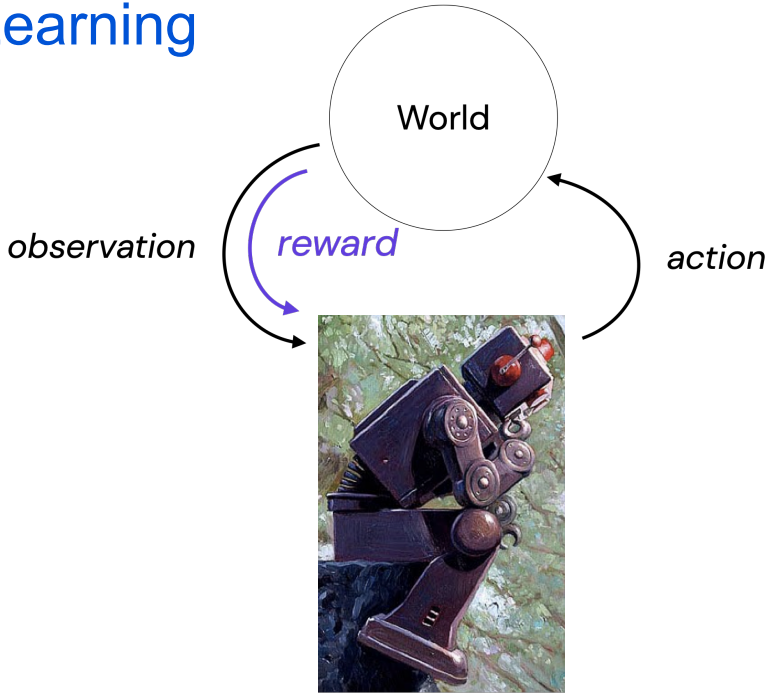
What is Reinforcement Learning for?

Reinforcement Learning



> *"Part of the appeal of reinforcement learning is that it is in a sense the whole AI problem in a microcosm."*
> – Sutton, 1992

1. RL for understanding intelligence

- A way to model processes in the brain
- A way to model cognitive processes in animals and people

Learning Values: Temporal-Difference Error

- Value estimate at time step *t*: $v(S_t)$
- Value estimate at time step *t+1*: $r(S_t, A_t) + \gamma v(S_{t+1})$
- *Temporal-difference error:*

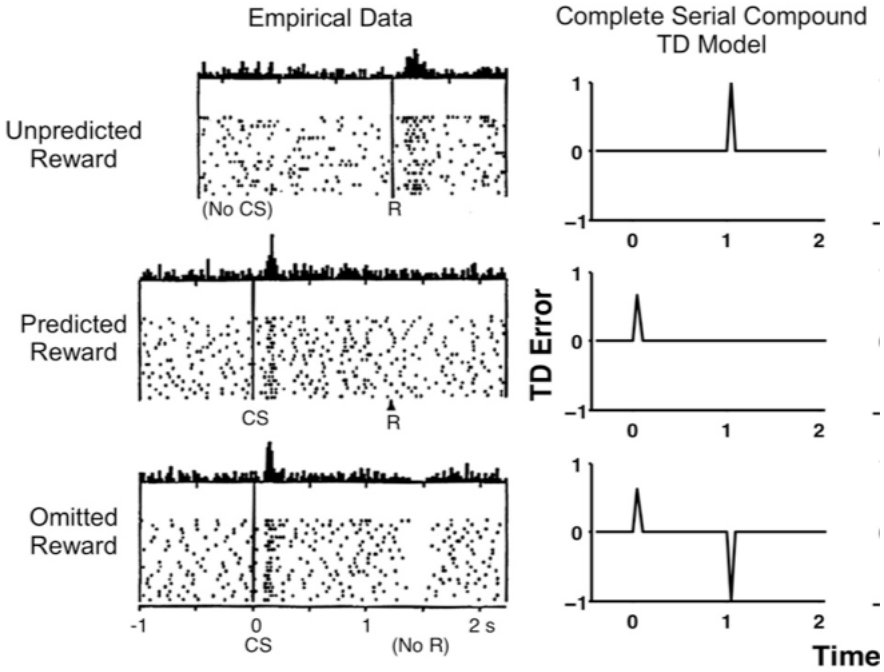
$$\delta_t = r(S_t, A_t) + \gamma v(S_{t+1}) - v(S_t)$$

- If v is parameterized by w, change w so as to minimize the TD-error:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \delta_t \nabla_{\mathbf{w}} v_{\mathbf{w}}(S_t)$$

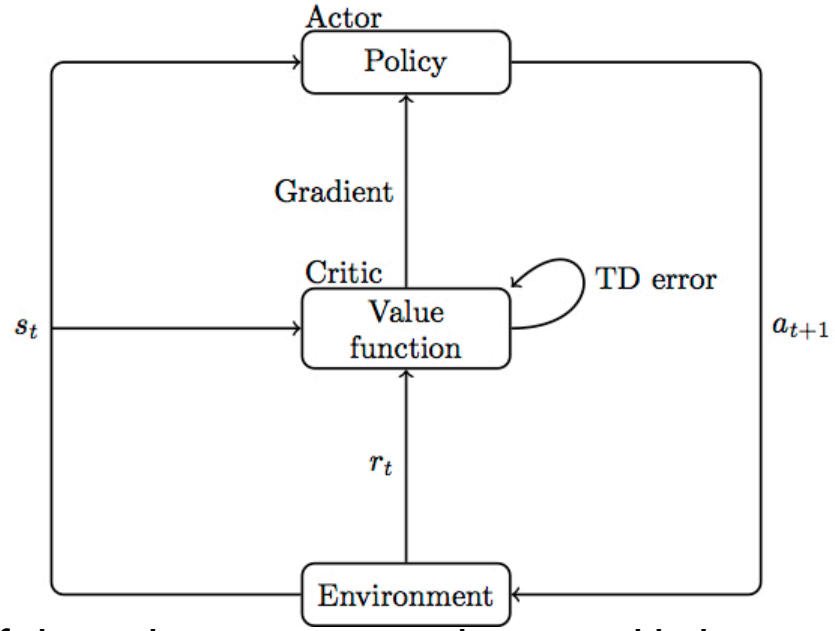
- Shultz, Dayan & Montague (1997): TD-errors model the activity of dopamine neurons

Dopamine neuron modelling



Cf. Shultz, Dayan et al, 1996; and lots of follow-up work including MNI, Psych.

Control: Actor-critic architecture



- Parameters of the policy move to make more likely action a that has positive advantage:

$$A(s,a) = r(s,a) + \gamma \mathbf{E}(v(s') \,|\, s,a) - v(s)$$

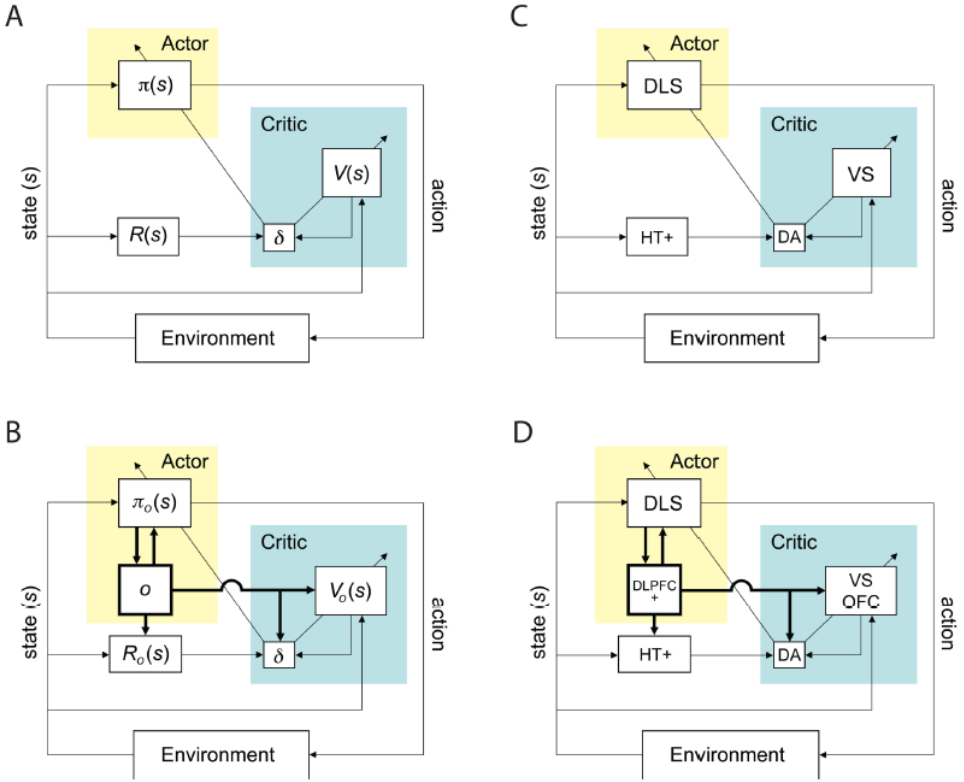
- O'Doherty et al (2004): fMRI evidence that dorsolateral striatum implements an actor and ventral striatum a critic

Generalizing Actions: Options Framework

- An *option* is a defined by a tuple $\langle I_\omega(s), \pi_\omega(a \mid s), \beta_\omega(s) \rangle$
  - An *initiation function* (precondition)
  - An *internal policy* (behavior)
  - A *termination function* (post-condition)
- Eg robot navigation: if no obstacle in front (initiation) go forward (policy) until something is too close (termination)

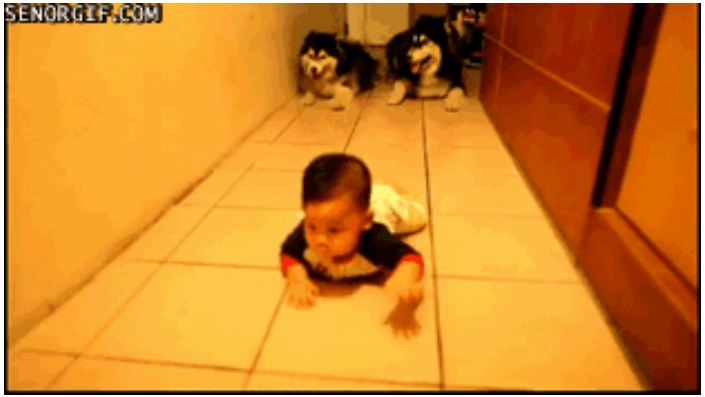
Cf. Sutton, Precup & Singh, 1998; Precup, 2000

Possible Neural Correlates of Options



From Botvinick, Niv & Barto, 2009

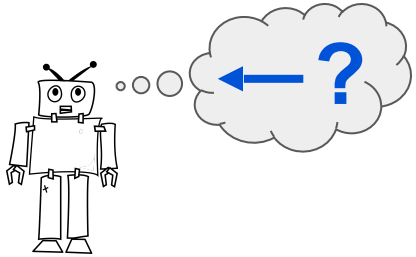
> Affordances […] relations between abilities of organisms and features of their environment.
>
> Gibson, 1977



Source: Giphy

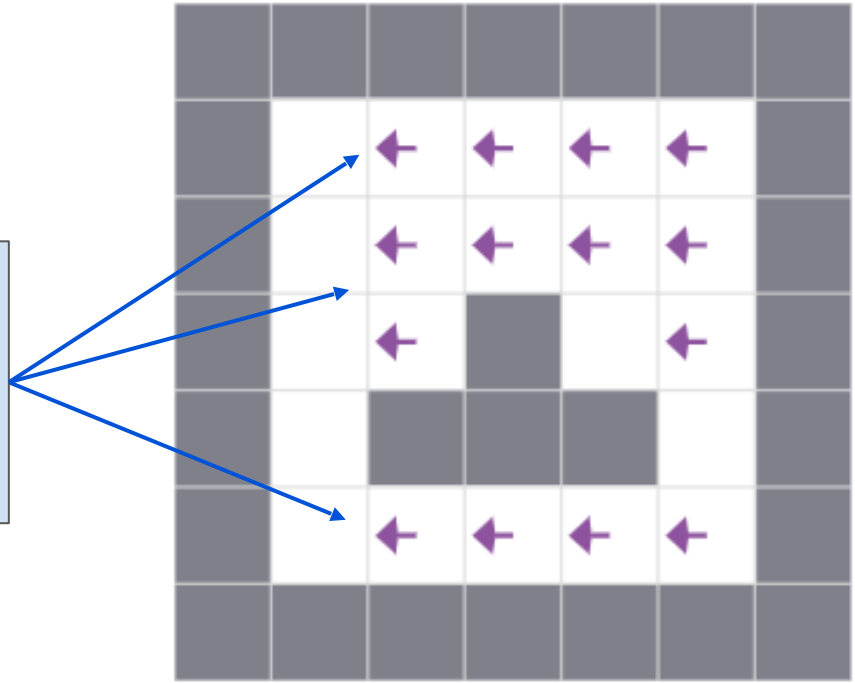
Affordances

- Captures states and actions that complete an intent



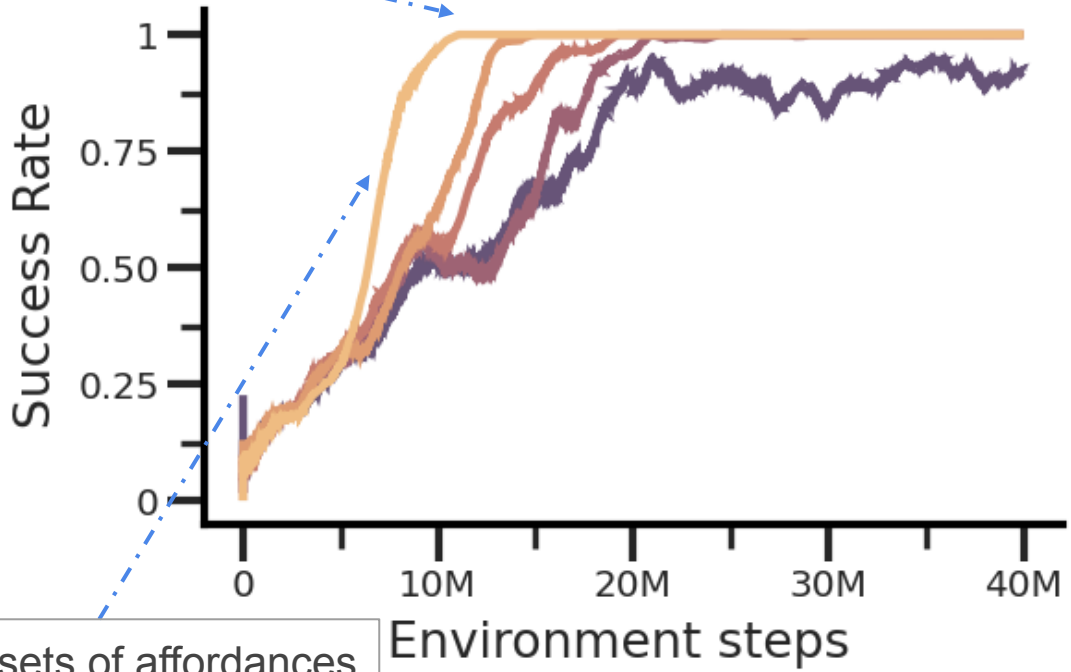
$$\mathcal{AF}_{\mathcal{I}} \subseteq \mathcal{S} \times \mathcal{A}$$

Affordances are the subset of states and actions which complete the intent to go left.



What is the impact of the affordance set size on performance ?

Performance gains



Threshold (k)

0
0.1
0.25
0.5
0.75

Decreasing Affordance set size

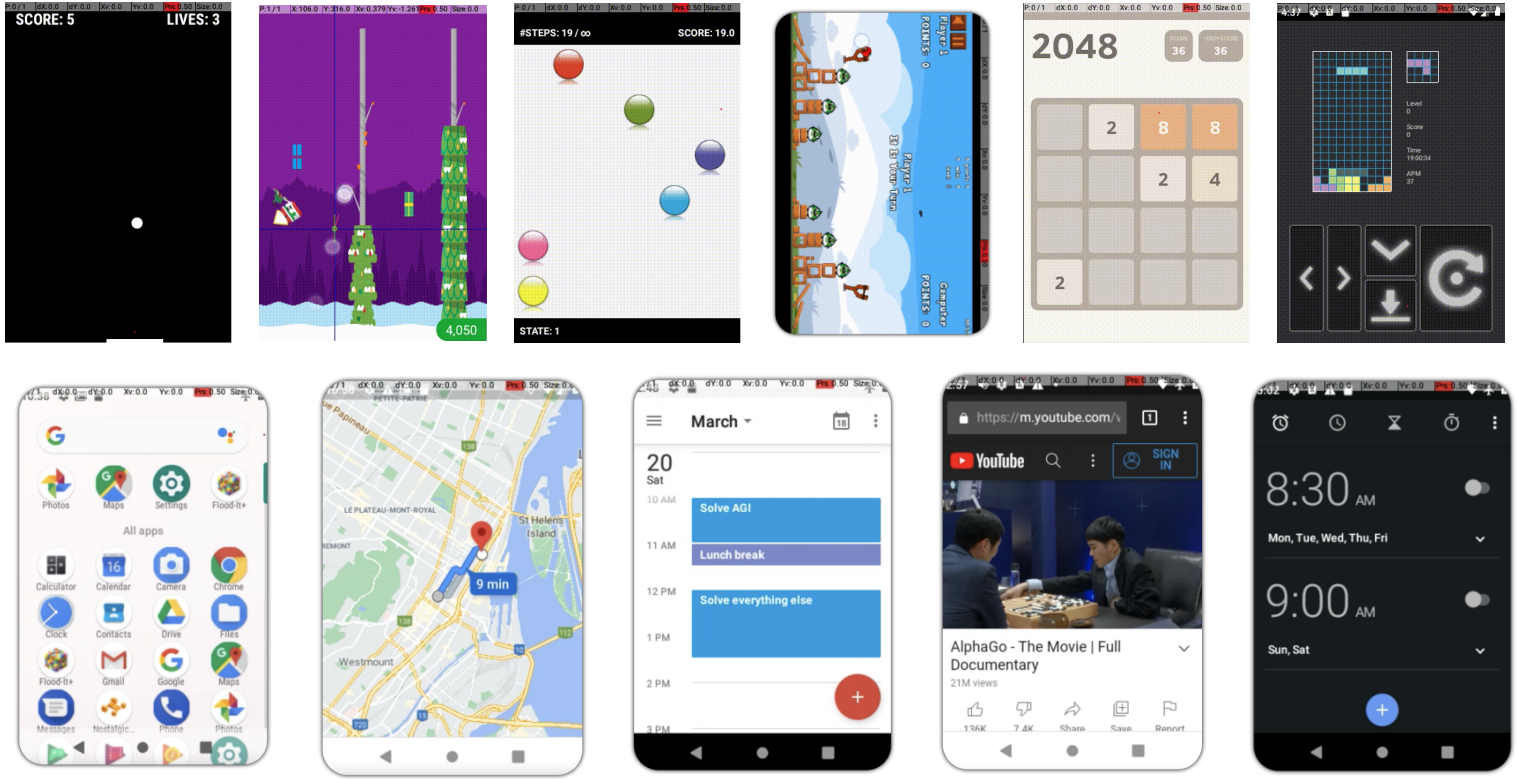
Smaller sets of affordances = quicker learning

2. RL for applications

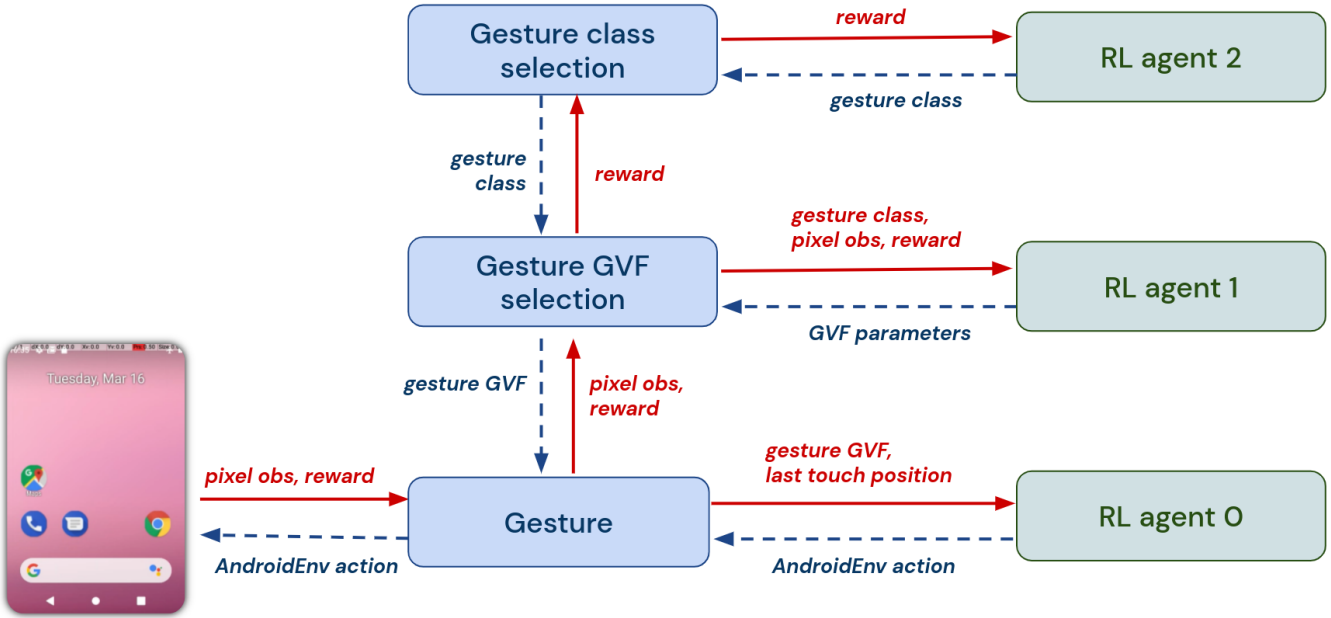
- Build (super-human) agents for language, games, computer control
- Tackle very complex control tasks (robotics, but not only)
- Learn to search and explore

Super-human performance: Games

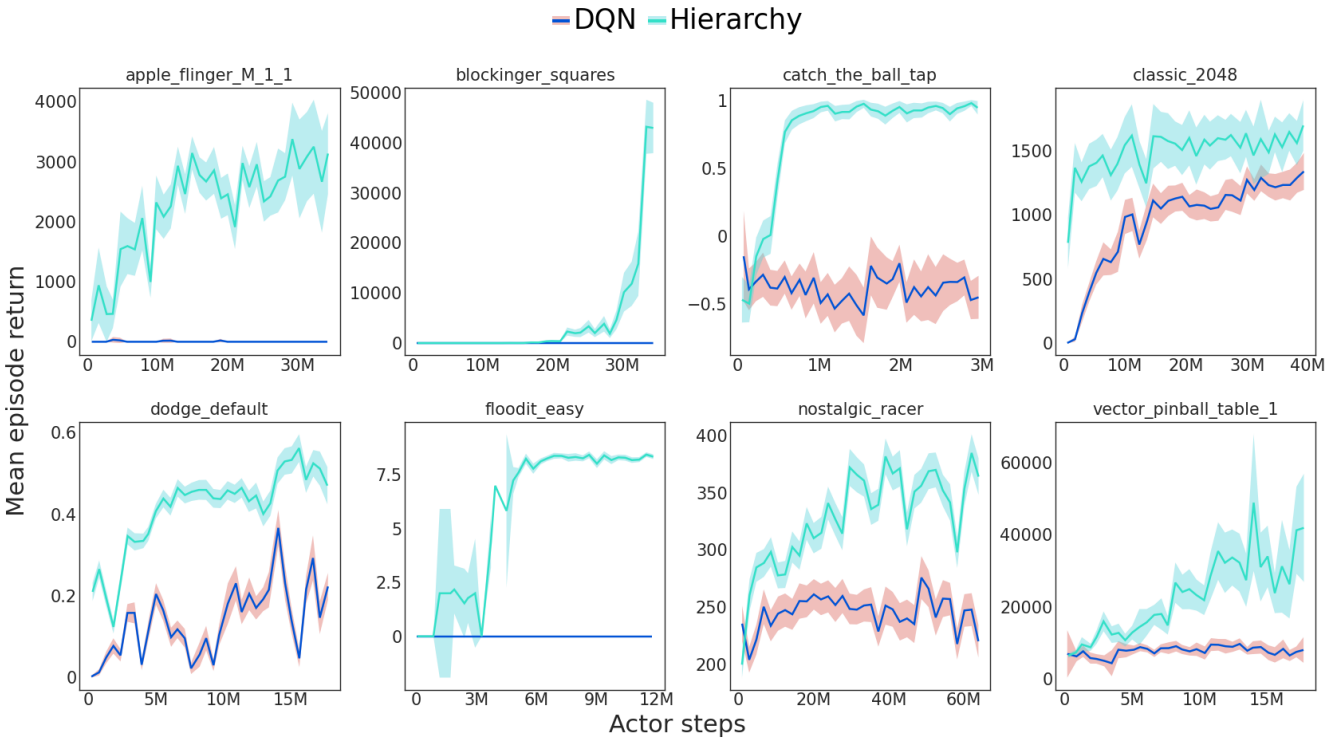
Example: Training to interact with all Android apps



How: Hierarchical RL (and now maybe large models)

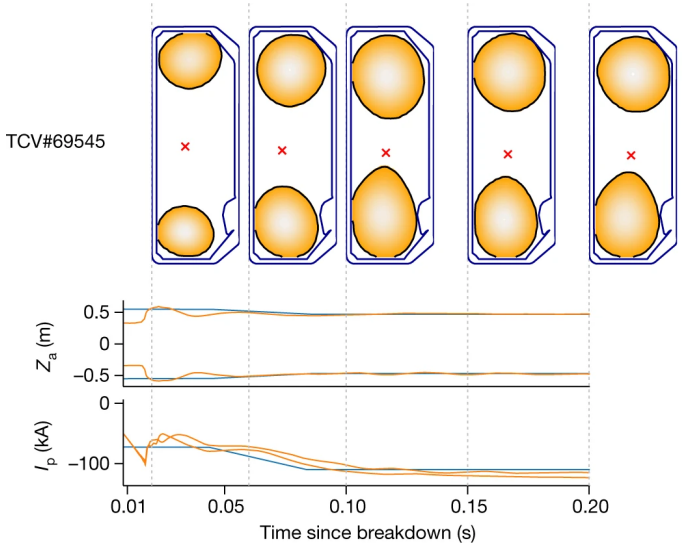


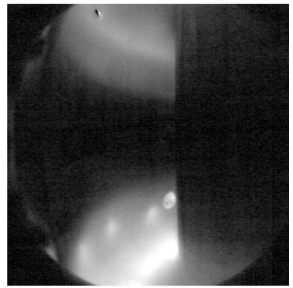
Some results, still lots to do



Complex Control Tasks

Bellemare et al, Nature, 2020



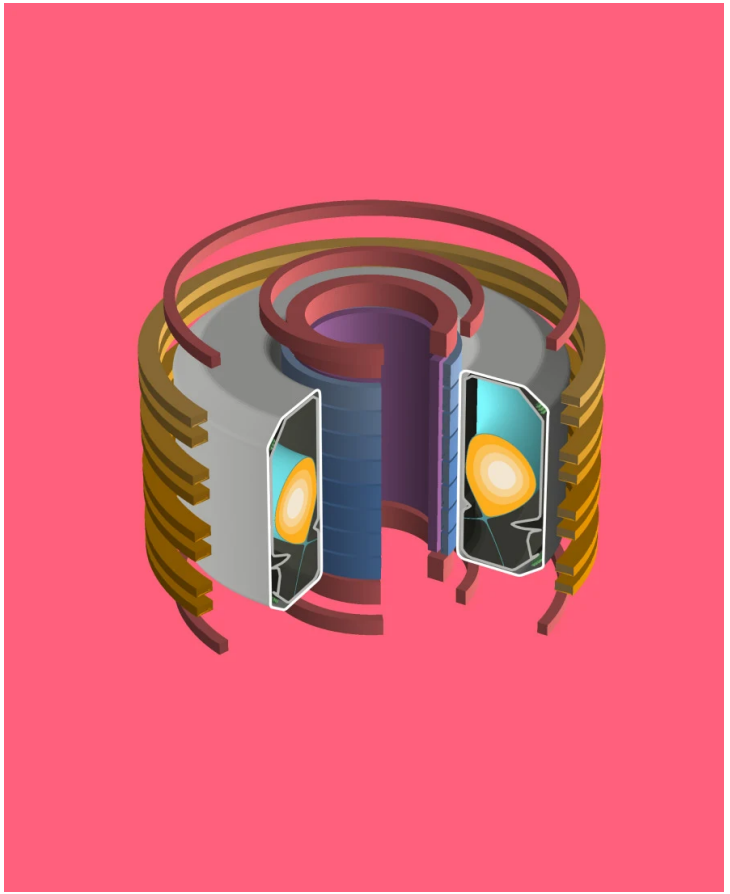


Degrave et al, Nature, 2022

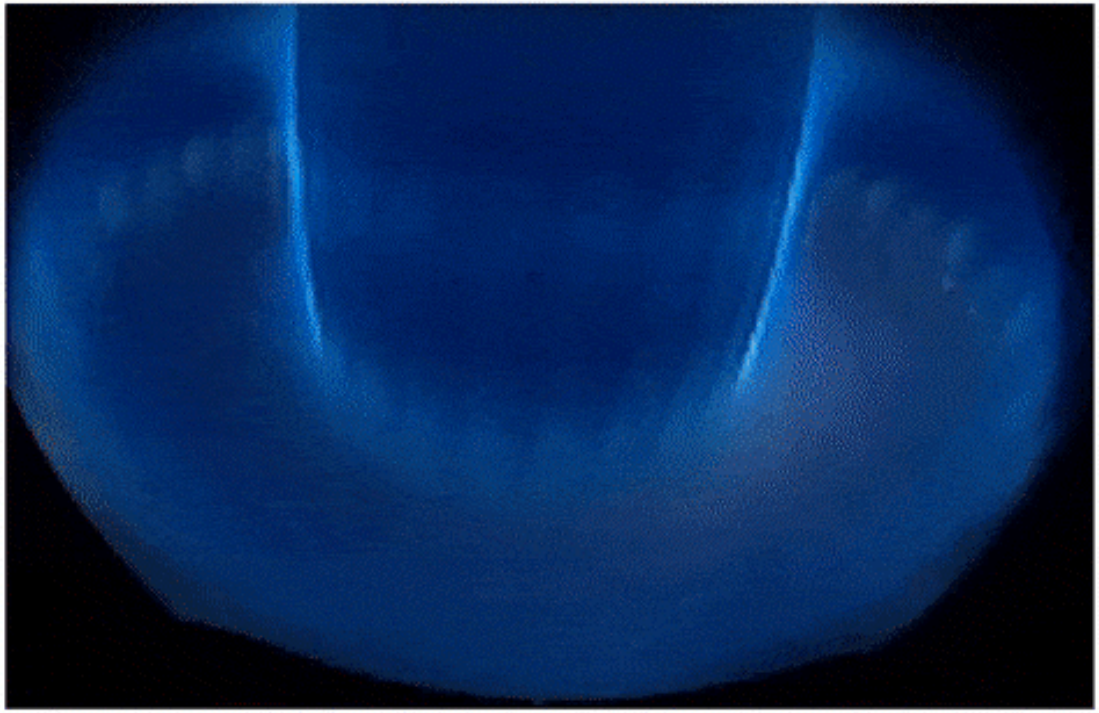
RL for controlling fusion reactors (Degrave et al, Nature 2022)

- Goal: achieve cheap clean energy!
- Tokamak reactor (EPFL): control 19 magnetic coils to get and maintain plasma into a specific shape
- True reward: energy output
- Proxy reward: penalize deviation from desired shape

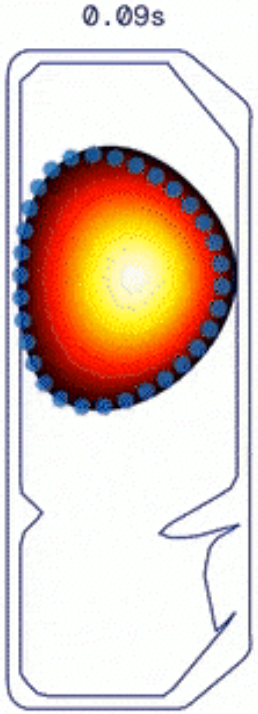
What does a Tokamak look like?



Inside a Tokamak reactor



View from inside the tokamak

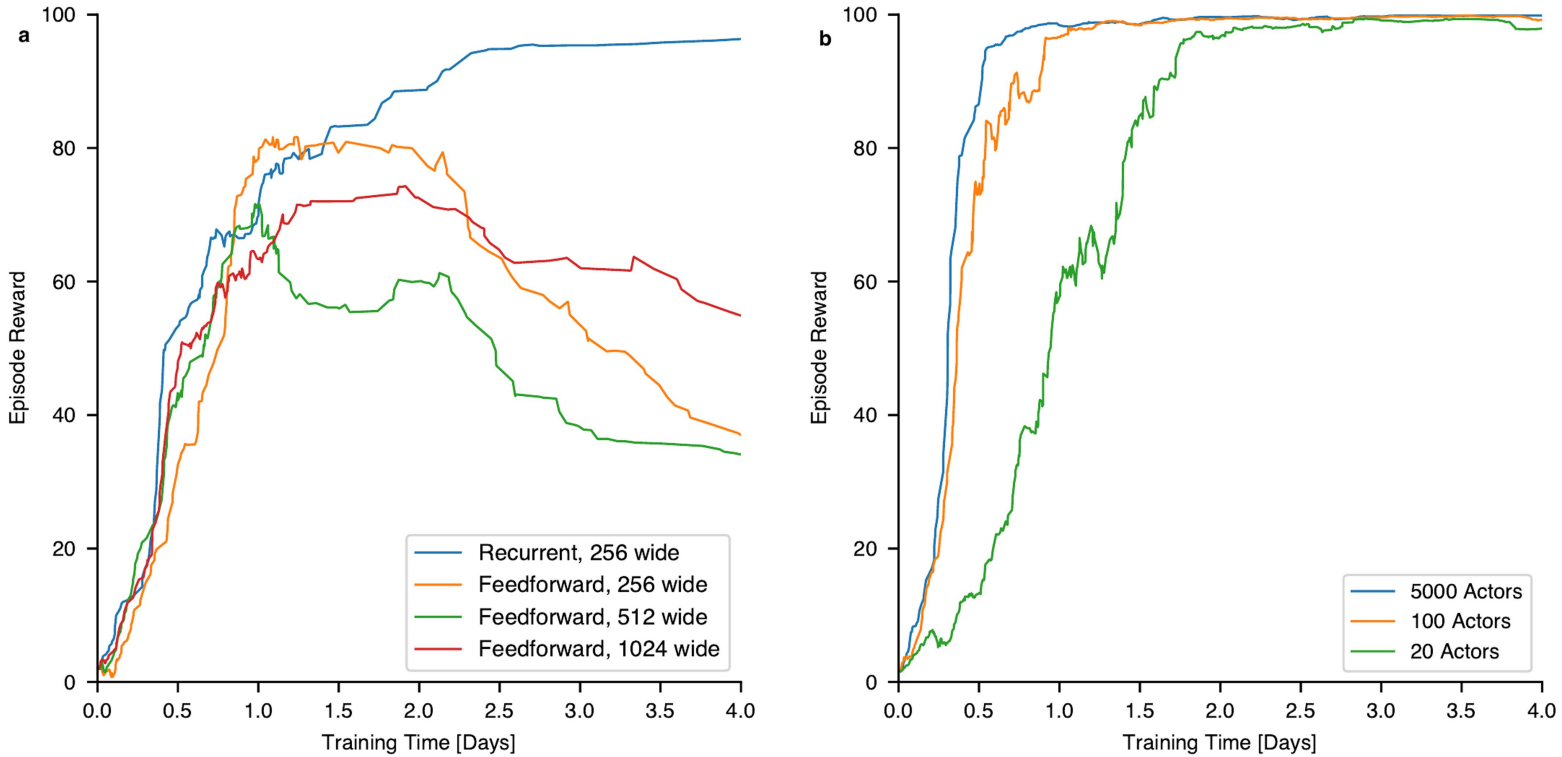


Plasma state reconstruction

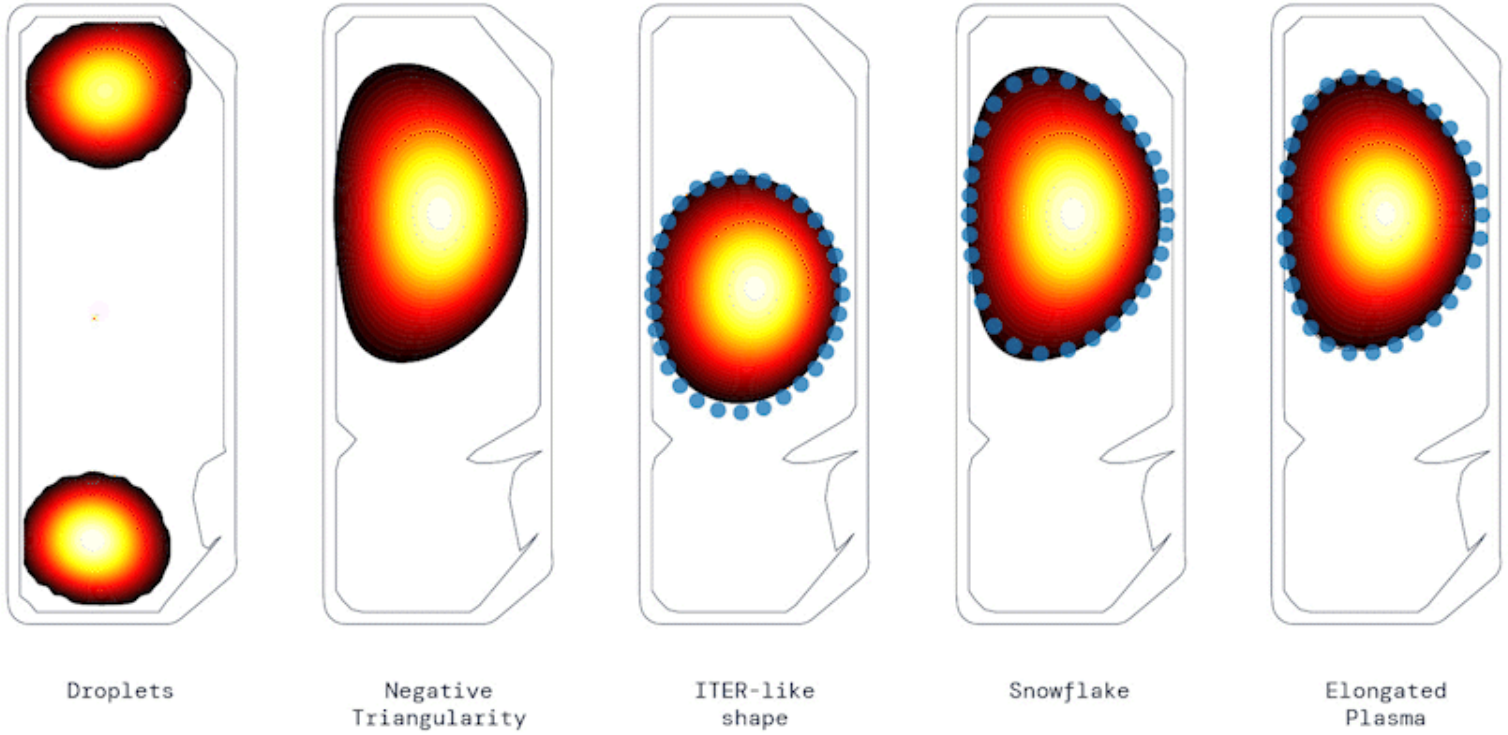
Recipe

- Build a simulator of the problem (using knowledge of physics
- Train an RL agent using policy optimization (MPO, Abdomaleki et al 2018)
- Take only the trained policy and deploy on a real reactor to evaluate
- Note control has to happen at 10kHz!

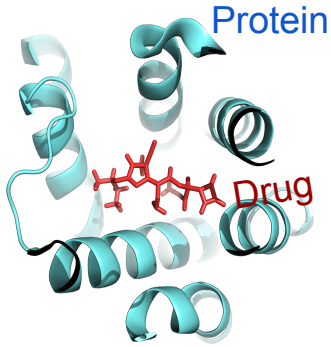
Quantitative results



Qualitative results



Small Molecule Drug Discovery



Initial data
{(x,y),..}

occasionally query “oracle"

generate molecule(s)

predict reward cheaply (DNN)

compute “real” reward

growing dataset

This part is expensive and/ or noisy! (w/ biased noise)

train generator

train reward predictor

Oracle?

- Ideal: send **diverse** batches (10-100k) of candidates to a lab, O(weeks)
- For now: use noisy physics simulator, O(15 CPUs)/molecule

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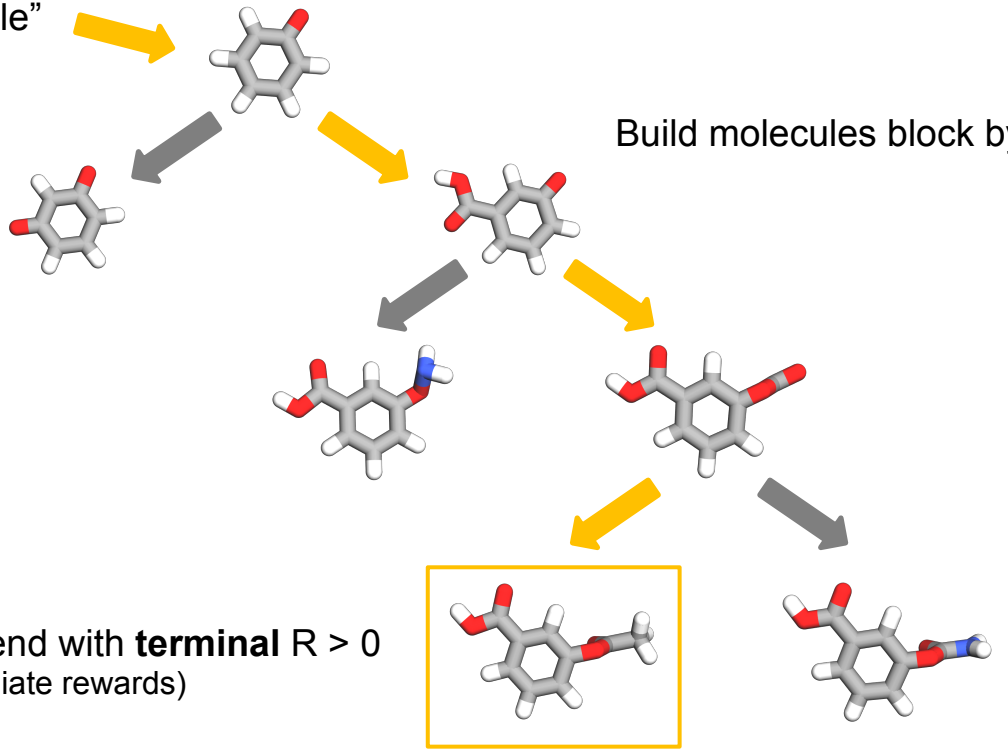
Mila

Drug Discovery as Reinforcement Learning Problem

“empty molecule”



Build molecules block by block

Episodes end with **terminal** R > 0
(no intermediate rewards)

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Just apply Reinforcement Learning?

- We have an environment (actions = build molecule)
- We have a (noisy, learned) reward
- RL! (Segler et al., 2017; De Cao & Kipf, 2018; Popova et al., 2019; Gottipati et al., 2020; Angermueller et al., 2020)

But RL greedily looks for one mode, even when we encourage entropy!
Not great for *diverse* batch oracle queries

What about the usual generative models?

- Trained from positive samples only (e.g. existing drugs)
  But we have a more informative (non-binary) signal! (reward)
- We don’t just want high reward, we want to avoid low reward (and have the data)
- Still possible to do well: Jin et al., 2018; Shi et al., 2020; Luo et al., 2021

GFlowNet

Flow Network based Generative Models for Non-Iterative Diverse Candidate Generation

Emmanuel Bengio[1,2], **Moksh Jain**[1,5], **Maksym Korablyov**[1]
Doina Precup[1,2,4], **Yoshua Bengio**[1,3]
[1]Mila, [2]McGill University, [3]Université de Montréal, [4]DeepMind, [5]Microsoft

NeurIPS 2021

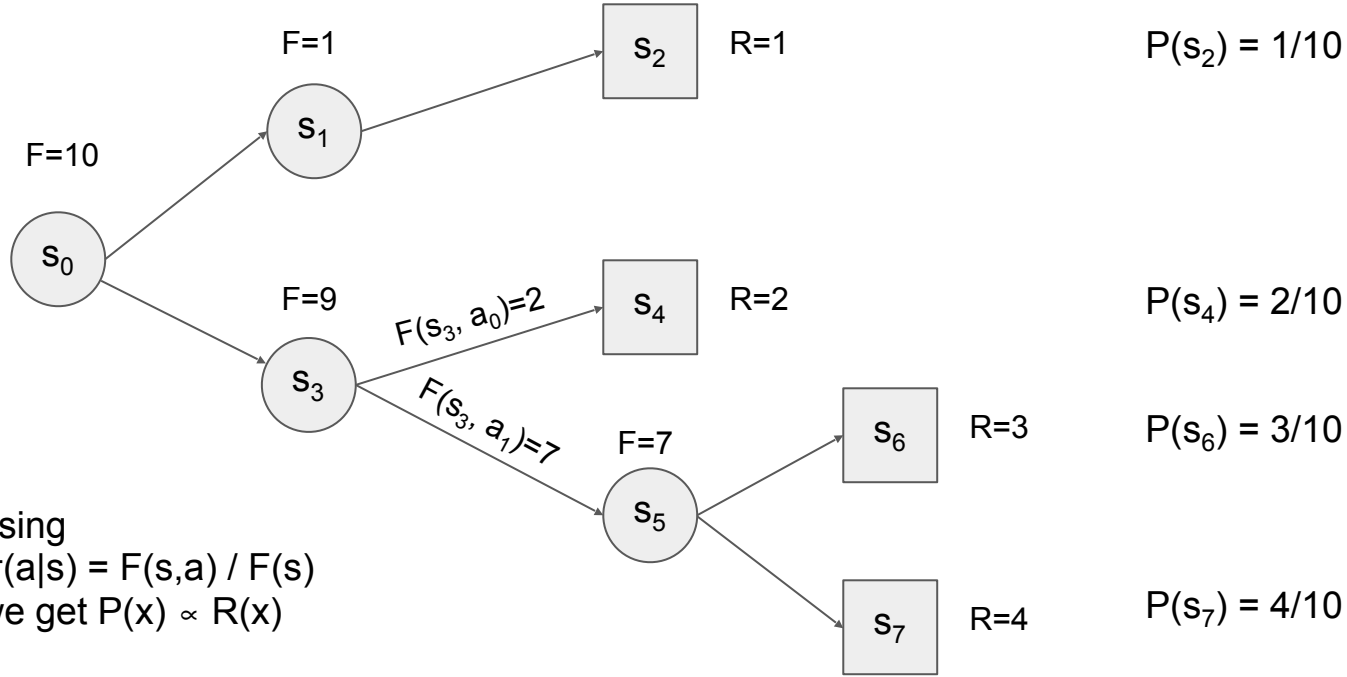
Generative framework for discrete objects which have a reward (or energy).

Desired: Reward-proportional sampling!

$$\pi(x) \approx \frac{R(x)}{Z} = \frac{R(x)}{\sum_{x' \in \mathcal{X}} R(x')}$$

Background: SumTrees (& control as inference: SoftAC/SoftQL)

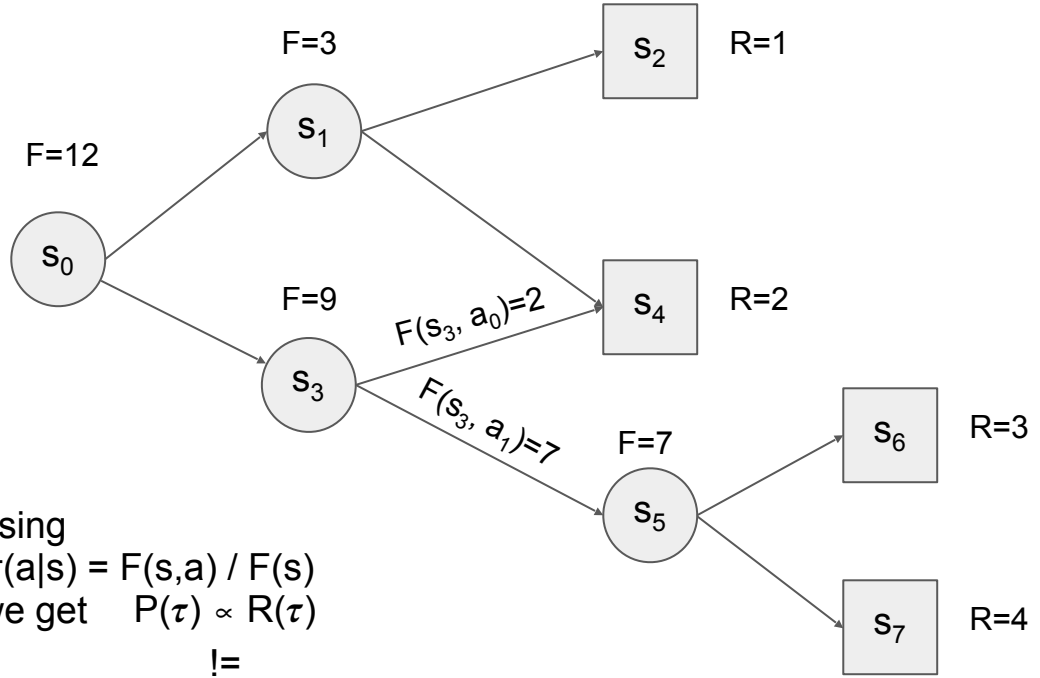
$\pi(a|s) = Q(s,a) / V(s) = F(s,a) / F(s)$



using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(x) \propto R(x)$

What if it's a DAG?

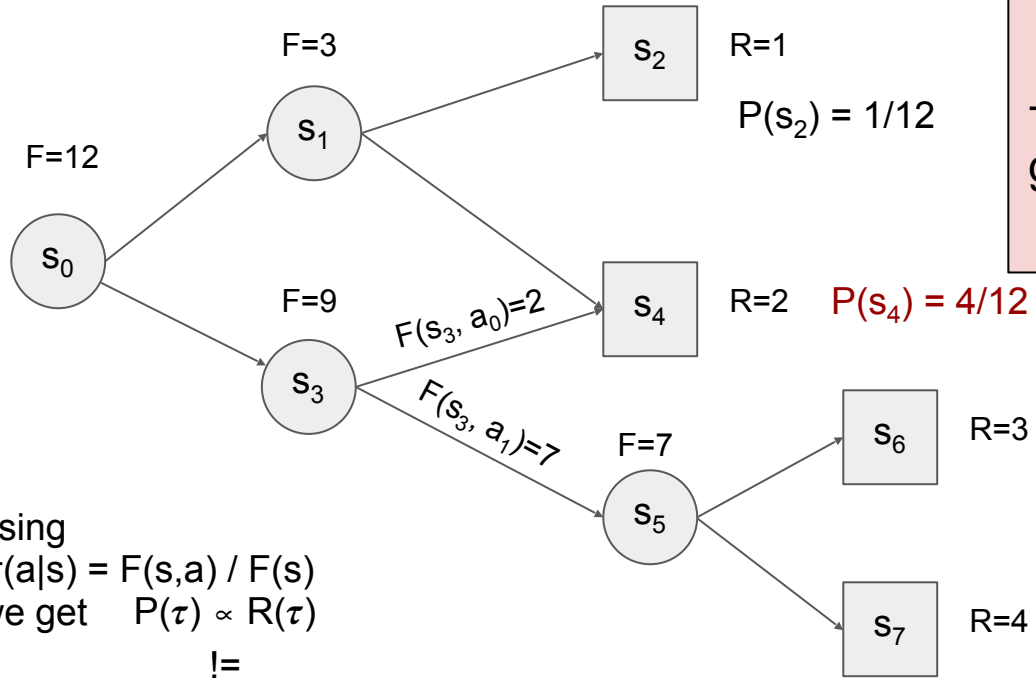
Naively applying SoftQL/SumTree yields the wrong solution



using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(\tau) \propto R(\tau)$
!=
$P(x) \propto R(x)$

What if it's a DAG?

Naively applying SoftQL/SumTree yields the wrong solution

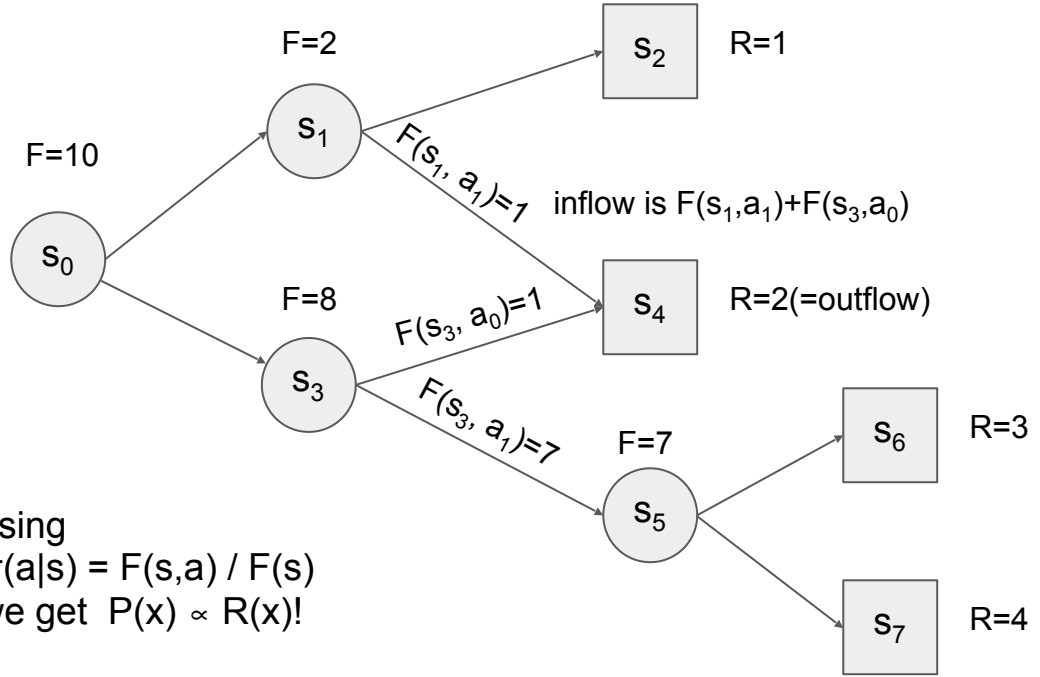


using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(\tau) \propto R(\tau)$
!=
$P(x) \propto R(x)$

- $P(\tau) \propto R(\tau)$ is bad if many τ lead to the same X!
- Exponentially bad in graph generation (combinatorial # of paths)

Interpreting the DAG as a flow network

F(s) such that inflow = outflow



using
$\pi(a|s) = F(s,a) / F(s)$
we get $P(x) \propto R(x)$!

Flow consistency

Satisfy flow conditions, for all s’

$$\sum_{s,a:T(s,a)=s'} F(s,a) = R(s') + \sum_{a' \in \mathcal{A}(s')} F(s',a')$$

in flow of s’ out flow of s’

This is very similar to a Bellman Equation, the bread and butter of RL!

Satisfying the flow equations yields the right sampling proportions

How to train GFlowNet

Take inspiration from RL to learn *F:*

$$\tilde{\mathcal{L}}_\theta(\tau) = \sum_{s' \in \tau \neq s_0} \left(\sum_{s,a:T(s,a)=s'} F_\theta(s,a) - R(s') - \sum_{a' \in \mathcal{A}(s')} F_\theta(s',a') \right)^2$$

Dangerous objective, $F(s_0,.)$ is going to be huge! $F(s_0) = Z$

How to train GFlowNet

Instead, learn the log, **and** match flows in log-space

$$\mathcal{L}_{\theta,\epsilon}(\tau) = \sum_{s' \in \tau \neq s_0} \left(\log \left[\epsilon + \sum_{s,a:T(s,a)=s'} \exp F_\theta^{\log}(s,a) \right] - \log \left[\epsilon + R(s') + \sum_{a' \in \mathcal{A}(s')} \exp F_\theta^{\log}(s',a') \right] \right)^2$$

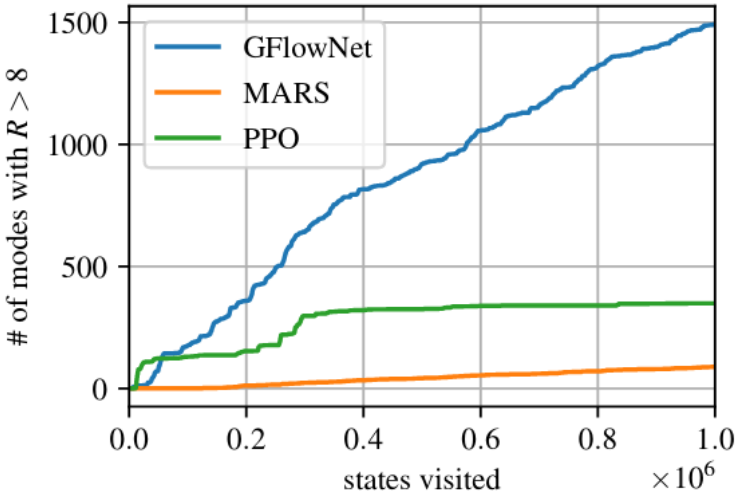
with an epsilon (care less about tiny flows)

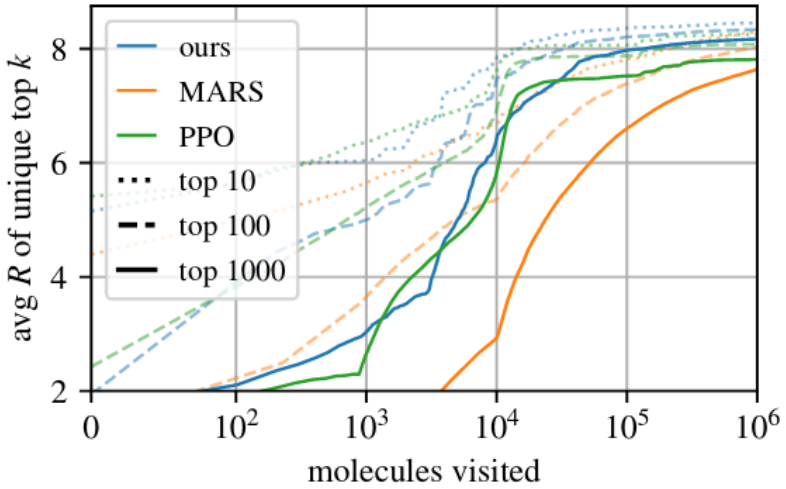
Relationship to MaxEntRL

- Quite similar in spirit but different mechanism (recent papers establish formal relationship)
- *Sampling of trajectories is always proportional to the reward at the end*
- If multiple policies are optimal their paths continue to be generated
- In fact, all paths continue to be generated
- Ongoing work: extensions to non-DAG, rewards at all states

Works well! Molecule results

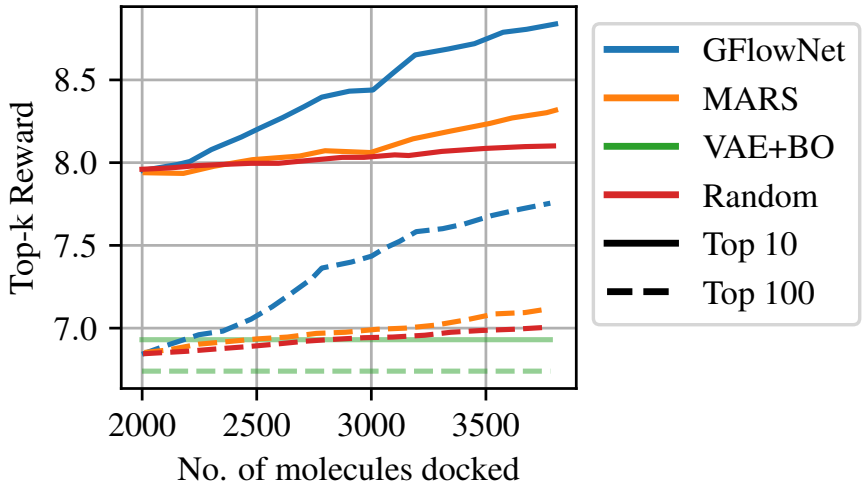
Pre-train reward function once on 300k molecules (computed on CPU simulator)
Modes are found faster, with better rewards





modes = Bemis-Murcko scaffolds

Works for Batch Active Learning too!



Average return over 3 runs of the top-k candidates in an iterative batch generation approach

Reinforcement Learning in practice

- Very big, largely untapped potential!
- **Reward design and ability to simulate can be crucial**
- **Need to consider specifics of the problem**

- Great opportunity to improve existing algorithms!
- **Sample efficiency of RL needs to be improved**