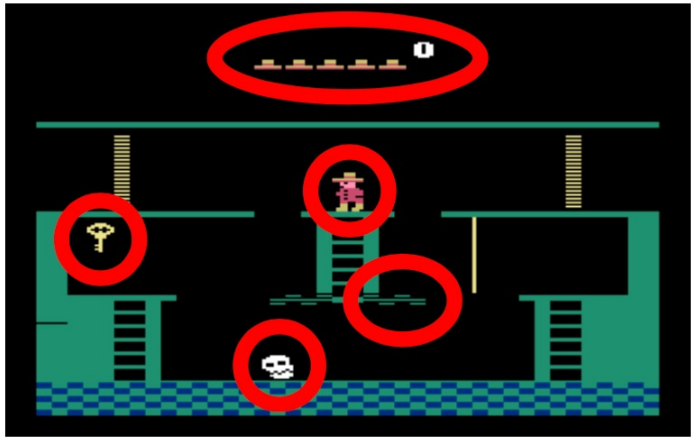
+ simple addition to any RL algorithm

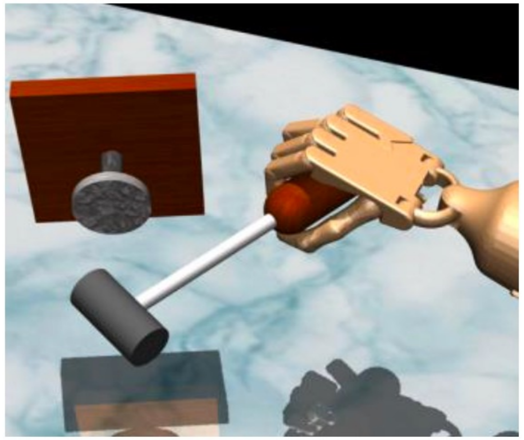
- need to tune bonus weight

# The trouble with counts

$$\text{use } r^+(\mathbf{s}, \mathbf{a}) = r(\mathbf{s}, \mathbf{a}) + \mathcal{B}(N(\mathbf{s}))$$

But wait… what's a count?





Uh oh… we never see the same thing twice!

But some states are more similar than others

# Fitting generative models

idea: fit a density model $p_\theta(\mathbf{s})$ (or $p_\theta(\mathbf{s}, \mathbf{a})$)

$p_\theta(\mathbf{s})$ might be high even for a new $\mathbf{s}$

if $\mathbf{s}$ is similar to previously seen states

can we use $p_\theta(\mathbf{s})$ to get a "pseudo-count"?

if we have small MDPs

the true probability is:

$$\underbrace{P(\mathbf{s})}_{\text{probability/density}} = \frac{\overbrace{N(\mathbf{s})}^{\text{count}}}{\underbrace{n}_{\text{total states visited}}}$$

after we see $\mathbf{s}$, we have:

$$P'(\mathbf{s}) = \frac{N(\mathbf{s}) + 1}{n + 1}$$

# Exploring with pseudo-counts

fit model $p_\theta(\mathbf{s})$ to all states $\mathcal{D}$ seen so far

take a step $i$ and observe $\mathbf{s}_i$

fit new model $p_{\theta'}(\mathbf{s})$ to $\mathcal{D} \cup \mathbf{s}_i$

use $p_\theta(\mathbf{s}_i)$ and $p_{\theta'}(\mathbf{s}_i)$ to estimate $\hat{N}(\mathbf{s})$

set $r_i^+ = r_i + \mathcal{B}(\hat{N}(\mathbf{s}))$ ← "pseudo-count"

how to get $\hat{N}(\mathbf{s})$? use the equations

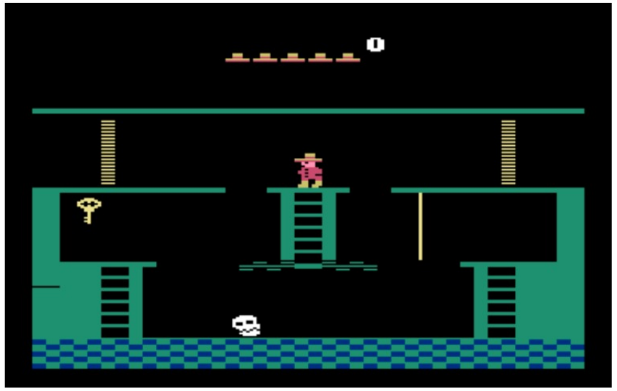
$$p_\theta(\mathbf{s}_i) = \frac{\hat{N}(\mathbf{s}_i)}{\hat{n}} \qquad p_{\theta'}(\mathbf{s}_i) = \frac{\hat{N}(\mathbf{s}_i) + 1}{\hat{n} + 1}$$

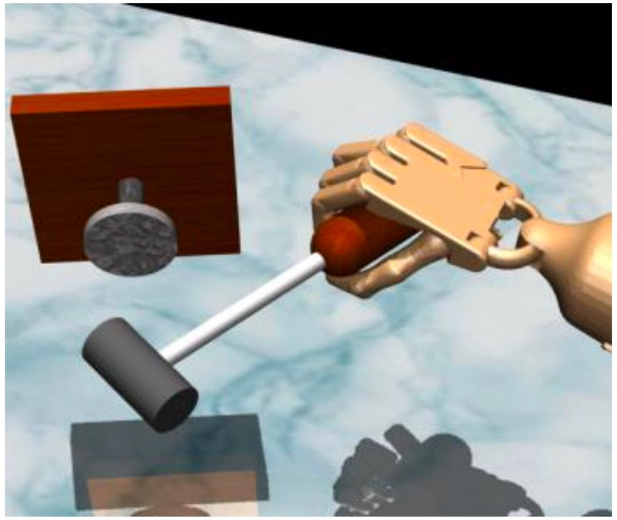
two equations and two unknowns!

$$\hat{N}(\mathbf{s}_i) = \hat{n} p_\theta(\mathbf{s}_i) \qquad \hat{n} = \frac{1 - p_{\theta'}(\mathbf{s}_i)}{p_{\theta'}(\mathbf{s}_i) - p_\theta(\mathbf{s}_i)} p_\theta(\mathbf{s}_i)$$

Bellemare et al. "Unifying Count-Based Exploration…"

# What kind of generative modeling to use?



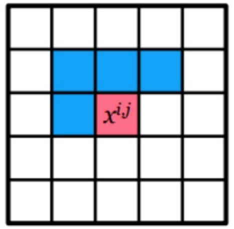


$$p_\theta(\mathbf{s})$$

need to be able to output densities, but doesn't necessarily need to produce great samples

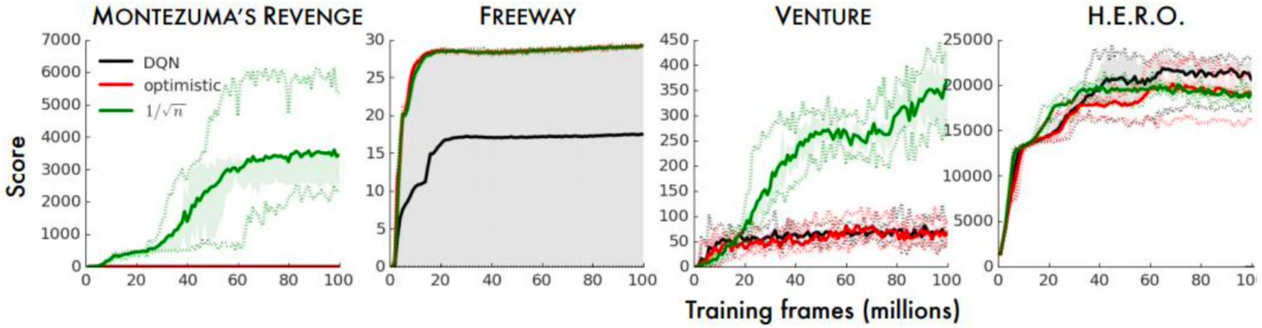
opposite considerations from many popular generative models in the literature (e.g., GANs)

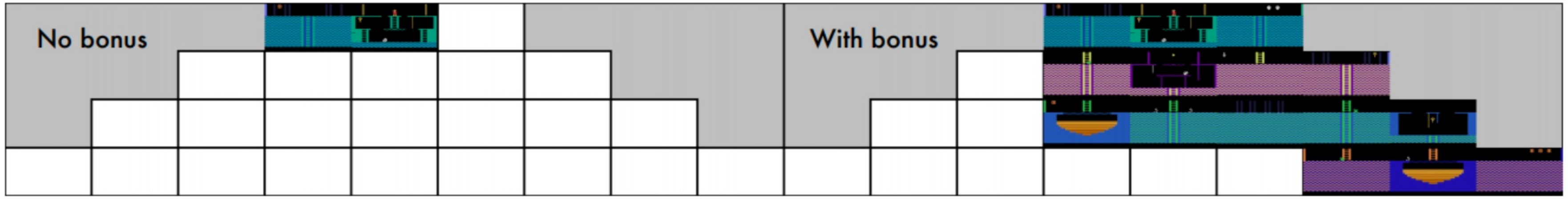
Bellemare et al.: "CTS" model: condition each pixel on its top-left neighborhood




Other models: stochastic neural networks, compression length, EX2

# Does it work?




Bellemare et al. "Unifying Count-Based Exploration…"

# Counting with hashes

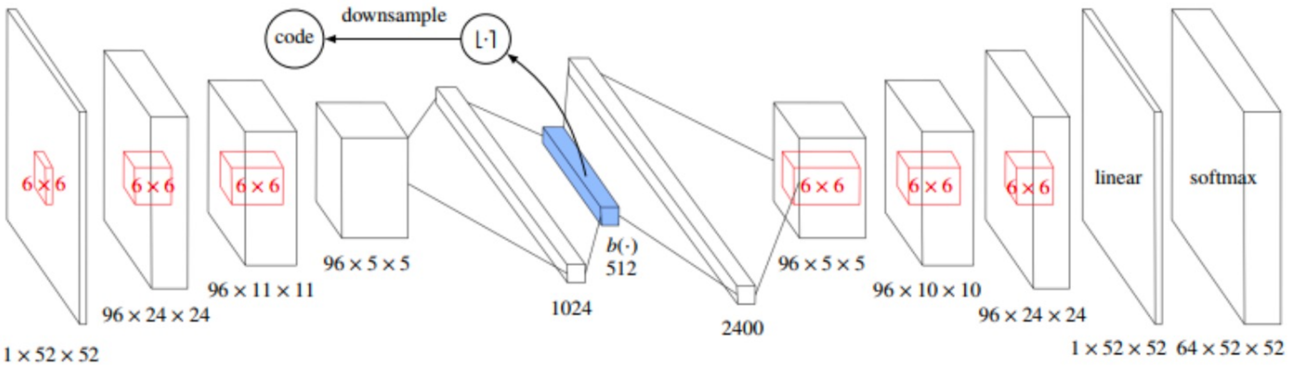
## What if we still count states, but in a different space?

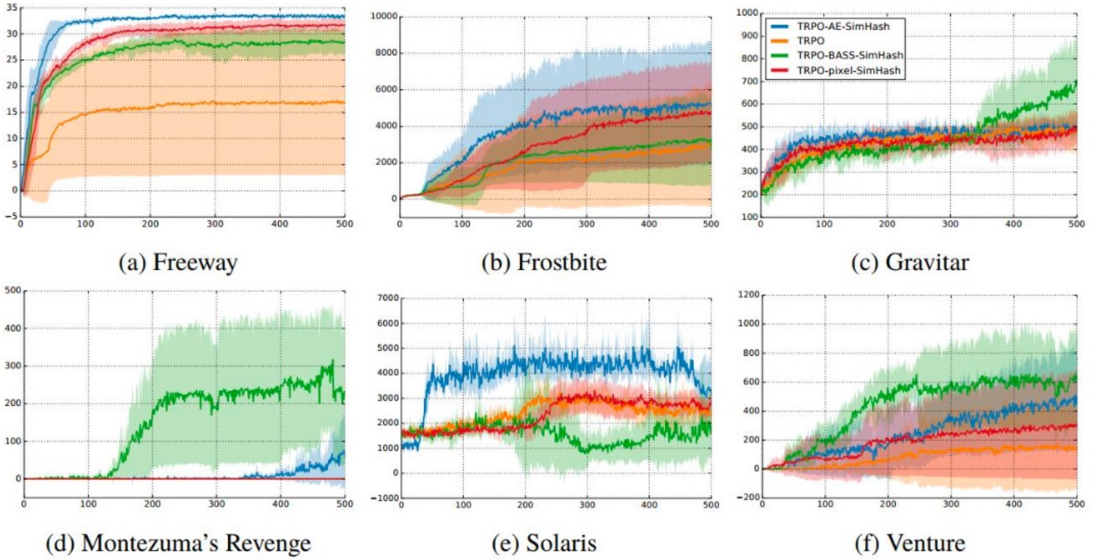
idea: compress $\mathbf{s}$ into a $k$-bit code via $\phi(\mathbf{s})$, then count $N(\phi(\mathbf{s}))$

shorter codes = more hash collisions

similar states get the same hash? maybe

improve the odds by *learning* a compression:




Tang et al. "#Exploration: A Study of Count-Based Exploration"

# Implicit density modeling with exemplar models

$p_\theta(\mathbf{s})$ need to be able to output densities, but doesn't necessarily need to produce great samples

Can we explicitly compare the new state to past states?

Intuition: the state is **novel** if it is **easy** to distinguish from all previous seen states by a classifier

for each observed state $\mathbf{s}$, fit a classifier to classify that state against all past states $\mathcal{D}$, use classifier error to obtain density

$$p_\theta(\mathbf{s}) = \frac{1 - D_{\mathbf{s}}(\mathbf{s})}{D_{\mathbf{s}}(\mathbf{s})}$$

probability that classifier assigns that $\mathbf{s}$ is "positive"
positives: $\{\mathbf{s}\}$
negatives: $\mathcal{D}$

Fu et al. "EX2: Exploration with Exemplar Models…"

# Implicit density modeling with exemplar models

$$D_{x^*} = \underset{D \in \mathcal{D}}{\arg\max} \left( E_{\delta_{x^*}}[\log D(x)] + E_{P_{\mathcal{X}}}[\log 1 - D(x)] \right) . \quad (1)$$

**Proposition 1.** *(Optimal Discriminator) For a discrete distribution $P_{\mathcal{X}}(x)$, the optimal discriminator $D_{x^*}$ for exemplar $x^*$ satisfies*

$$D_{x^*}(x) = \frac{\delta_{x^*}(x)}{\delta_{x^*}(x) + P_{\mathcal{X}}(x)} \quad \textit{and} \quad D_{x^*}(x^*) = \frac{1}{1 + P_{\mathcal{X}}(x^*)}.$$

*Proof.* The proof is obtained by taking the derivative of the loss in Eq. (1) with respect to $D(x)$, setting it to zero, and solving for $D(x)$. □

# Implicit density modeling with exemplar models

hang on... aren't we just checking if $\mathbf{s} = \mathbf{s}$?

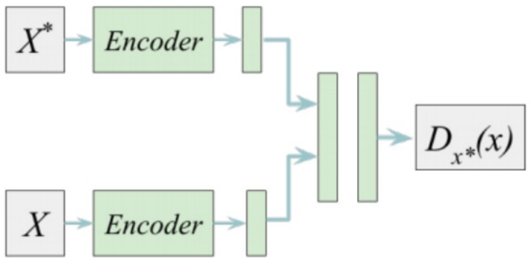
if $\mathbf{s} \in \mathcal{D}$, then the optimal $D_{\mathbf{s}}(\mathbf{s}) \neq 1$

in fact: $D^\star_{\mathbf{s}}(\mathbf{s}) = \frac{1}{1 + p(\mathbf{s})}$ $\longrightarrow$ $p_\theta(\mathbf{s}) = \frac{1 - D_{\mathbf{s}}(\mathbf{s})}{D_{\mathbf{s}}(\mathbf{s})}$

in reality, each state is unique, so we *regularize* the classifier

isn't one classifier per state a bit much?

train one *amortized* model: single network that takes in exemplar as input!



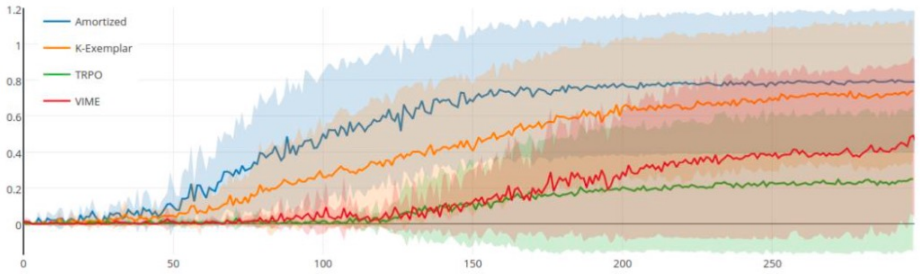




Figure 9: DoomMyWayHome+

Fu et al. "EX2: Exploration with Exemplar Models…"

# Heuristic estimation of counts via errors

$p_\theta(\mathbf{s})$ need to be able to output densities, but doesn't necessarily need to produce great samples

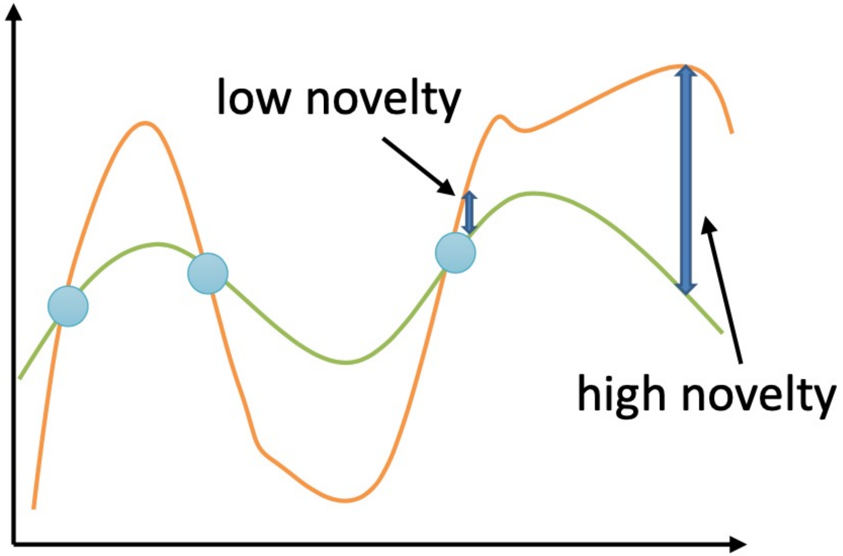
…and doesn't even need to output great densities

…just need to tell if state is **novel** or not!

let's say we have some **target** function $f^\star(\mathbf{s}, \mathbf{a})$

given our buffer $\mathcal{D} = \{(\mathbf{s}_i, \mathbf{a}_i)\}$, fit $\hat{f}_\theta(\mathbf{s}, \mathbf{a})$

use $\mathcal{E}(\mathbf{s}, \mathbf{a}) = ||\hat{f}_\theta(\mathbf{s}, \mathbf{a}) - f^\star(\mathbf{s}, \mathbf{a})||^2$ as bonus



# Heuristic estimation of counts via errors

what should we use for $f^{\star}(\mathbf{s}, \mathbf{a})$?

one common choice: set $f^{\star}(\mathbf{s}, \mathbf{a}) = \mathbf{s}'$ – i.e., next state prediction

even simpler: $f^{\star}(\mathbf{s}, \mathbf{a}) = f_{\phi}(\mathbf{s}, \mathbf{a})$, where $\phi$ is a *random* parameter vector

Burda et al. Exploration by random network distillation. 2018.

# Posterior sampling in deep RL

**Thompson sampling:**

$$\theta_1, \ldots, \theta_n \sim \hat{p}(\theta_1, \ldots, \theta_n)$$

$$a = \arg\max_a E_{\theta_a}[r(a)]$$

What do we sample?

How do we represent the distribution?

bandit setting: $\hat{p}(\theta_1, \ldots, \theta_n)$ is distribution over *rewards*

MDP analog is the $Q$-function!

1. sample Q-function $Q$ from $p(Q)$
2. act according to $Q$ for one episode
3. update $p(Q)$

since Q-learning is off-policy, we don't care which Q-function was used to collect data

how can we represent a distribution over functions?

Osband et al. "Deep Exploration via Bootstrapped DQN"

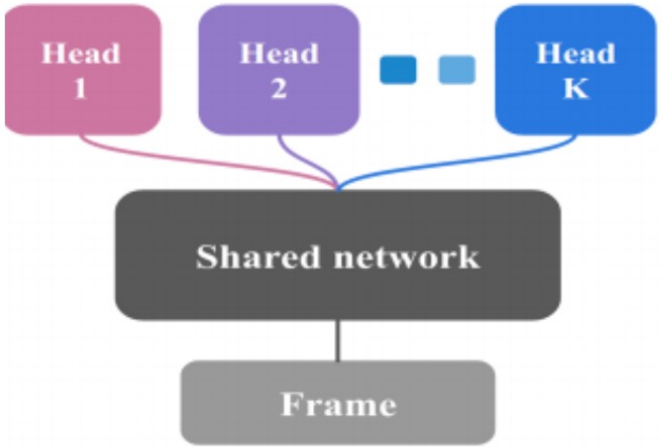
# Bootstrap

given a dataset $\mathcal{D}$, resample with replacement $N$ times to get $\mathcal{D}_1, \dots, \mathcal{D}_N$

train each model $f_{\theta_i}$ on $\mathcal{D}_i$

to sample from $p(\theta)$, sample $i \in [1, \dots, N]$ and use $f_{\theta_i}$

training $N$ big neural nets is expensive, can we avoid it?




Osband et al. "Deep Exploration via Bootstrapped DQN"

# Bootstrap

**Algorithm 1** Bootstrapped DQN

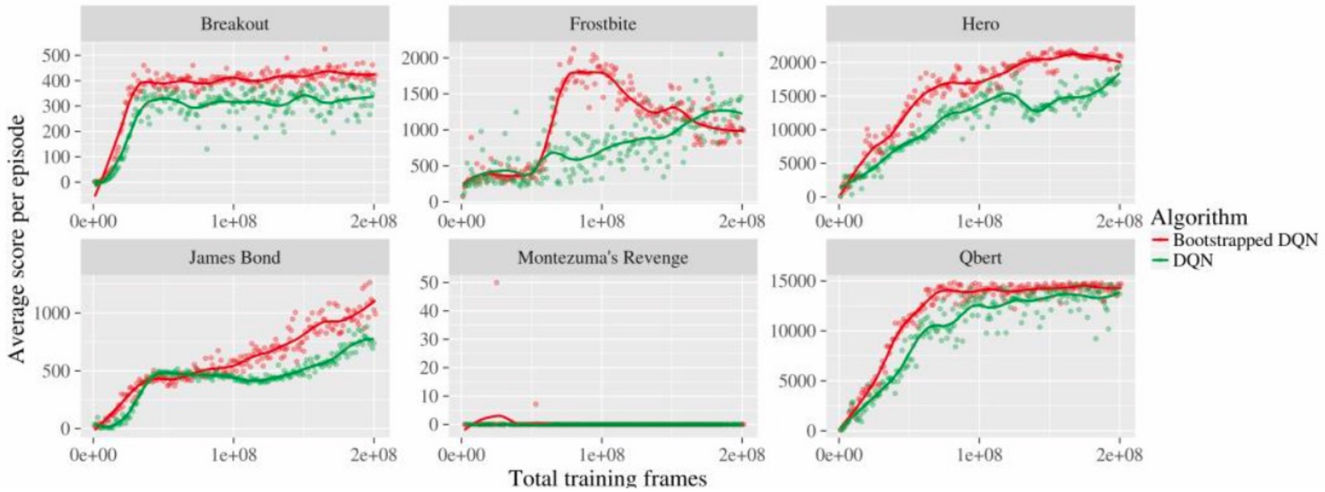
```
Input: Value function networks Q with K outputs {Q_k}_{k=1}^K. Masking distribution M.
Let B be a replay buffer storing experience for training.
for each episode do
    Obtain initial state from environment s_0
    Pick a value function to act using k ~ Uniform{1, ..., K}
    for step t = 1, ... until end of episode do
        Pick an action according to a_t ∈ arg max_a Q_k(s_t, a)
        Receive state s_{t+1} and reward r_t from environment, having taking action a_t
        Sample bootstrap mask m_t ~ M
        Add (s_t, a_t, r_{t+1}, s_{t+1}, m_t) to replay buffer B
    end for
end for
```

Osband et al. "Deep Exploration via Bootstrapped DQN"

# Why does this work?

Exploring with random actions (e.g., epsilon-greedy): oscillate back and forth, might not go to a coherent or interesting place

Exploring with random Q-functions: commit to a randomized but internally consistent strategy for an entire episode


+ no change to original reward function

- very good bonuses often do better

Osband et al. “Deep Exploration via Bootstrapped DQN”