Exploration

CS 294-112: Deep Reinforcement Learning

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Class Notes

1. Homework 4 due on Wednesday
2. Project proposal feedback sent

Today's Lecture

1. What is exploration? Why is it a problem?
2. Multi-armed bandits and theoretically grounded exploration
3. Optimism-based exploration
4. Posterior matching exploration
5. Information-theoretic exploration

- Goals:
  - Understand what the exploration is
  - Understand how theoretically grounded exploration methods can be derived
  - Understand how we can do exploration in deep RL in practice

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!

Put yourself in the algorithm's shoes

Mao

- "the only rule you may be told is this one"
- Incur a penalty when you break a rule
- Can only discover rules through trial and error
- Rules don't always make sense to you

- Temporally extended tasks like Montezuma's revenge become increasingly difficult based on
  - How extended the task is
  - How little you know about the rules
- Imagine if your goal in life was to win 50 games of Mao…
- (and you didn't know this in advance)

Another example

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?
- Actually the same problem:
  - Exploitation: doing what you *know* will yield highest reward
  - Exploration: doing things you haven’t done before, in the hopes of getting even higher reward

Exploration and exploitation examples

- Restaurant selection
  - Exploitation: go to your favorite restaurant
  - Exploration: try a new restaurant
- Online ad placement
  - Exploitation: show the most successful advertisement
  - Exploration: show a different random advertisement
- Oil drilling
  - Exploitation: drill at the best known location
  - Exploration: drill at a new location

Examples from D. Silver lecture notes: http://www0.cs.ucl.ac.uk/staff/d.silver/web/Teaching_files/XX.pdf

Exploration is hard

Can we derive an **optimal** exploration strategy?

what does optimal even mean?

regret vs. Bayes-optimal strategy? more on this later…

multi-armed bandits (1-step stateless RL problems)	contextual bandits (1-step RL problems)	small, finite MDPs (e.g., tractable planning, model-based RL setting)	large, infinite MDPs, continuous spaces

← →

theoretically tractable … theoretically intractable

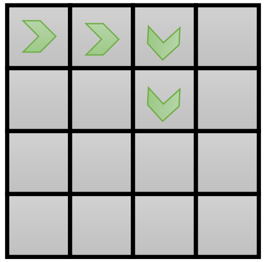
What makes an exploration problem tractable?

multi-arm bandits

contextual bandits

can formalize exploration as POMDP identification

policy learning is trivial even with POMDP



small, finite MDPs

can frame as Bayesian model identification, reason explicitly about value of information

large or infinite MDPs

optimal methods don't work

...but can take inspiration from optimal methods in smaller settings

use hacks

Bandits

What's a bandit anyway?

the drosophila of exploration problems

$\mathcal{A} = \{\text{pull arm}\}$

$r(\text{pull arm}) = ?$

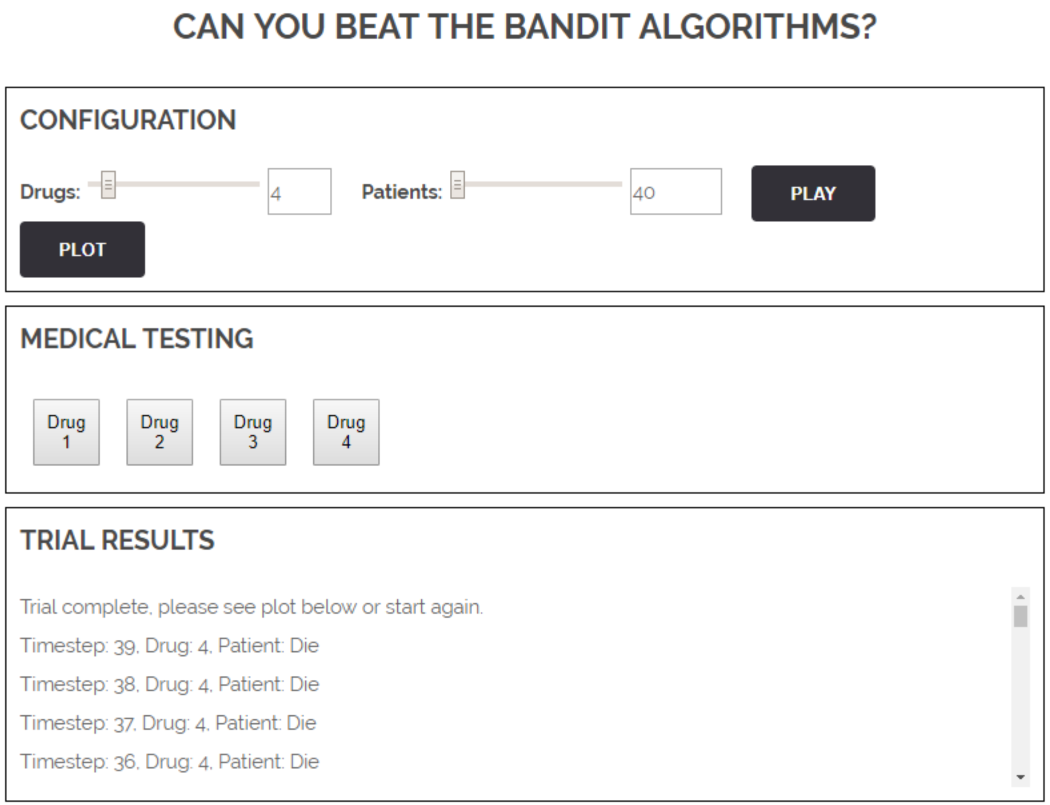
$\mathcal{A} = \{\text{pull}_1, \text{pull}_2, \ldots, \text{pull}_n\}$

$r(a_n) = ?$

assume $r(a_n) \sim p(r|a_n)$

unknown *per-action* reward distribution!

Let’s play!



- Drug prescription problem
- Bandit arm = drug (1 of 4)
- Reward
  - 1 if patient lives
  - 0 if patient dies
  - (stakes are high)
- How well can you do?

http://iosband.github.io/2015/07/28/Beat-the-bandit.html

How can we define the bandit?

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

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

actual reward of action actually taken

How can we beat the bandit?

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

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

actual reward of action
actually taken

- Variety of relatively simple strategies
- Often can provide theoretical guarantees on regret
  - Variety of optimal algorithms (up to a constant factor)
  - But empirical performance may vary…
- Exploration strategies for more complex MDP domains will be inspired by these strategies

Optimistic exploration

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

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

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

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

$\text{Reg}(T)$ 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:

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

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

Info gain:

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

- 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

Why should we care?

- Bandits are easier to analyze and understand
- Can derive foundations for exploration methods
- Then apply these methods to more complex MDPs

- Not covered here:
  - Contextual bandits (bandits with state, essentially 1-step MDPs)
  - Optimal exploration in small MDPs
  - Bayesian model-based reinforcement learning (similar to information gain)
  - Probably approximately correct (PAC) exploration

Break

Classes of exploration methods in deep RL

- Optimistic exploration:
  - new state = good state
  - requires estimating state visitation frequencies or novelty
  - typically realized by means of exploration bonuses
- Thompson sampling style algorithms:
  - learn distribution over Q-functions or policies
  - sample and act according to sample
- Information gain style algorithms
  - reason about information gain from visiting new states

Optimistic exploration in RL

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

"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

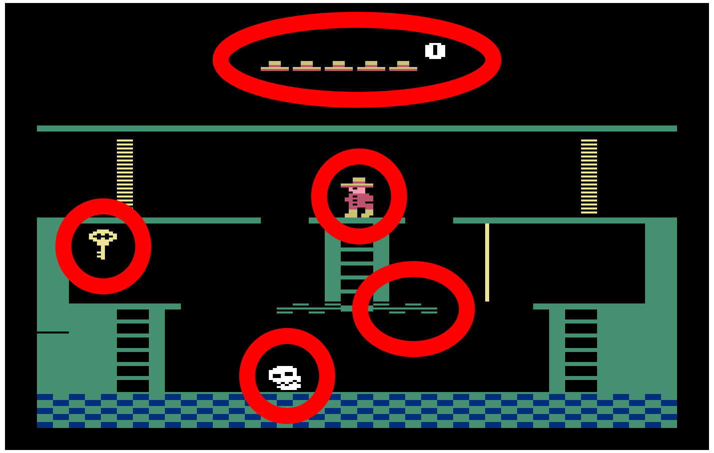
+ simple addition to any RL algorithm

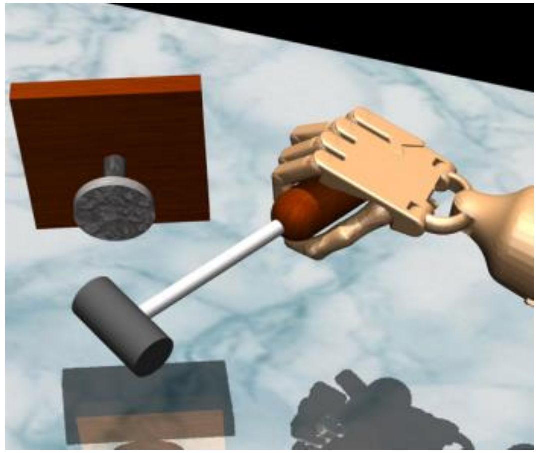
- need to tune bonus weight

The trouble with counts

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

But wait… what's a count?

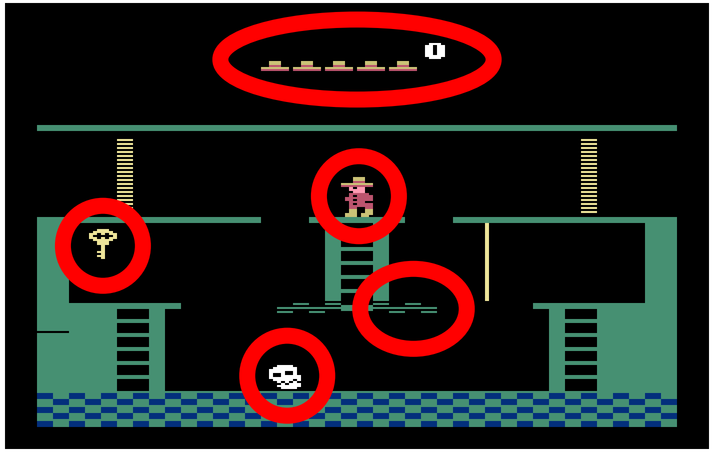




Uh oh… we never see the same thing twice!

But some states are more similar than others

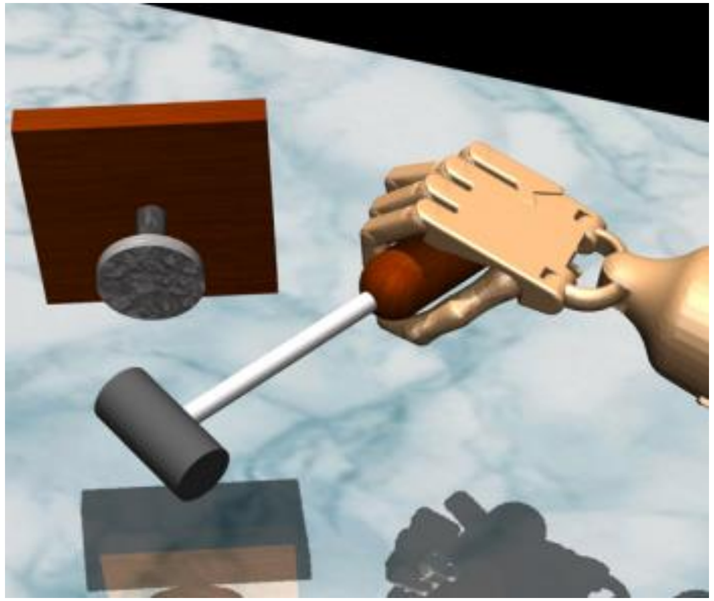
Fitting generative models



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:

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

count

probability/density

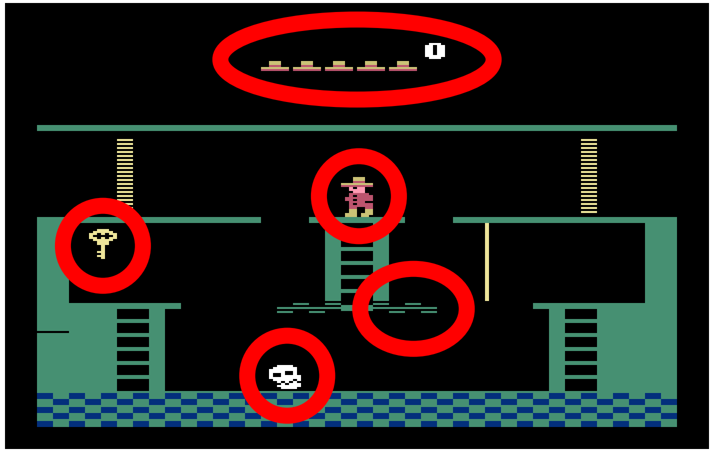
total states visited

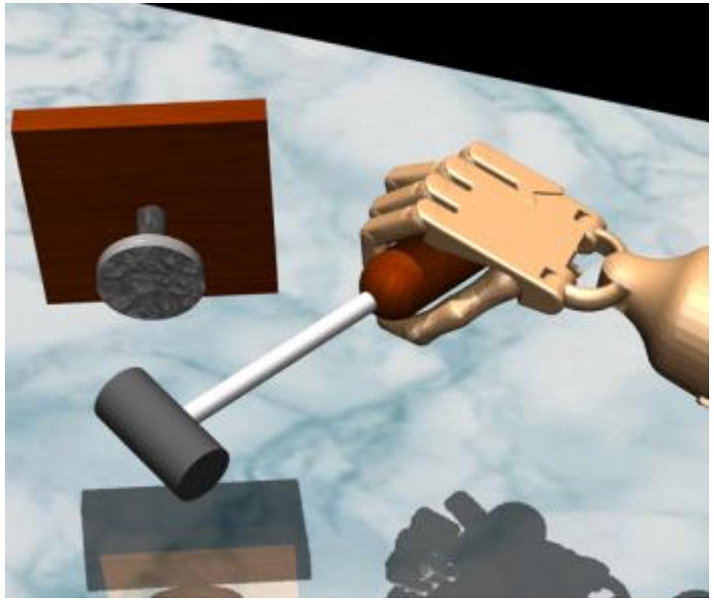
after we see $\mathbf{s}$, we have:

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

can we get $p_\theta(\mathbf{s})$ and $p_{\theta'}(\mathbf{s})$ to obey these equations?

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 bonus to use?

Lots of functions in the literature, inspired by optimal methods for bandits or small MDPs

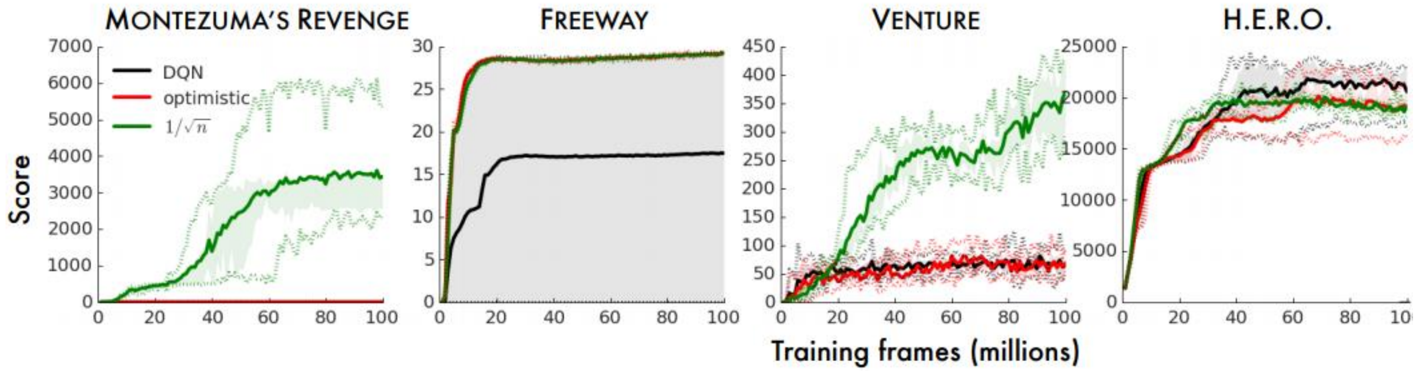
UCB: $$\mathcal{B}(N(\mathbf{s})) = \sqrt{\frac{2 \ln n}{N(\mathbf{s})}}$$

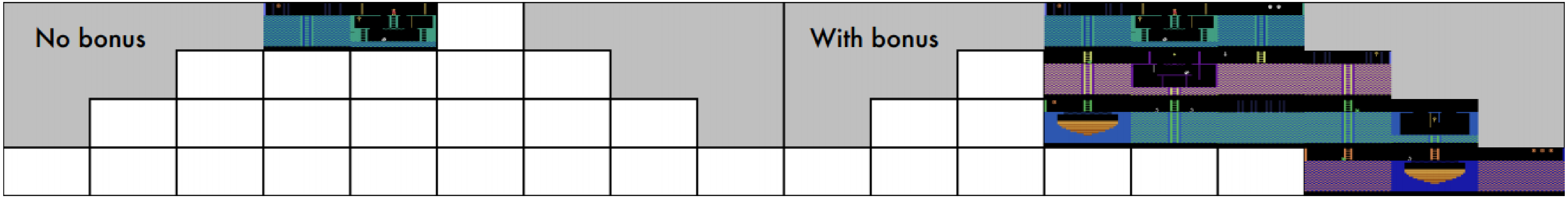
MBIE-EB (Strehl & Littman, 2008): $$\mathcal{B}(N(\mathbf{s})) = \sqrt{\frac{1}{N(\mathbf{s})}}$$

this is the one used by Bellemare et al. ‘16

BEB (Kolter & Ng, 2009): $$\mathcal{B}(N(\mathbf{s})) = \frac{1}{N(\mathbf{s})}$$

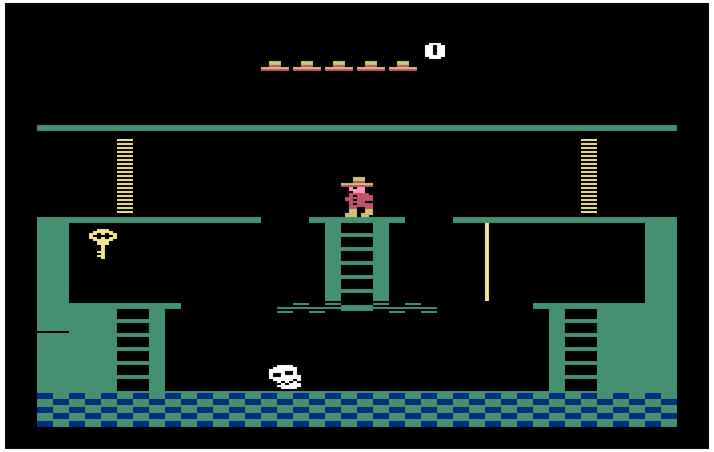
Does it work?

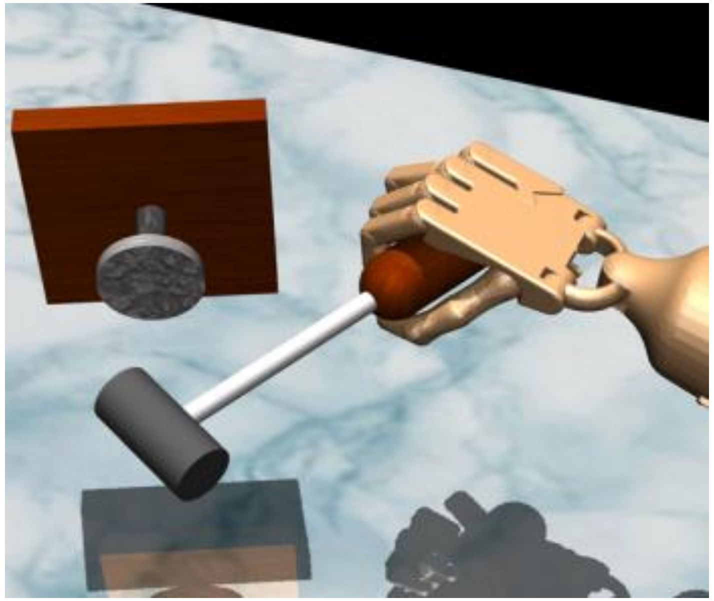




Bellemare et al. "Unifying Count-Based Exploration…"

What kind of model to use?



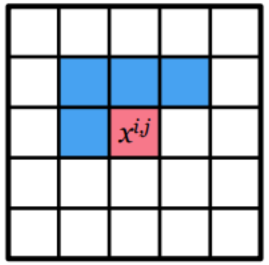


$$p_\theta(\mathbf{s})$$

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

Counting with hashes

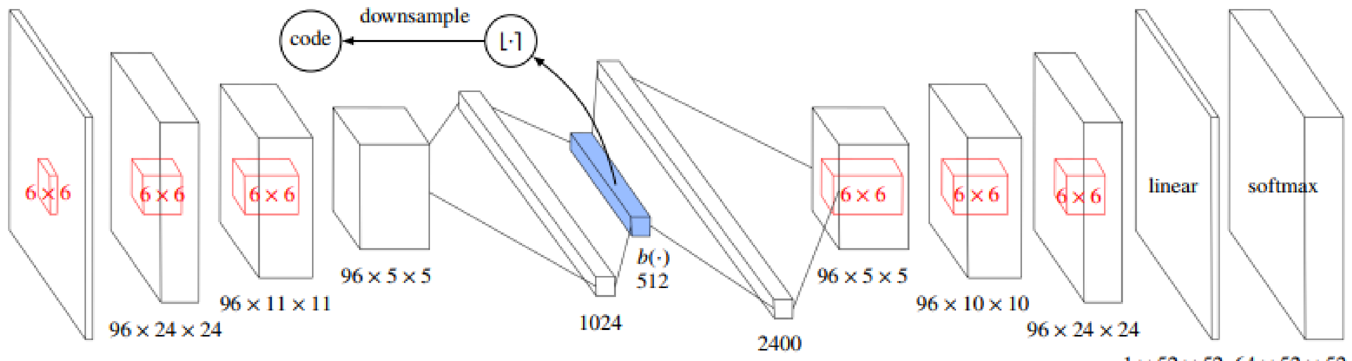
What if we still count states, but in a different space?

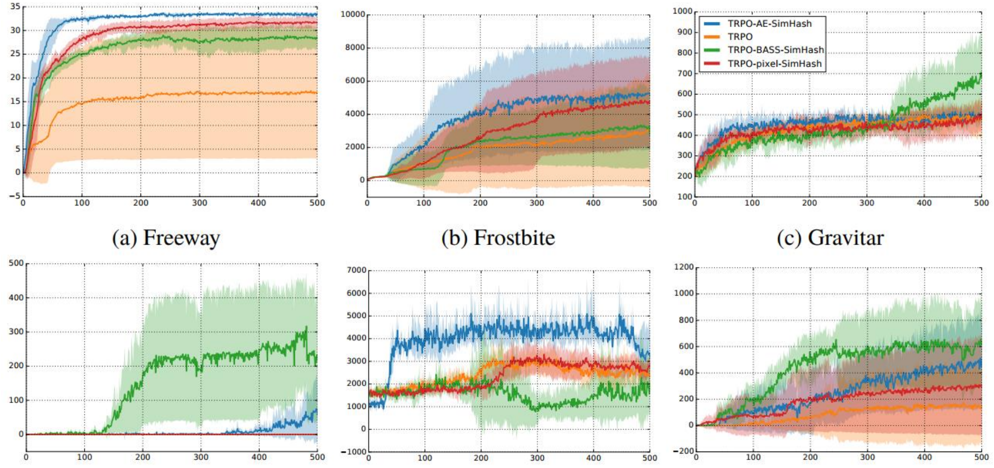
idea: compress $\mathbf{s}$ into a k-bit code via $\phi(\mathbf{s})$, then count $N(\phi(\mathbf{s}))$

shorter codes $=$ more hash collisions

similar states get the same hash? maybe

improve the odds by *learning* a compression:





(a) Freeway (b) Frostbite (c) Gravitar

(d) Montezuma's Revenge (e) Solaris (f) Venture

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

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

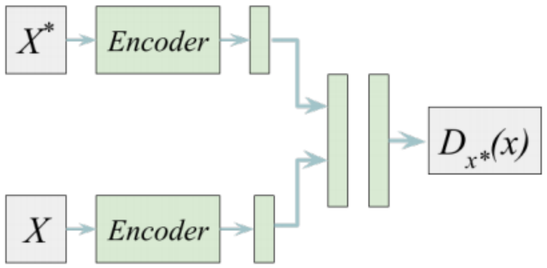
if $\mathbf{s} \in \mathcal{D}$, then the optimal $D_{\mathbf{s}}(\mathbf{s}) \neq 1$

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

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!



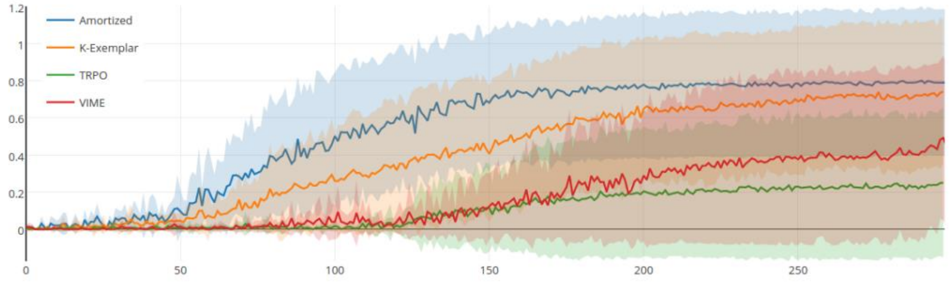


Figure 9: DoomMyWayHome+

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

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?

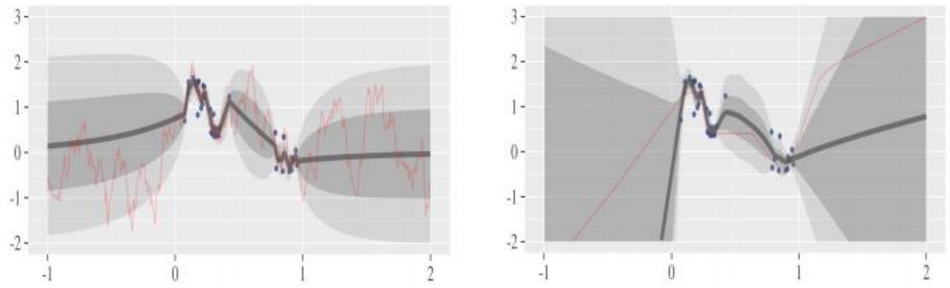
Osband et al. "Deep Exploration via Bootstrapped DQN"

Bootstrap

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

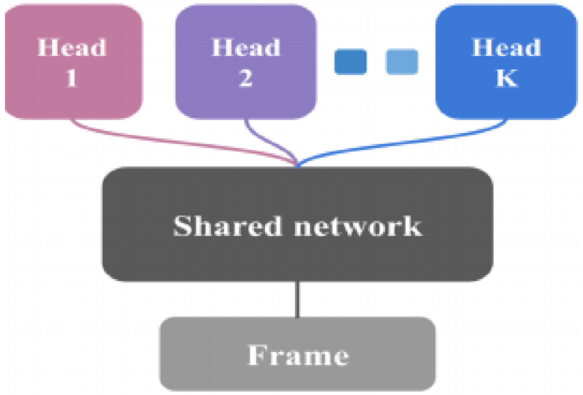
train each model f_{θ_i} on $\mathcal{D}_i$

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



(b) Gaussian process posterior (c) Bootstrapped neural nets

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

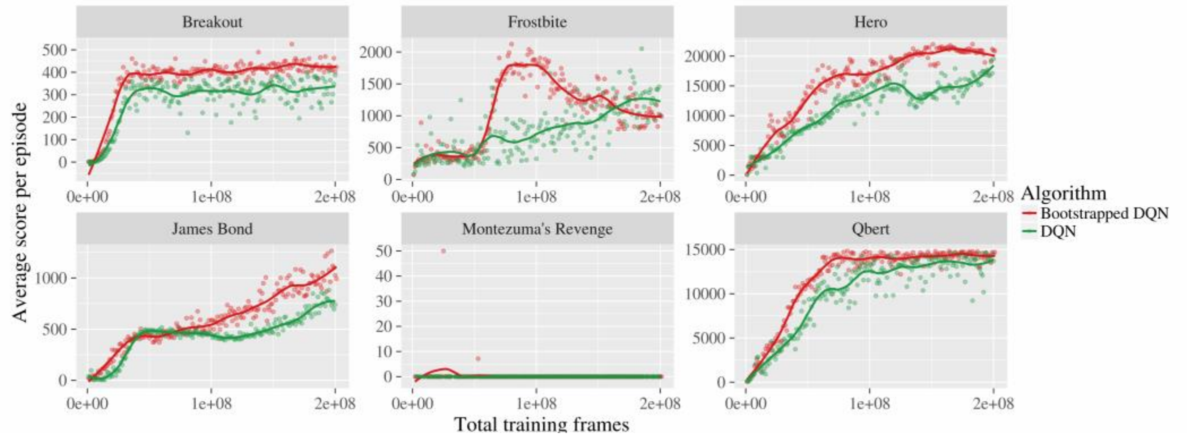


Osband et al. “Deep Exploration via Bootstrapped DQN”

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”

Reasoning about information gain (approximately)

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

information gain about *what*?

information gain about reward $r(\mathbf{s}, \mathbf{a})$?	not very useful if reward is sparse
state density $p(\mathbf{s})$?	a bit strange, but actually makes sense!
information gain about dynamics $p(\mathbf{s}'|\mathbf{s}, \mathbf{a})$?	good proxy for *learning* the MDP, though still heuristic

Generally intractable to use exactly, regardless of what is being estimated!

Reasoning about information gain (approximately)

Generally intractable to use exactly, regardless of what is being estimated

A few approximations:

prediction gain: $\log p_{\theta'}(\mathbf{s}) - \log p_\theta(\mathbf{s})$ (Schmidhuber '91, Bellemare '16)

intuition: if density changed a lot, the state was novel

variational inference: (Houthooft et al. "VIME")

IG can be equivalently written as $D_{\mathrm{KL}}(p(\theta|h, \underline{s_t, a_t, s_{t+1}})\|p(\theta|h))$

model parameters for $p_\theta(s_{t+1}|s_t, a_t)$

newly observed transition

history of all prior transitions

intuition: a transition is more informative if it causes belief over θ to change

idea: use variational inference to estimate $q(\theta|\phi) \approx p(\theta|h)$

given new transition (s, a, s'), update ϕ to get ϕ'

Reasoning about information gain (approximately)

VIME implementation:

IG can be equivalently written as $D_{\mathrm{KL}}(p(\theta|h, \underline{s_t, a_t, s_{t+1}})\|p(\theta|h))$

- θ: model parameters for $p_\theta(s_{t+1}|s_t, a_t)$
- h: history of all prior transitions
- s_t, a_t, s_{t+1}: newly observed transition

$q(\theta|\phi) \approx p(\theta|h)$ specifically, optimize variational lower bound $D_{\mathrm{KL}}(q(\theta|\phi)\|p(h|\theta)p(\theta))$

represent $q(\theta|\phi)$ as product of independent Gaussian parameter distributions
with mean ϕ (see Blundell et al. "Weight uncertainty in neural networks")

given new transition (s, a, s'), update ϕ to get ϕ'
this corresponds to updating the network mean parameters

use $D_{\mathrm{KL}}(q(\theta|\phi')\|q(\theta|\phi))$ as approximate bonus

Houthooft et al. "VIME"

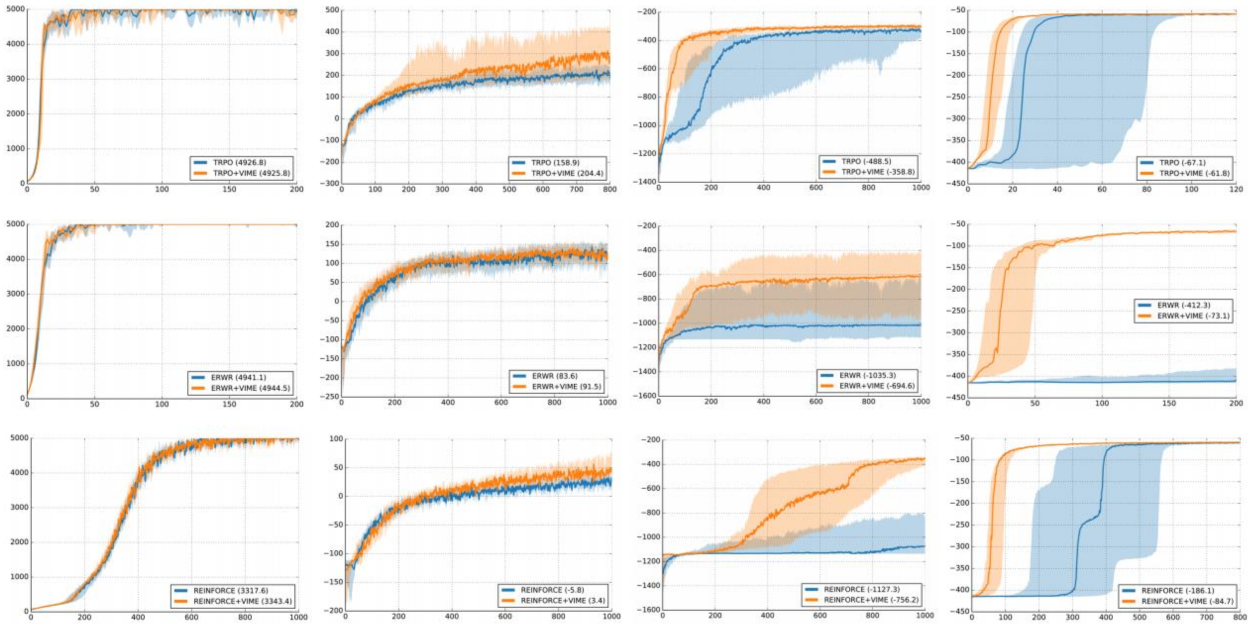
Reasoning about information gain (approximately)

VIME implementation:

IG can be equivalently written as $D_{\mathrm{KL}}(p(\theta|h, s_t, a_t, s_{t+1}) \| p(\theta|h))$

$q(\theta|\phi) \approx p(\theta|h)$ specifically, optimize variational lower bound $D_{\mathrm{KL}}(q(\theta|\phi) \| p(h|\theta)p(\theta))$

use $D_{\mathrm{KL}}(q(\theta|\phi') \| q(\theta|\phi))$ as approximate bonus



(a) CartPole (b) CartPoleSwingup (c) DoublePendulum (d) MountainCar

Approximate IG:

+ appealing mathematical formalism

- models are more complex, generally harder to use effectively

Houthooft et al. "VIME"

Exploration with model errors

$D_{\mathrm{KL}}(q(\theta|\phi')\|q(\theta|\phi))$ can be seen as change in network (mean) parameters ϕ

if we forget about IG, there are many other ways to measure this

Stadie et al. 2015:
- encode image observations using auto-encoder
- build predictive model on auto-encoder latent states
- use model error as exploration bonus

Schmidhuber et al. (see, e.g. “Formal Theory of Creativity, Fun, and Intrinsic Motivation):
- exploration bonus for model error
- exploration bonus for model gradient
- many other variations

Suggested readings

Schmidhuber. (1992). **A Possibility for Implementing Curiosity and Boredom in Model-Building Neural Controllers.**

Stadie, Levine, Abbeel (2015). **Incentivizing Exploration in Reinforcement Learning with Deep Predictive Models.**

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