Policy Gradient Methods

http://bicmr.pku.edu.cn/~wenzw/bigdata2023.html

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Outline

Policy gradient methods

- In Q-learning function approximation was used to approximate Q-function, and policy was a greedy policy based on estimated Q-function. In policy gradient methods, we approximate a stochastic policy directly using a parametric function approximator.
- More formally, given an MDP (S, A, s_1, R, P), let $\pi_\theta : S \to \Delta^A$ denote a randomized policy parameterized by parameter vector $\theta \in \mathbb{R}^d$ For a scalable formulation, we want $d << |S|$.
- For example, the policy π_θ might be represented by a neural network whose input is a representation of the state, whose output is action selection probabilities, and whose weights form the policy parameters θ. (The architecture for such a [deep] neural network is similar to that for a multi-label classifier, with input being a state, and labels being different actions. The network should be trained to predict the probability of different actions given an input state).

Policy gradient methods

- For simplicity, assume that π_θ is differentiable with respect to θ, i.e. $\frac{\partial \pi_\theta(s,a)}{\partial \theta}$ exists. This is true for example, if a neural network with differentiable activation functions is used to define π_θ. Let $\rho(\pi_\theta)$ denote the gain of policy π_θ.This may be defined as long term average reward, long term discounted reward or total reward in an episode or finite horizon. Therefore, solving for optimal policy reduces to the problem of solving

$$\max_\theta \rho(\pi_\theta)$$

- In order to use stochastic gradient descent algorithm for finding a stationary point of the above problem, we need to compute (an unbiased) estimate of gradient of $\rho(\pi_\theta)$ with respect to θ.

Finite horizon MDP

- Here performance measure to optimize is total expected reward over a finite horizon H.

$$\rho(\pi) = \mathbb{E}\left[\sum_{t=1}^{H} \gamma^{t-1} r_t | \pi, s_1\right]$$

- Let $\pi(s,a)$ denote the probability of action a in state s for randomized policy π. Let $D^{\pi}(\tau)$ denote the probability distribution of a trajectory (state-action sequence) $\tau = (s_1, a_1, s_2, \ldots, a_{H-1}, s_H)$ of states on starting from state s_1 and following policy π. That is,

$$D^{\pi}(\tau) := \prod_{i=1}^{H-1} \pi(s_i, a_i) P(s_i, a_i, s_{i+1})$$

Finite horizon MDP

Theorem 2

For finite horizon MDP (S, A, s_1, P, R, H), let $R(\tau)$ be the total reward for an sample trajectory τ, on following π_θ for H steps, starting from state s_1. Then,

$$\nabla_\theta \rho\left(\pi_\theta\right) = \mathbb{E}_\tau\left[R(\tau) \nabla_\theta \log\left(D^{\pi_\theta}(\tau)\right)\right] = \mathbb{E}_\tau\left[R(\tau) \sum_{t=1}^{H-1} \nabla_\theta \log\left(\pi_\theta\left(s_t, a_t\right)\right)\right]$$

Proof. Let $R(\tau)$ be expected total reward for an entire sample trajectory τ, on following π_θ for H steps, starting from states_1. That is, given a sample trajectory $\tau = (s_1, a_1, s_2, \ldots, a_{H-1}, s_H)$ from distribution D^{π_θ},

$$R(\tau) := \sum_{t=1}^{H-1} \gamma^{t-1} R\left(s_t, a_t\right)$$

Proof of Theorem 2

Then,

$$\rho\left(\pi_\theta\right) = \mathbb{E}_{\tau \sim D^{\pi_\theta}}[R(\tau)]$$

Now, (the calculations below implicitly assume finite state and action space, so that the distribution $D(\tau)$ has a finite support)

$$\begin{aligned}
\frac{\partial \rho\left(\pi_\theta\right)}{\partial \theta} &= \frac{\partial}{\partial \theta} \mathbb{E}_{\tau \sim D^{\pi_\theta}}\left[R(\tau)\right] \\
&= \frac{\partial}{\partial \theta} \sum_{\tau : D^{\pi_\theta}(\tau) > 0} D^{\pi_\theta}(\tau) R(\tau) \\
&= \sum_{\tau : D^{\pi_\theta}(\tau) > 0} D^{\pi_\theta}(\tau) \frac{\partial}{\partial \theta} \log\left(D^{\pi_\theta}(\tau)\right) R(\tau) \\
&= \mathbb{E}_{\tau \sim D^{\pi_\theta}}\left[\frac{\partial}{\partial \theta} \log\left(D^{\pi_\theta}(\tau)\right) R(\tau)\right]
\end{aligned}$$

Proof of Theorem 2

Further, for a given sample trajectory τ^i.

$$\begin{aligned}\nabla_\theta \log\left(D^{\pi_\theta}\left(\tau^i\right)\right) &= \sum_{t=1}^{H-1} \nabla_\theta \log\left(\pi_\theta\left(s_t^i, a_t^i\right)\right) + \nabla_\theta \log P\left(s_t^i, a_t^i, s_{t+1}^i\right) \\ &= \sum_{t=1}^{H-1} \nabla_\theta \log\left(\pi_\theta\left(s_t^i, a_t^i\right)\right)\end{aligned}$$

Finite horizon MDP

- The gradient representation given by above theorem is extremely useful, as given a sample trajectory this can be computed only using the policy parameter, and does not require knowledge of the transition model $P(\cdot,\cdot,\cdot)$! This does seem to require knowledge of reward model, but that can be handled by replacing $R\left(\tau^i\right)$ by $\hat{R}\left(\tau^i\right) = r_1 + \gamma r_2 + \ldots, \gamma^{H-2} r_{H-1}$, the total of sample rewards observed in this trajectory.
- Since, given a trajectory τ, the quantity $D^{\pi_\theta}(\tau)$ is determined, and $\mathbb{E}[\hat{R}(\tau)|\tau] = R(\tau)$

$$\begin{aligned}
\nabla_\theta \rho\left(\pi_\theta\right) &= \mathbb{E}_\tau\left[R(\tau)\nabla_\theta \log\left(D^{\pi_\theta}(\tau)\right)\right] \\
&= \mathbb{E}_\tau\left[\hat{R}(\tau)\nabla_\theta \log\left(D^{\pi_\theta}(\tau)\right)\right] \\
&= \mathbb{E}_\tau\left[\hat{R}(\tau)\sum_{t=1}^{H-1}\nabla_\theta \log\left(\pi_\theta\left(s_t, a_t\right)\right)\right]
\end{aligned}$$

Unbiased estimator of gradient from samples

- From above, given sample trajectories τ^i, $i = 1, \ldots, m$, an unbiased estimator for gradient $\nabla_\theta \rho(\pi_\theta)$ is given as:

$$\begin{aligned} \hat{\mathbf{g}} &= \frac{1}{m} \sum_{i=1}^{m} \hat{R}(\tau^i) \nabla_\theta \log\left(D^{\pi_\theta}(\tau^i)\right) \\ &= \frac{1}{m} \sum_{i=1}^{m} \hat{R}(\tau^i) \sum_{t=1}^{H-1} \nabla_\theta \log\left(\pi_\theta\left(s_t^i, a_t^i\right)\right) \end{aligned}$$

Baseline

- Note that for any constant b (or b that is conditionally independent of sampling from π_θ given θ), we have:

$$\mathbb{E}_\tau \left[b \frac{\partial}{\partial \theta_j} \log \left(D^{\pi_\theta}(\tau) \right) | \theta, s_1 \right] = b \int_\tau \frac{\partial}{\partial \theta_j} \left(D^{\pi_\theta}(\tau) \right) = b \frac{\partial}{\partial \theta_j} \int_\tau D^{\pi_\theta}(\tau) = 0$$

- Therefore, choosing any 'baseline' b, following is also an unbiased estimator of the $\nabla_\theta \rho \left(\pi_\theta \right)$:

$$\hat{\mathbf{g}} = \frac{1}{m} \sum_{i=1}^{m} \sum_{t=1}^{H-1} \left(\hat{R} \left(\tau^i \right) - b \right) \nabla_\theta \log \left(\pi_\theta \left(s_t^i, a_t^i \right) \right)$$

Baseline

- Or, more generally, one could even use a state and time dependent baseline $b_t\left(s_t^i\right)$ conditionally is independent of sampling from π_θ given s_t^i, θ, to get estimator:

$$\hat{\mathbf{g}} = \frac{1}{m}\sum_{i=1}^{m}\sum_{t=1}^{H-1}\left(\hat{R}\left(\tau^i\right) - b_t\left(s_t^i\right)\right)\nabla_\theta \log\left(\pi_\theta\left(s_t^i, a_t^i\right)\right) \tag{1}$$

- Below we show this is unbiased. The expectations below are over trajectories $\left(s_1, a_1, \ldots, a_{H-1}, s_H\right)$, where $a_t \sim \pi\left(s_t, \cdot\right)$, given s_t. For any fixed θ, t, the baseline $b_t\left(s_t\right)|s_t$ needs to be deterministic or independent of $a_t|s_t$. For simplicity we assume it is deterministic.

Baseline

$$
\begin{aligned}
& \mathbb{E}_{\tau}\left[\sum_{t=1}^{H-1} b_t\left(s_t\right) \frac{\partial}{\partial \theta_j} \log\left(\pi_\theta\left(s_t, a_t\right)\right) | \theta, s_1\right] \\
= \quad & \mathbb{E}\left[\sum_{t=1}^{H-1} \mathbb{E}\left[b_t\left(s_t\right) \frac{\partial}{\partial \theta_j} \log\left(\pi_\theta\left(s_t, a_t\right)\right) | s_t\right] | \theta, s_1\right] \\
= \quad & \mathbb{E}\left[\sum_{t=1}^{H-1} b_t\left(s_t\right) \mathbb{E}\left[\frac{\partial}{\partial \theta_j} \log\left(\pi_\theta\left(s_t, a_t\right)\right) | s_t\right] | \theta, s_1\right] \\
= \quad & \mathbb{E}\left[\sum_{t=1}^{H-1} b_t\left(s_t\right) \sum_a \pi_\theta\left(s_t, a\right) \frac{\partial}{\partial \theta_j} \log\left(\pi_\theta\left(s_t, a\right)\right) | \theta, s_1\right] \\
= \quad & \mathbb{E}\left[\sum_{t=1}^{H-1} b_t\left(s_t\right) \sum_a \frac{\partial}{\partial \theta_j} \pi_\theta\left(s_t, a\right) | \theta, s_1\right]
\end{aligned}
$$

Baseline

$$
\begin{aligned}
&= \mathbb{E}\left[\sum_{t=1}^{H-1} b_t(s_t)\,\frac{\partial}{\partial\theta_j}\sum_a \pi_\theta(s_t,a) \mid \theta, s_1\right] \\
&= \mathbb{E}\left[\sum_{t=1}^{H-1} b_t(s_t)\,\frac{\partial}{\partial\theta_j} 1 \mid \theta, s_1\right] \\
&= 0
\end{aligned}
$$

- An example of such state dependent baseline $b_t(s)$, given s and θ, is $V_{H-t}^{\pi_\theta}(s)$, i.e., the value of policy π_θ, starting from state s at time t. We will see later that such a baseline is useful in reducing the variance of gradient estimates.

Vanilla policy gradient algorithm

Initialize policy parameter θ, and baseline.
In each iteration,

- Execute current policy π_θ to obtain several sample trajectories τ^i, $i = 1, \ldots, m$.
- Use these sample trajectories and chosen baseline to compute the gradient estimator $\hat{\mathbf{g}}$ as in (1)
- Update $\theta \leftarrow \theta + \alpha \hat{g}$
- Update baseline as required.

Above is essentially same as the REINFORCE algorithm introduced by [Williams, 1988, 1992].

Softmax policies

- Consider policy set parameterized by $\theta \in \mathbb{R}^d$ such that given $s \in S$, probability of picking action $a \in A$ is given by:

$$\pi_\theta(s,a) = \frac{e^{\theta^\top \phi_{sa}}}{\sum_{a' \in A} e^{\theta^\top \phi_{sa'}}}$$

where each ϕ_{sa} is an d-dimensional feature vector characterizing state-action pair s, a. This is a popular form of policy space called softmax policies. Here,

$$\nabla_\theta \log\left(\pi_\theta(s,a)\right) = \phi_{sa} - \left(\sum_{a' \in A} \phi_{sa'} \pi_\theta\left(s,a'\right)\right) = \phi_{sa} - \mathbb{E}_{a' \sim \pi(s)}\left[\phi_{sa'}\right]$$

Gaussian policy for continuous action spaces

- In continuous action spaces, it is natural to use Gaussian policies. Given state s, the probability of action a is given as:

$$\pi_\theta(s,a) = \mathcal{N}\left(\phi(s)^T\theta, \sigma^2\right)$$

for some constant σ. Here $\phi(s)$ is a feature representation of s. Then,

$$\nabla_\theta \log\left(\pi_\theta(s,a)\right) = \nabla_\theta \frac{-\left(a-\theta^\top\phi(s)\right)^2}{2\sigma^2} = \frac{\left(\theta^\top\phi(s)-a\right)}{\sigma^2}\phi(s)$$

Outline

Actor-critic methods

- Actor-only methods (vanilla policy gradient) work with a parameterized family of policies.
- The gradient of the performance, with respect to the actor parameters, is directly estimated by simulation, and the parameters are updated in a direction of improvement.
- A possible drawback of such methods is that the gradient estimators may have a large variance.
- As the policy changes, a new gradient is estimated independently of past estimates (by sampling trajectories).
- There is no "learning", in the sense of accumulation and consolidation of older information.

Actor-critic methods

- Critic-only methods (e.g., Q-learning, TD-learning) rely exclusively on value function approximation and aim at learning an approximate solution to the Bellman equation, which will then hopefully prescribe a near-optimal policy.
- Such methods are indirect in the sense that they do not try to optimize directly over a policy space.
- A method of this type may succeed in constructing a "good" approximation of the value function, yet lack reliable guarantees in terms of near-optimality of the resulting policy.

Actor-critic methods

- Actor-critic methods aim at combining the strong points of actor-only and critic-only methods, by incorporating value function approximation in the policy gradient methods.
- We already saw the potential of using value function approximation for picking baseline for variance reduction.
- Another more obvious place to incorporate Q-value approximation is for approximating Q-function in the policy gradient expression. Recall, by policy gradient theorem:

$$\nabla_\theta \rho\left(\pi_\theta\right) = \sum_s d^{\pi_\theta}(s) \mathbb{E}_{a\sim\pi(s)}\left[\left(Q^{\pi_\theta}(s,a) - b^{\pi_\theta}(s)\right) \nabla_\theta \log\left(\pi_\theta(s,a)\right)\right]$$

for any baseline $b^{\pi_\theta}(\cdot)$.

Theorem 1 (Sutton et al. [1999])

If function f_ω is compatible with policy parametrization θ in the sense that for every s, a,

$$\nabla_\omega f_\omega(s,a) = \frac{1}{\pi_\theta(s,a)} \nabla_\theta \pi_\theta(s,a) = \nabla_\theta \log\left(\pi_\theta(s,a)\right)$$

And, further we are given parameter ω which is a stationary point of the following least squares problem:

$$\min_\omega \mathbb{E}_{s\sim d^{\pi_\theta}, a\sim\pi_\theta(s,)} \left[\left(Q^{\pi_\theta}(s,a) - b(s;\theta) - f_\omega(s,a)\right)^2\right]$$

where $b(\cdot;\theta)$ is any baseline, which may depend on the current policy π_θ. Then,

$$\nabla_\theta \rho\left(\pi_\theta\right) = \mathbb{E}_{s\sim d^{\pi_\theta}} \mathbb{E}_{a\in\pi_\theta(s)} \left[f_\omega(s,a) \nabla_\theta \log\left(\pi_\theta(s,a)\right)\right]$$

That is, function approximation f_ω can be used in place of Q-function to obtain gradient with respect to θ.

Proof of Policy gradient theorem

(Here, we abuse the notation and use $\mathbb{E}_{s\sim d^{\pi_\theta}}[x]$ as a shorthand for $\sum_s d^{\pi_\theta}(s)x$. This is not technically correct in the discounted case since in that case $d^{\pi_\theta}(s) = \mathbb{E}_{s_1}\left[\sum_{t=1}^{\infty} \Pr(s_t = s; \pi, s_1)\gamma^{t-1}\right]$, which is not a distribution. In fact in discounted case, $(1-\gamma)d^{\pi_\theta}$ is a distribution.)
Proof. Given θ, for stationary point ω of the least squares problem:

$$\mathbb{E}_{s\sim d^{\pi}\theta, a\sim\pi_\theta(s,\cdot)}\left[\left(Q^{\pi_\theta}(s,a) - b(s;\theta) - f_\omega(s,a)\right)\nabla_\omega f_\omega(s,a)\right] = 0$$

Substituting the compatibility condition:

$$\mathbb{E}_{s\sim d^{\pi_\theta}, a\sim\pi_\theta(s,\cdot)}\left[\left(Q^{\pi_\theta}(s,a) - b(s;\theta) - f_\omega(s,a)\right)\nabla_\theta \pi_\theta(s,a)\frac{1}{\pi_\theta(s,a)}\right] = 0$$

Proof of Policy gradient theorem

Or,

$$\sum_s d^{\pi_\theta}(s) \sum_a \nabla_\theta \pi_\theta(s,a) \left(Q^{\pi_\theta}(s,a) - b(s;\theta) - f_\omega(s,a)\right) = 0$$

Since $b(s;\theta) \sum_a \nabla_\theta \pi_\theta(s,a) = 0$

$$\sum_s d^{\pi_\theta}(s) \sum_a \nabla_\theta \pi_\theta(s,a) \left(Q^{\pi_\theta}(s,a) - f_\omega(s,a)\right) = 0$$

using this with the policy gradient theorem, we get

$$\nabla_\theta \rho(\pi_\theta) = \sum_s d^{\pi_\theta}(s) \sum_a \nabla_\theta \pi_\theta(s,a) f_\omega(s,a)$$

Example: softmax policy

- Consider policy set parameterized by θ such that given $s \in S$, probability of picking action $a \in A$ is given by:

$$\pi_\theta(s,a) = \frac{e^{\theta^\top \phi_{sa}}}{\sum_{a' \in A} e^{\theta^\top \phi_{sa'}}}$$

where each ϕ_{sa} is an ℓ-dimensional feature vector characterizing state-action pair s, a. This is a popular form of parameterization. Here,

$$\nabla_\theta \pi_\theta(s,a) = \phi_{sa}\pi_\theta(s,a) - \left(\sum_{a' \in A} \phi_{sa'}\pi_\theta\left(s,a'\right)\right)\pi_\theta(s,a)$$

Example: softmax policy

- Meeting the compatibility condition in Theorem 1 requires that

$$\nabla_\omega f_\omega(s,a) = \frac{1}{\pi_\theta(s,a)} \nabla_\theta \pi_\theta(s,a) = \phi_{sa} - \sum_{a' \in A} \phi_{sa'} \pi_\theta\left(s,a'\right)$$

- A natural form of $f_\omega(s,a)$ satisfying this condition is:

$$f_\omega(s,a) = \omega^\top \left(\phi_{sa} - \sum_{b \in A} \phi_{sb} \pi_\theta(s,b) \right)$$

- Thus f_ω must be linear in the same features as the policy, except normalized to be mean zero for each state. In this sense it is better to think of f_ω as an approximation of the advantage function, $A^\pi(s,a) = Q^\pi(s,a) - V^\pi(s)$, rather than Q^π.

Example: Gaussian policy for continuous action spaces

- In continuous action spaces, it is natural to use Gaussian policy. Given state s, the probability of action a is given as:

$$\pi_\theta(s,a) = \mathcal{N}\left(\phi(s)^T\theta, \sigma^2\right)$$

for some constant σ. Here $\phi(s)$ is a feature representation of s. Then, compatibility condition for $f_\omega(s,a)$:

$$\nabla_\omega f_\omega(s,a) = \nabla_\theta \log\left(\pi_\theta(s,a)\right) = \nabla_\theta \frac{-\left(a-\theta^\top\phi(s)\right)^2}{2\sigma^2} = \frac{\left(\theta^\top\phi(s)-a\right)}{\sigma^2}\phi(s)$$

- For f_ω to satisfy this, it must be linear in ω, e.g., $f_\omega(s,a) = \frac{\left(\theta^\top\phi(s)-a\right)}{\sigma^2}\phi(s)^\top\omega$

Policy iteration algorithm with function approximation

Let $f_\omega(\cdot,\cdot)$ be such that $\nabla f_\omega(s,a) = \nabla_\theta \log \pi_\theta(s,a)$ for all ω, θ, s, a.
Initialize θ_1, $\pi_1 := \pi_{\theta_1}$. Pick step sizes $\alpha_1, \alpha_2, \ldots,$.
In iteration $k = 1, 2, 3, \ldots,$

- Policy evaluation: Find $w_k = w$ such that

$$\mathbb{E}_{s\sim d^{\pi_k}} \mathbb{E}_{a\sim\pi_k(s)} \left[\left(Q^{\pi_k}(s,a) - b_k(s) - f_\omega(s,a) \right) \nabla_\theta \log \left(\pi_k(s,a) \right) \right] = 0$$

  (Here, d^{π_k} is not normalized to 1, and sums to $1/(1-\gamma)$.)

- Policy improvement:

$$\theta_{k+1} \leftarrow \theta_k + \alpha_k \mathbb{E}_{s\sim d^{\pi_k}} \mathbb{E}_{a\sim\pi_k(s)} \left[f_\omega(s,a) \nabla_\theta \log \left(\pi_k(s,a) \right) \right]$$

A similar algorithm appears in Konda and Tsitsiklis [1999].

Convergence Guarantees

Following version of convergence guarantees were provided by Sutton et al. [1999] for infinite horizon MDPs (average or discounted).

Theorem 2 (Sutton et al. [1999])

Given $\alpha_1, \alpha_2, \ldots,$ such that

$$\lim_{T\to\infty} \sum_{k=1}^{T} \alpha_k = \infty, \lim_{T\to\infty} \sum_{k=1}^{T} \alpha_k^2 < \infty$$

and $\max_{\theta,s,a,i,j} \frac{\partial^2 \pi_\theta(s,a)}{\partial\theta_i\theta_j} < \infty$. Then, for $\theta_1, \theta_2, \ldots,$ obtained by the above algorithm,

$$\lim_{k\to\infty} \nabla_\theta \rho\left(\theta\right)|_{\theta_k} = 0$$

Pseudocode: Vanilla Policy Gradient Algorithm

Algorithm 1 Vanilla Policy Gradient Algorithm

1: Input: initial policy parameters θ_0, initial value function parameters ϕ_0
2: **for** $k = 0, 1, 2, \ldots$ **do**
3: Collect set of trajectories $\mathcal{D}_k = \{\tau_i\}$ by running policy $\pi_k = \pi(\theta_k)$ in the environment.
4: Compute rewards-to-go $\hat{R}_t$.
5: Compute advantage estimates, $\hat{A}_t$ (using any method of advantage estimation) based on the current value function V_{ϕ_k}.
6: Estimate policy gradient as

$$\hat{g}_k = \frac{1}{|\mathcal{D}_k|} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \nabla_\theta \log \pi_\theta(a_t|s_t)|_{\theta_k} \hat{A}_t.$$

7: Compute policy update, either using standard gradient ascent,

$$\theta_{k+1} = \theta_k + \alpha_k \hat{g}_k,$$

or via another gradient ascent algorithm like Adam.
8: Fit value function by regression on mean-squared error:

$$\phi_{k+1} = \arg\min_\phi \frac{1}{|\mathcal{D}_k| T} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \left(V_\phi(s_t) - \hat{R}_t\right)^2,$$

typically via some gradient descent algorithm.
9: **end for**

Outline

Trust Region Policy Optimization (John Schulman, etc)

- Assume start-state distribution d_0 is independent with policy
- Total expected discounted reward with policy π

$$\eta(\pi) = E_\pi[\sum_{t=0}^{\infty} \gamma^t r(s_t)]$$

- Advantage function: $A_\pi(s,a) = Q_\pi(s,a) - V_\pi(s)$
- Between any two different policy $\widetilde{\pi}$ and π

$$\begin{aligned}
\eta(\widetilde{\pi}) &= \eta(\pi) + E_{\widetilde{\pi}}[\sum_{t=0}^{\infty} \gamma^t A_\pi(s_t, a_t)] \\
&= \eta(\pi) + \sum_{t=0}^{\infty} \sum_s P(s_t = s|\widetilde{\pi}) \sum_a \widetilde{\pi}(a|s) \gamma^t A_\pi(s,a) \\
&= \eta(\pi) + \sum_s \sum_{t=0}^{\infty} \gamma^t P(s_t = s|\widetilde{\pi}) \sum_a \widetilde{\pi}(a|s) A_\pi(s,a) \\
&= \eta(\pi) + \sum_s d_{\widetilde{\pi}}(s) \sum_a \widetilde{\pi}(a|s) A_\pi(s,a).
\end{aligned}$$

Trust Region Policy Optimization

- Find new policy $\widetilde{\pi}$ to maximize $\eta(\widetilde{\pi}) - \eta(\pi)$ for given π, that is

$$\max_{\widetilde{\pi}} \eta(\pi) + \sum_s d_{\widetilde{\pi}}(s) \sum_a \widetilde{\pi}(a|s) A_\pi(s,a)$$

- For simpleness, maximize the approximator

$$L_\pi(\widetilde{\pi}) = \eta(\pi) + \sum_s d_\pi(s) \sum_a \widetilde{\pi}(a|s) A_\pi(s,a)$$

- Parameterize the policy $\pi(a|s) := \pi_\theta(a|s)$

$$L_{\pi_{\theta_{old}}}(\pi_\theta) = \eta(\pi_{\theta_{old}}) + \sum_s d_{\pi_{\theta_{old}}}(s) \sum_a \pi_\theta(a|s) A_{\pi_{\theta_{old}}}(s,a)$$

Why $L_{\pi_{\theta_{old}}}(\pi_\theta)$?

- A sufficiently small step $\theta_{old} \rightarrow \theta$ improves $L_{\pi_{\theta_{old}}}(\pi_\theta)$ also improves η

$$L_{\pi_{\theta_{old}}}(\pi_{\theta_{old}}) = \eta(\pi_{\theta_{old}}),$$
$$\nabla_\theta L_{\pi_{\theta_{old}}}(\pi_\theta)|_{\theta=\theta_{old}} = \nabla_\theta \eta(\pi_\theta)|_{\theta=\theta_{old}}.$$

- Lower bounds on the improvement of η

$$\eta(\pi_{\theta_{new}}) \geq L_{\pi_{\theta_{old}}}(\pi_{\theta_{new}}) - \frac{2\epsilon\gamma}{(1-\gamma)^2}\alpha^2$$

where

$$\epsilon = \max_s |E_{a\sim\pi_{\theta_{new}}} A_{\pi_{\theta_{old}}}(s,a)|$$
$$\alpha = D_{TV}^{max}(\pi_{\theta_{old}}||\pi_{\theta_{new}}) = \max_s D_{TV}(\pi_{\theta_{old}}(\cdot|s)||\pi_{\theta_{new}}(\cdot|s))$$

Lower bound

- TV divergence between two distribution p, q (discrete case)

$$D_{TV}(p\|q) = \frac{1}{2}\sum_X |p(X) - q(X)|$$

- KL divergence between two distribution p, q (discrete case)

$$D_{KL}(p\|q) = \sum_X p(X)\log\frac{p(X)}{q(X)}$$

- $(D_{TV}(p||q))^2 \leq D_{KL}(p||q)$ (Pollard(2000),Ch.3)

- Thus obtain a lower bound

$$\eta(\pi_{\theta_{new}}) \geq L_{\pi_{\theta_{old}}}(\pi_{\theta_{new}}) - \frac{2\epsilon\gamma}{(1-\gamma)^2}\alpha$$

where

$$\alpha = D_{KL}^{max}(\pi_{\theta_{old}}||\pi_{\theta_{new}}) := \max_s D_{KL}(\pi_{\theta_{old}}(\cdot|s)||\pi_{\theta_{new}}(\cdot|s))$$

Practical algorithm

- The penalty coefficient $\frac{2\epsilon\gamma}{(1-\gamma)^2}$ is large in practice, which yields small update
- Take a constraint on the KL divergence, i.e., a trust region constraint:

$$\begin{aligned} \max_{\theta} \quad & L_{\pi_{\theta_{old}}}(\pi_\theta) \\ \text{s.t.} \quad & D_{KL}^{max}(\pi_{\theta_{old}}||\pi_\theta) \leq \delta \end{aligned}$$

- A heuristic approximation

$$\begin{aligned} \max_{\theta} \quad & L_{\pi_{\theta_{old}}}(\pi_\theta) \\ \text{s.t.} \quad & \overline{D}_{KL}^{\rho_{\pi_{\theta_{old}}}}(\pi_{\theta_{old}}||\pi_\theta) \leq \delta \end{aligned}$$

where

$$\overline{D}_{KL}^{\rho_{\pi_{\theta_{old}}}}(\pi_{\theta_{old}}||\pi_\theta) = E_{\pi_{\theta_{old}}}(D_{KL}(\pi_{\theta_{old}}(\cdot|s)||\pi_\theta(\cdot|s))$$

TRPO

- The objective and constraint are both zero when $\theta = \theta_k$. Furthermore, the gradient of the constraint with respect to θ is zero when $\theta = \theta_k$.
- The theoretical TRPO update isn't the easiest to work with, so TRPO makes some approximations to get an answer quickly. We Taylor expand the objective and constraint to leading order around θ_k:

$$L_{\theta_k}(\theta) \approx g^T(\theta - \theta_k)$$
$$\bar{D}_{KL}(\theta_k||\theta) \approx \frac{1}{2}(\theta - \theta_k)^T H(\theta - \theta_k)$$

resulting in an approximate optimization problem,

$$\theta_{k+1} = \arg\max_{\theta} g^T(\theta - \theta_k)$$
$$\text{s.t. } \frac{1}{2}(\theta - \theta_k)^T H(\theta - \theta_k) \leq \delta.$$

TRPO

- By happy coincidence, the gradient g of the surrogate advantage function with respect to θ, evaluated at $\theta = \theta_k$, is exactly equal to the policy gradient, $\nabla_\theta J(\pi_\theta)$
- This approximate problem can be analytically solved by the methods of Lagrangian duality, yielding the solution:

$$\theta_{k+1} = \theta_k + \sqrt{\frac{2\delta}{g^T H^{-1} g}} H^{-1} g.$$

- TRPO adds a modification to this update rule: a backtracking line search,

$$\theta_{k+1} = \theta_k + \alpha^j \sqrt{\frac{2\delta}{g^T H^{-1} g}} H^{-1} g,$$

where $\alpha \in (0, 1)$ is the backtracking coefficient, and j is the smallest nonnegative integer such that $\pi_{\theta_{k+1}}$ satisfies the KL constraint and produces a positive surrogate advantage.

TRPO

- computing and storing the matrix inverse, H^{-1}, is painfully expensive when dealing with neural network policies with thousands or millions of parameters. TRPO sidesteps the issue by using the 'conjugate gradient' algorithm to solve $Hx = g$ for $x = H^{-1}g$, requiring only a function which can compute the matrix-vector product Hx instead of computing and storing the whole matrix H directly.

$$Hx = \nabla_\theta \left(\left(\nabla_\theta \bar{D}_{KL}(\theta_k || \theta) \right)^T x \right)$$

Pseudocode: TRPO

Algorithm 2 Trust Region Policy Optimization

Input: initial policy θ_0, initial value function ϕ_0, KL-divergence limit δ, backtracking coefficient α

for $k = 0, 1, 2, \ldots$ **do**

Collect set of trajectories $\mathcal{D}_k = \{\tau_i\}$ by running policy $\pi_k = \pi(\theta_k)$ in the environment.

Compute rewards-to-go $\hat{R}_t$.

Compute advantage estimates, $\hat{A}_t$ (using any method of advantage estimation) based on the current value function V_{ϕ_k}.

Estimate policy gradient as

$$\hat{g}_k = \frac{1}{|\mathcal{D}_k|} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \nabla_\theta \log \pi_\theta(a_t|s_t)|_{\theta_k} \hat{A}_t.$$

Use the conjugate gradient algorithm to compute $\hat{x}_k \approx \hat{H}_k^{-1} \hat{g}_k$, where $\hat{H}_k$ is the Hessian of the sample average KL-divergence.

Update the policy by backtracking line search with $\theta_{k+1} = \theta_k + \alpha^j \sqrt{\frac{2\delta}{\hat{x}_k^T \hat{H}_k \hat{x}_k}} \hat{x}_k$, where j is the smallest value which improves the sample loss and satisfies the sample KL-divergence constraint.

Fit value function by regression on mean-squared error:

$$\phi_{k+1} = \arg\min_\phi \frac{1}{|\mathcal{D}_k| T} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \left(V_\phi(s_t) - \hat{R}_t \right)^2,$$

typically via some gradient descent algorithm.

end for

Proximal Policy Optimization (PPO)

- PPO is motivated by the same question as TRPO: how can we take the biggest possible improvement step on a policy using the data we currently have, without stepping so far that we accidentally cause performance collapse? Where TRPO tries to solve this problem with a complex second-order method, PPO is a family of first-order methods that use a few other tricks to keep new policies close to old.
- **PPO-Penalty** approximately solves a KL-constrained update like TRPO, but penalizes the KL-divergence in the objective function instead of making it a hard constraint, and automatically adjusts the penalty coefficient over the course of training so that it's scaled appropriately.
- **PPO-Clip** doesn't have a KL-divergence term in the objective and doesn't have a constraint at all. Instead relies on specialized clipping in the objective function to remove incentives for the new policy to get far from the old policy.

Key Equations

- PPO-clip updates policies via

$$\theta_{k+1} = \arg\max_{\theta} \underset{s,a \sim \pi_{\theta_k}}{\mathrm{E}} \left[L(s, a, \theta_k, \theta) \right],$$

typically taking multiple steps of (usually minibatch) SGD to maximize the objective. Here L is given by

$$L(s, a, \theta_k, \theta) = \min \left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A^{\pi_{\theta_k}}(s, a), \quad \text{clip} \left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)}, 1 - \epsilon, 1 + \epsilon \right) A^{\pi_{\theta_k}}(s, a) \right),$$

in which ϵ is a (small) hyperparameter which roughly says how far away the new policy is allowed to go from the old.

- `https://openai.com/research/openai-baselines-ppo`

- This is a pretty complex expression, and it's hard to tell at first glance what it's doing, or how it helps keep the new policy close to the old policy. As it turns out, there's a considerably simplified version of this objective which is a bit easier to grapple with

$$L(s, a, \theta_k, \theta) = \min \left(\frac{\pi_\theta(a|s)}{\pi_{\theta_k}(a|s)} A^{\pi_{\theta_k}}(s, a), \quad g(\epsilon, A^{\pi_{\theta_k}}(s, a)) \right),$$

  where

$$g(\epsilon, A) = \begin{cases} (1+\epsilon)A & A \geq 0 \\ (1-\epsilon)A & A < 0. \end{cases}$$

- To figure out what intuition to take away from this, let's look at a single state-action pair (s, a), and think of cases.

Pseudocode: PPO

Algorithm 3 PPO-Clip

Input: initial policy parameters θ_0, initial value function parameters ϕ_0

for $k = 0, 1, 2, \ldots$ **do**

Collect set of trajectories $\mathcal{D}_k = \{\tau_i\}$ by running policy $\pi_k = \pi(\theta_k)$ in the environment.

Compute rewards-to-go $\hat{R}_t$.

Compute advantage estimates, $\hat{A}_t$ (using any method of advantage estimation) based on the current value function V_{ϕ_k}.

Update the policy by maximizing the PPO-Clip objective:

$$\theta_{k+1} = \arg\max_{\theta} \frac{1}{|\mathcal{D}_k|T} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \min\left(\frac{\pi_\theta(a_t|s_t)}{\pi_{\theta_k}(a_t|s_t)} A^{\pi_{\theta_k}}(s_t, a_t), \quad g(\epsilon, A^{\pi_{\theta_k}}(s_t, a_t)) \right),$$

typically via stochastic gradient ascent with Adam.

Fit value function by regression on mean-squared error:

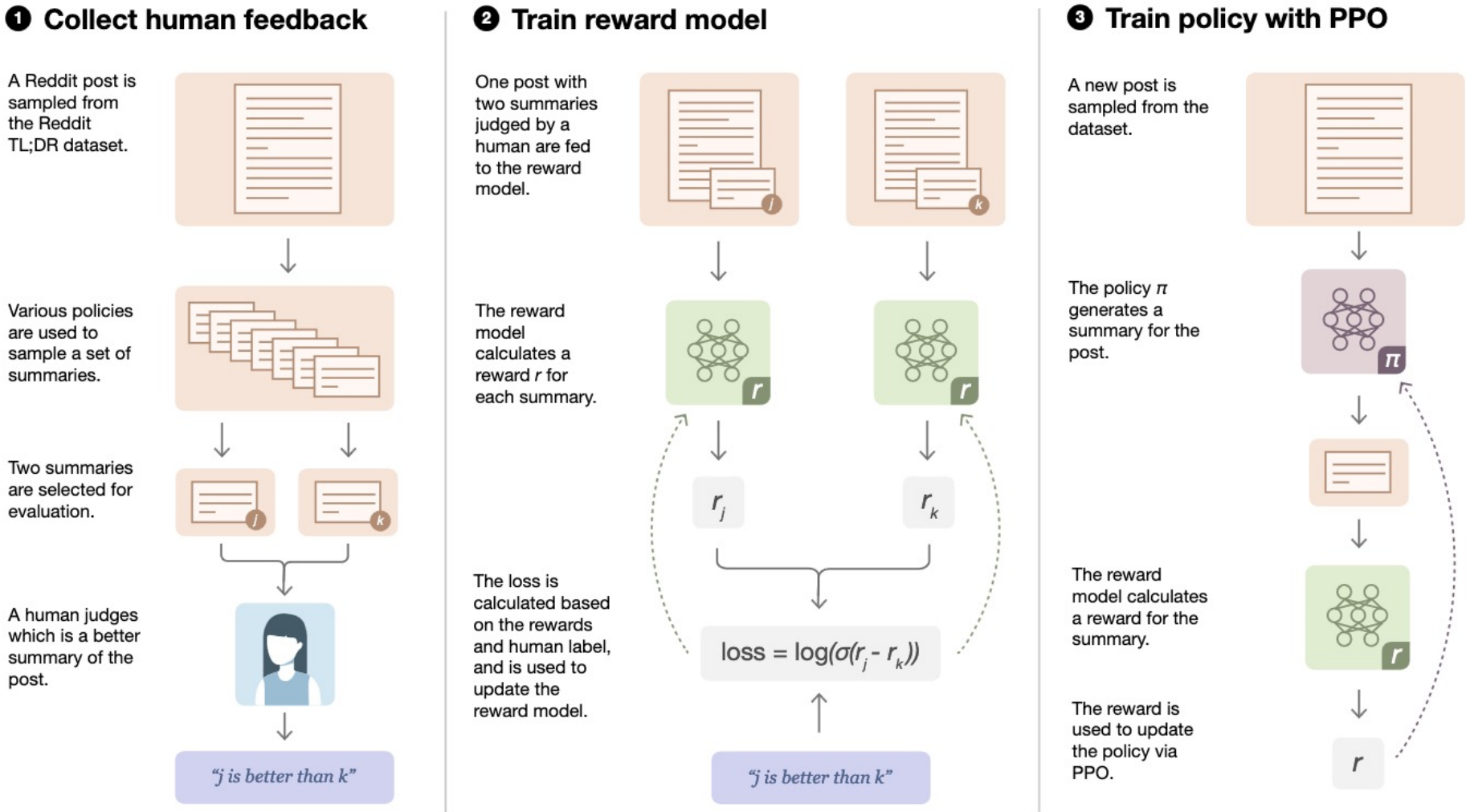
$$\phi_{k+1} = \arg\min_{\phi} \frac{1}{|\mathcal{D}_k|T} \sum_{\tau \in \mathcal{D}_k} \sum_{t=0}^{T} \left(V_\phi(s_t) - \hat{R}_t \right)^2,$$

typically via some gradient descent algorithm.

end for

Reinforcement Learning from Human Feedback

RLHF: Nisan Stiennon, etc, Learning to summarize with human feedback, NeurIPS 2020



InstructGPT

provide detailed, accurate, and instructive responses to user queries.

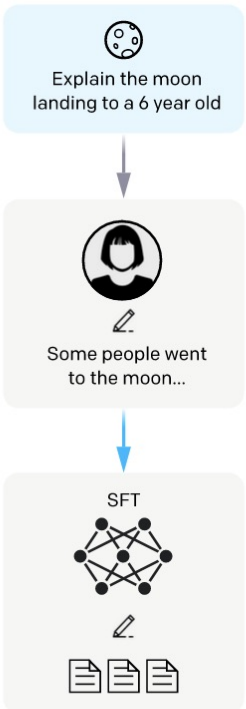
Step 1

Collect demonstration data, and train a supervised policy.

A prompt is sampled from our prompt dataset.

A labeler demonstrates the desired output behavior.

This data is used to fine-tune GPT-3 with supervised learning.



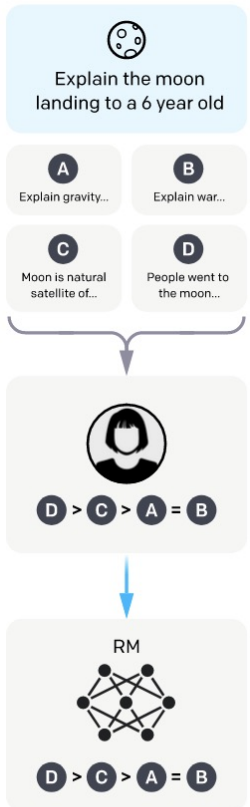
Step 2

Collect comparison data, and train a reward model.

A prompt and several model outputs are sampled.

A labeler ranks the outputs from best to worst.

This data is used to train our reward model.



Step 3

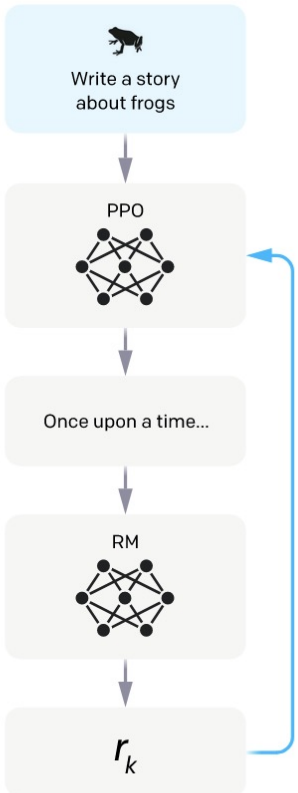
Optimize a policy against the reward model using reinforcement learning.

A new prompt is sampled from the dataset.

The policy generates an output.

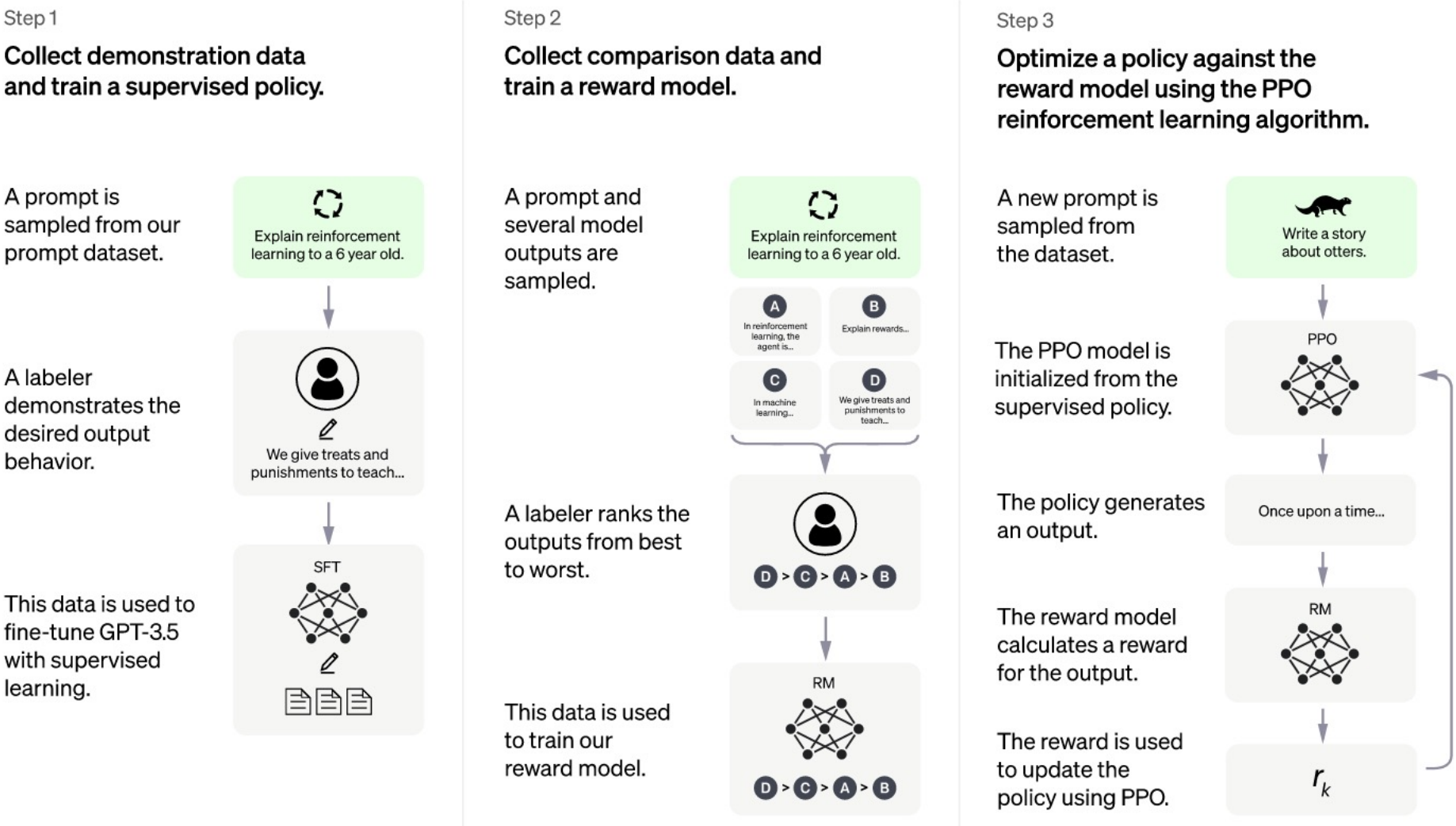
The reward model calculates a reward for the output.

The reward is used to update the policy using PPO.



ChatGPT

generate human-like text based on the input it's given, and it can carry out a wide-ranging conversation on various topics.



Outline

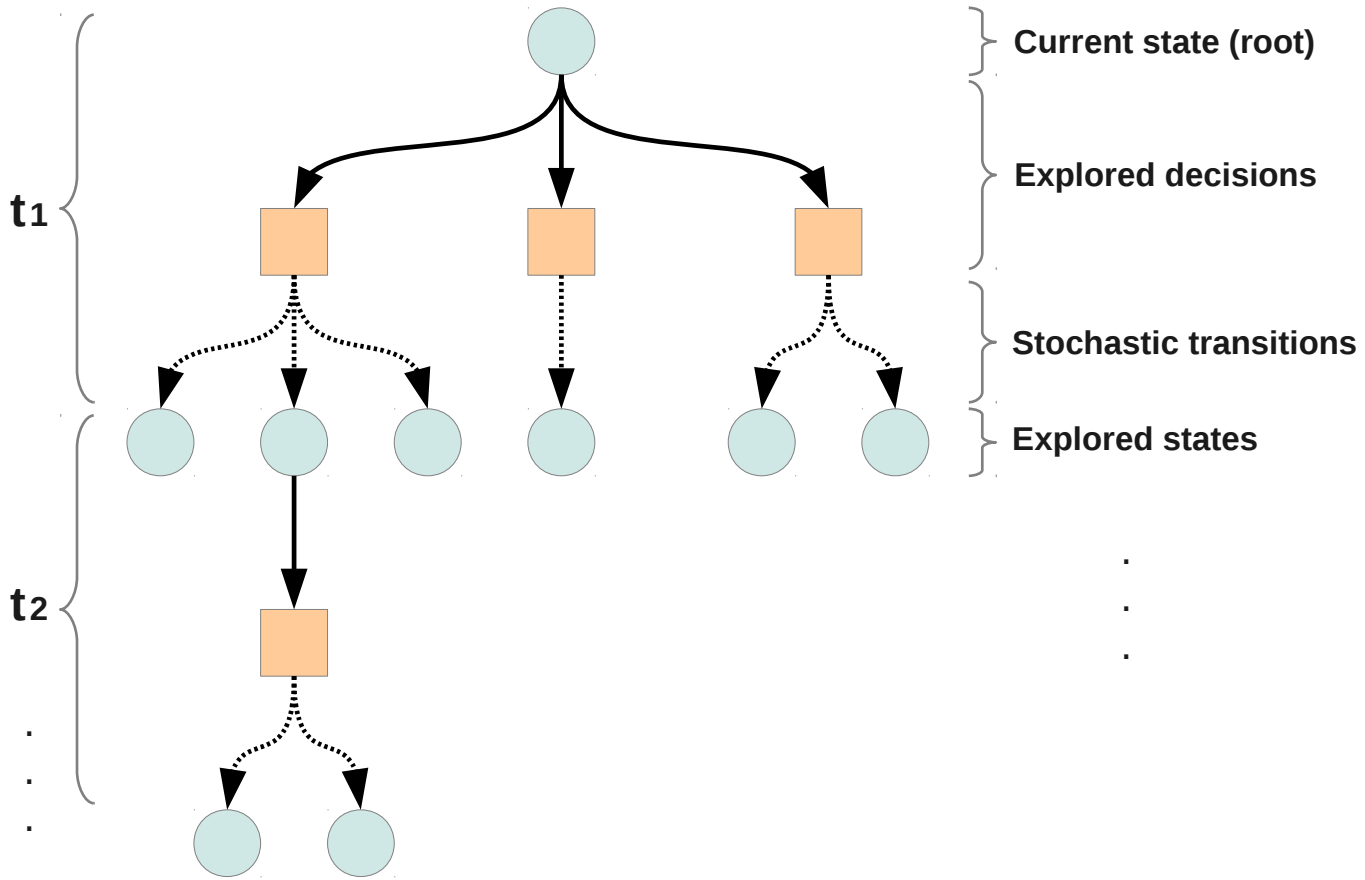
Monte-Carlo Tree Search (MCTS)

- MCTS is a recent algorithm for *sequential decision making*
- MCTS is a versatile algorithm (it does not require knowledge about the problem)
- especially, does not require any knowledge about the Bellman value function
- stable on high dimensional problems
- it outperforms all other algorithms on some problems (difficult games like Go, general game playing, . . .)

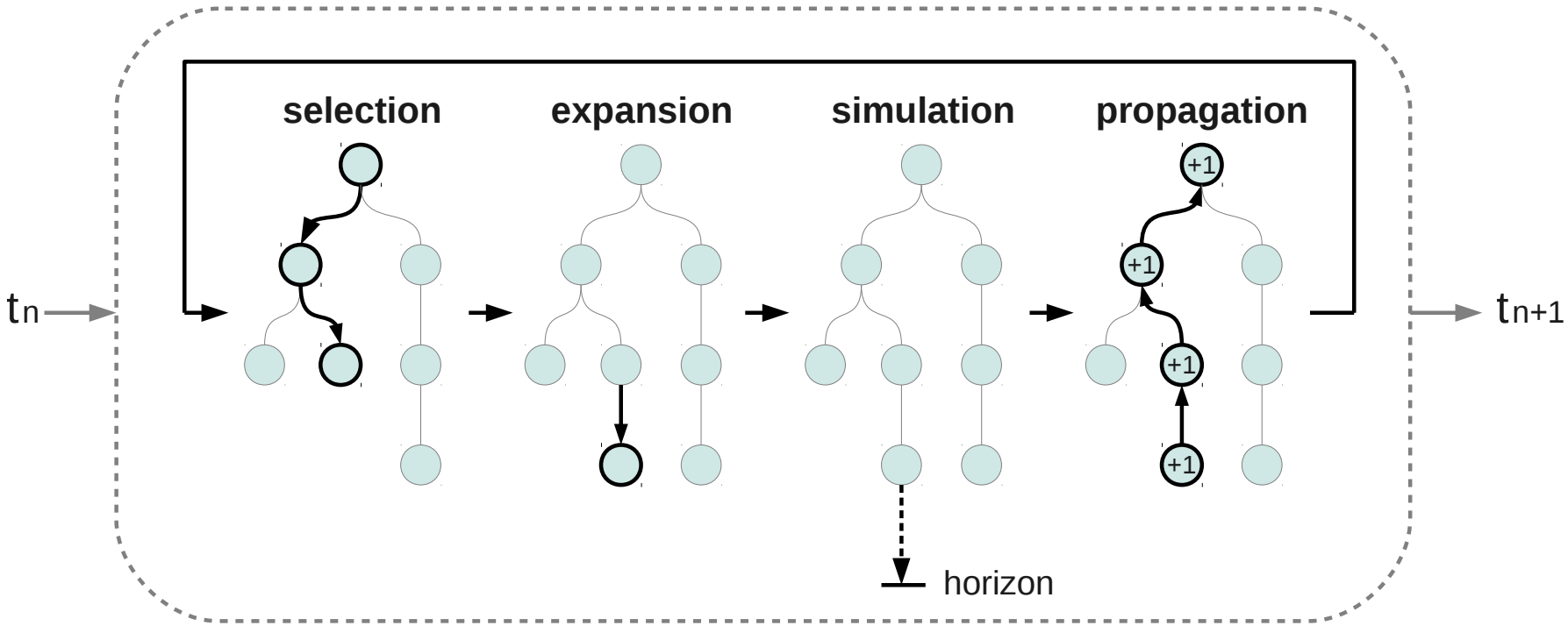
MCTS

Problems are represented as a tree structure:

- blue circles = states
- plain edges + red squares = decisions
- dashed edges = stochastic transitions between two states



Main steps of MCTS

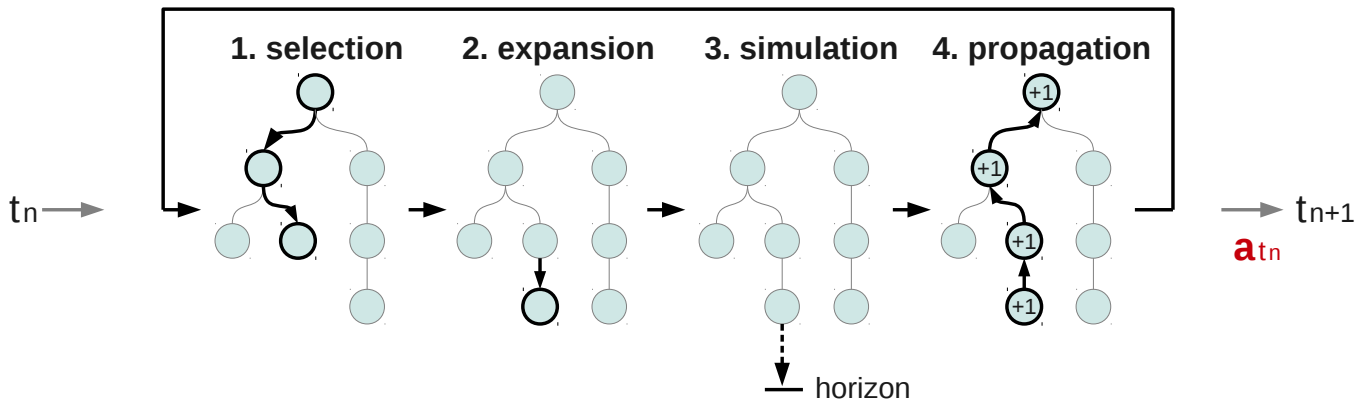


Main steps of MCTS

Starting from an initial state:

1. **Selection**: select the state we want to expand from
2. **Expansion**: One (or more) child nodes are added to expand the tree, according to the available actions.
3. **Simulation**: A simulation is run from the new node(s) according to the default policy (pick actions randomly) to produce an outcome.
4. **Back-propagation** of some information:
   - $N(s,a)$: number of times decision a has been simulated in s
   - $N(s)$: number of time s has been visited in simulations
   - $Q(s,a)$: mean reward of simulations where a was chosen in s

Main steps of MCTS

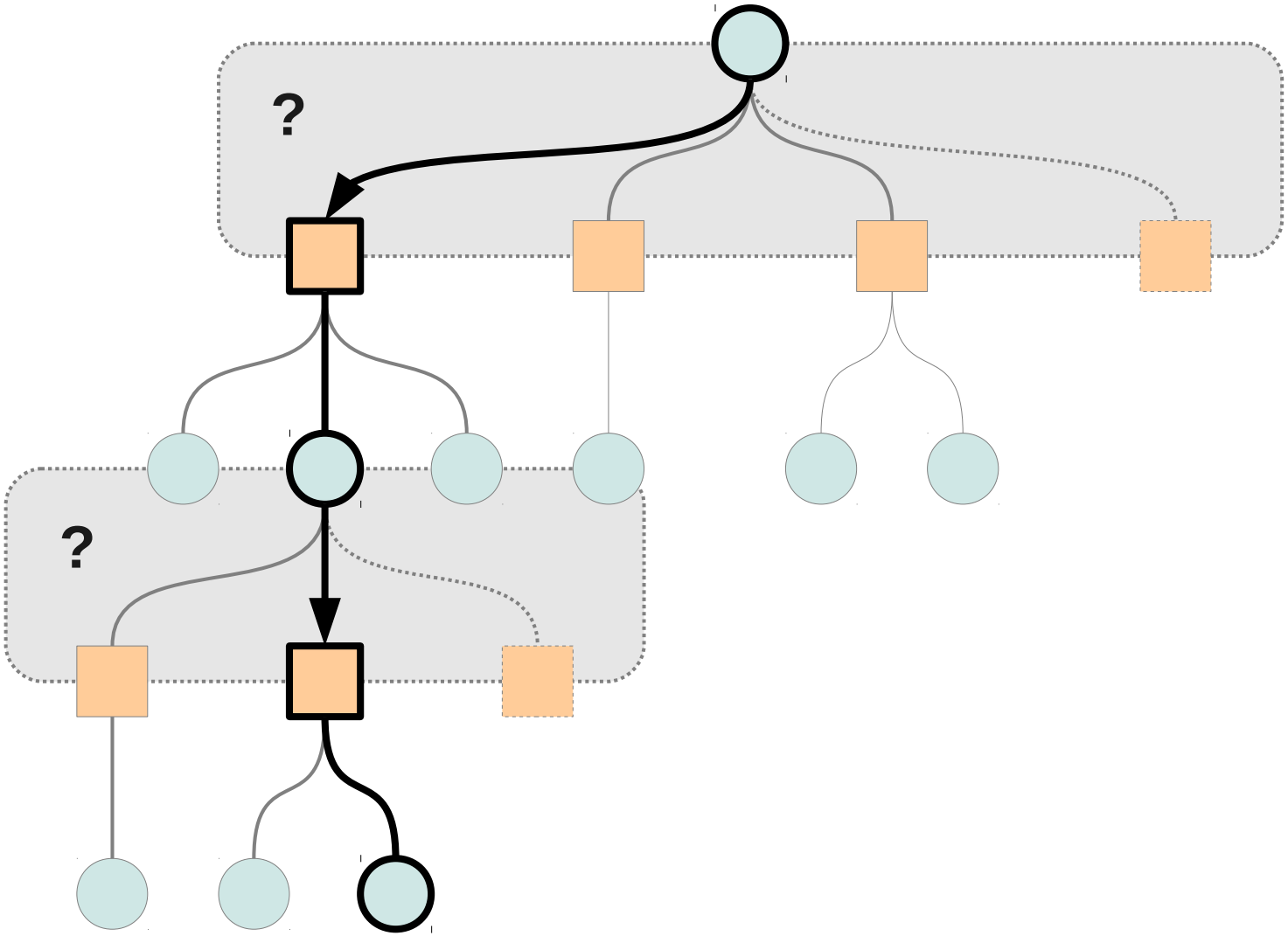


The selected decision

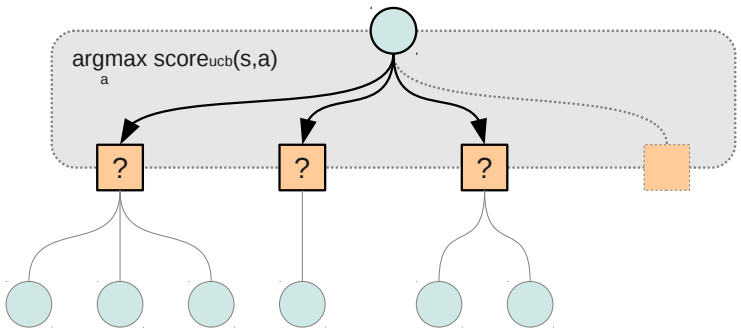
a_{t_n} = the most visited decision from the current state (root node)

Selection step

How to select the state to expand ?



How to select the state to expand ?

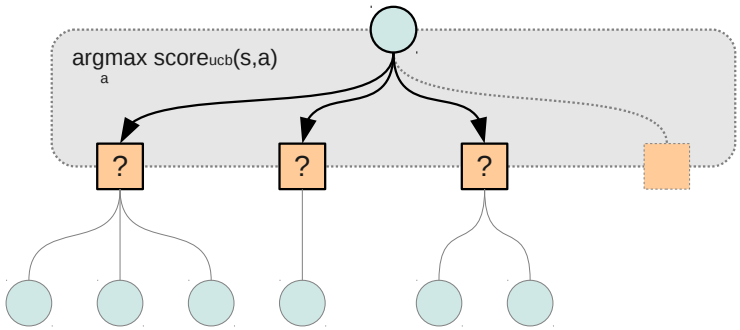


The *selection* phase is driven by Upper Confidence Bound (UCB):

$$\text{score}_{\text{ucb}}(s,a) = \underbrace{Q(s,a)}_{1} + \underbrace{\sqrt{\frac{\log(2+N(s))}{2+N(s,a)}}}_{2}$$

1. mean reward of simulations including action a in state s
2. the uncertainty on this estimation of the action's value

How to select the state to expand ?



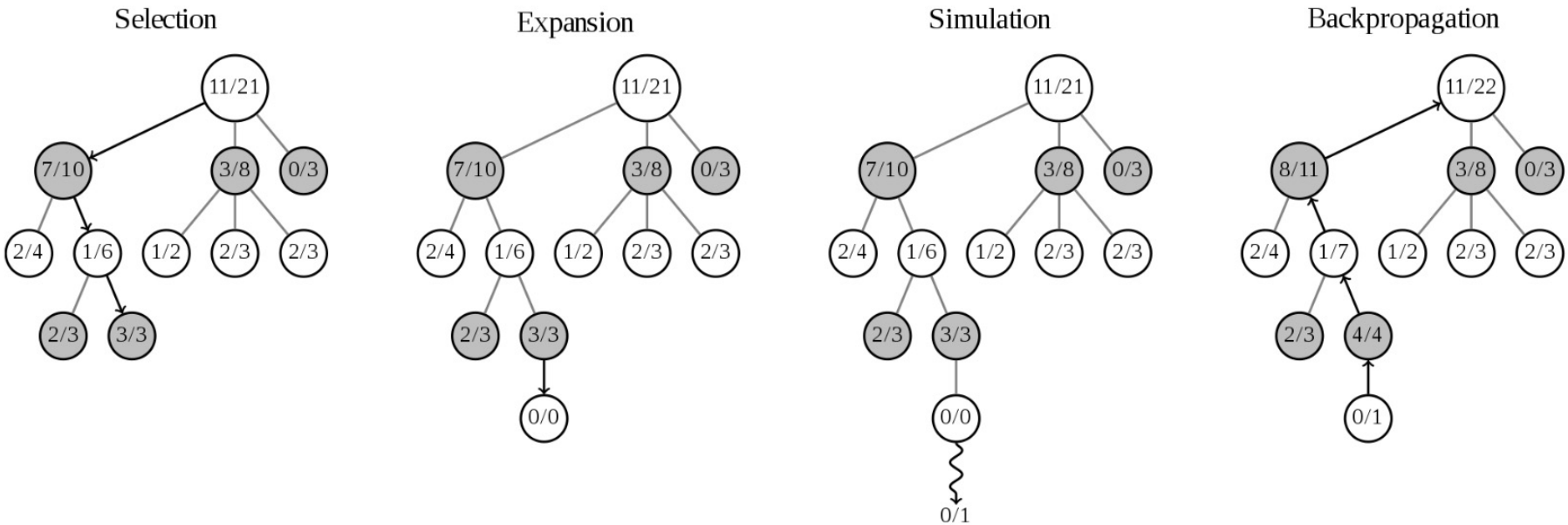
The *selection* phase is driven by Upper Confidence Bound (UCB):

$$\text{score}_{\text{ucb}}(s,a) = \underbrace{Q(s,a)}_{1} + \underbrace{\sqrt{\frac{\log(2+N(s))}{2+N(s,a)}}}_{2}$$

The selected action:

$$a^\star = \arg\max_a \ \text{score}_{\text{ucb}}(s,a)$$

Example: Back-propagation



AlphaZero

2018/12/7, AlphaZero at “Science”. It demonstrates learning chess, shogi and go, tabula rasa without any domain-specific human knowledge or data, only using self-play. The evaluation is performed against strongest programs available.

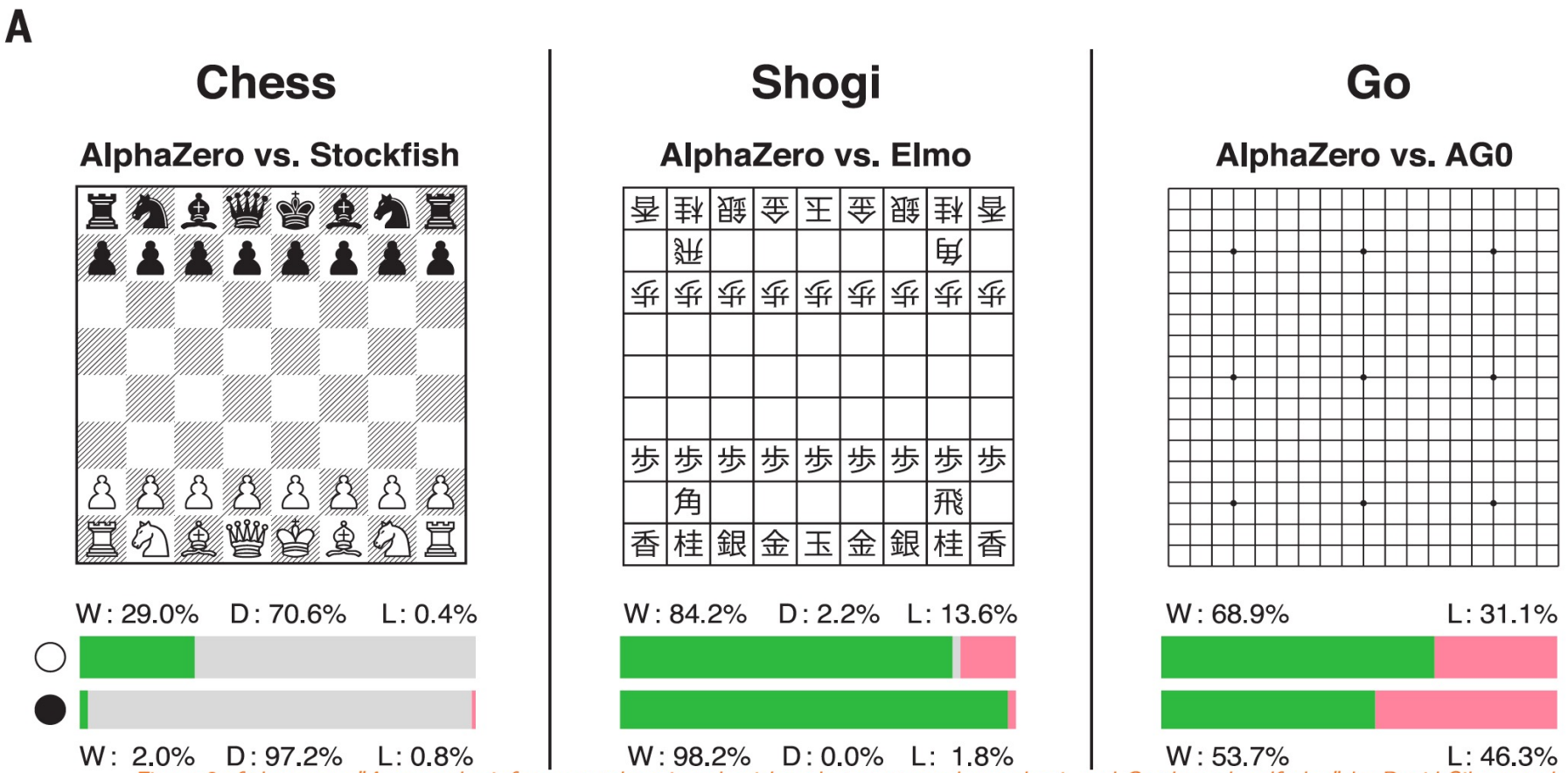


Figure 2 of the paper "A general reinforcement learning algorithm that masters chess, shogi, and Go through self-play" by David Silver et al.

AlphaZero

- AlphaZero uses a neural network predicting $(p(s), v(s)) = f(s, \theta)$ for a given state s
  - $p(s)$ is a vector of move probabilities
  - $v(s)$ is expected outcome of the game in range $[-1, 1]$.
- Unlike the standard MCTS, Alpha Go Zero does not use a default policy to perform a rollout in order to achieve an estimate of the value of a state.
- By a sequence of simulated self-play games, the search can improve the estimate of p and v, and can be considered a powerful policy evaluation operator given a network f predicting policy p and value estimate v, MCTS produces a more accurate policy π and better value estimate w for a given state:

$$(\pi(s), w(s)) \leftarrow \text{MCTS}(p(s), v(s), f) \text{ for } (p(s), v(s)) = f(s, \theta).$$

AlphaZero: MCTS

MCTS keeps a tree of currently explored states from a fixed root state. Each node corresponds to a game state and to every non-root node we got by performing an action a from the parent state. Each state-action pair (s, a) stores the following set of statistics:

- visit count $N(s, a)$
- total action-value $W(s, a)$
- mean action-value $Q(s, a) = W(s, a)/N(s, a)$, which is not stored explicitly
- prior probability $P(s, a)$ of selecting action a in state s

AlphaZero: UCB

- Each simulation starts in the root node and finishes in a leaf node s_L. In a state s_t, an action is selected using a variant of PUCT algorithm as

$$a_t = \arg\max_a \quad Q(s_t, a) + U(s_t, a)$$

where

$$U(s,a) = C(s)P(s,a)\frac{\sqrt{N(s)}}{1+N(s,a)},$$

with $C(s) = \log\left(\frac{1+N(s)+c_{base}}{c_{base}}\right) + c_{init}$.

- In the Alphazero paper, $c_{init} = 1.25$ and $c_{base} = 19652$.

AlphaZero

When reaching a leaf node s_L,

- evaluate it by the network, generating (p, v)
- add all its children with $N = W = 0$ and the prior probability p,
- in the backward pass for all $t \leq L$, we update the statistics in nodes by performing
  - $N(s_t, a_t) \leftarrow N(s_t, a_t) + 1$, and
  - $W(s_t, a_t) \leftarrow W(s_t, a_t) \pm v$, depending on the player on turn.

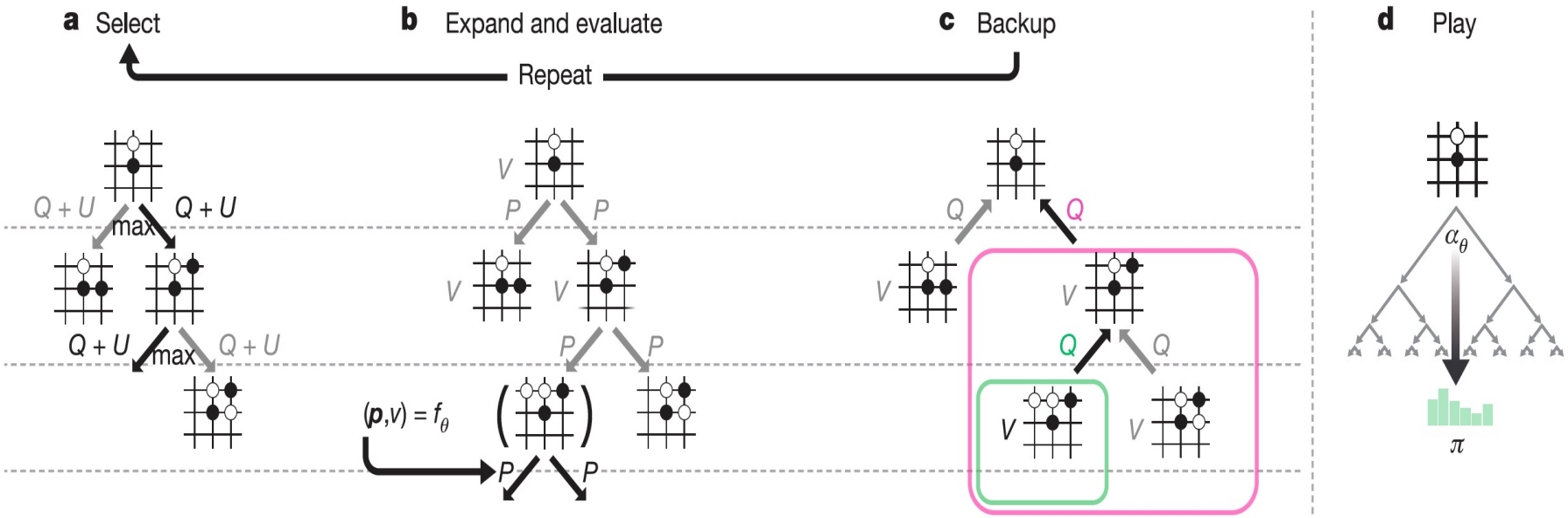


Figure 2 of the paper "Mastering the game of Go without human knowledge" by David Silver et al.

AlphaZero

- The MCTS runs usually several hundreds simulations in a single tree. The result is a distribution proportional to exponentiated visit counts $N(s_{root}, a)^{1/\tau}$ using a temperature ($\tau = 1$ is mostly used), together with the predicted value function.
- The next move is chosen as either:
  - proportional to visit counts $N(s_{root}, \cdot)^{1/\tau}$

$$\pi_{root}(a) \sim N(s_{root}, \cdot)^{1/\tau}$$

  - deterministically as the most visited action

$$\pi_{root} = \arg\max_a N(s_{root}, a)$$

- During self-play, the stochastic policy is used for the first 30 moves of the game, while the deterministic is used for the rest of the moves. (This does not affect the internal MCTS search, there we always sample according to PUCT rule.)

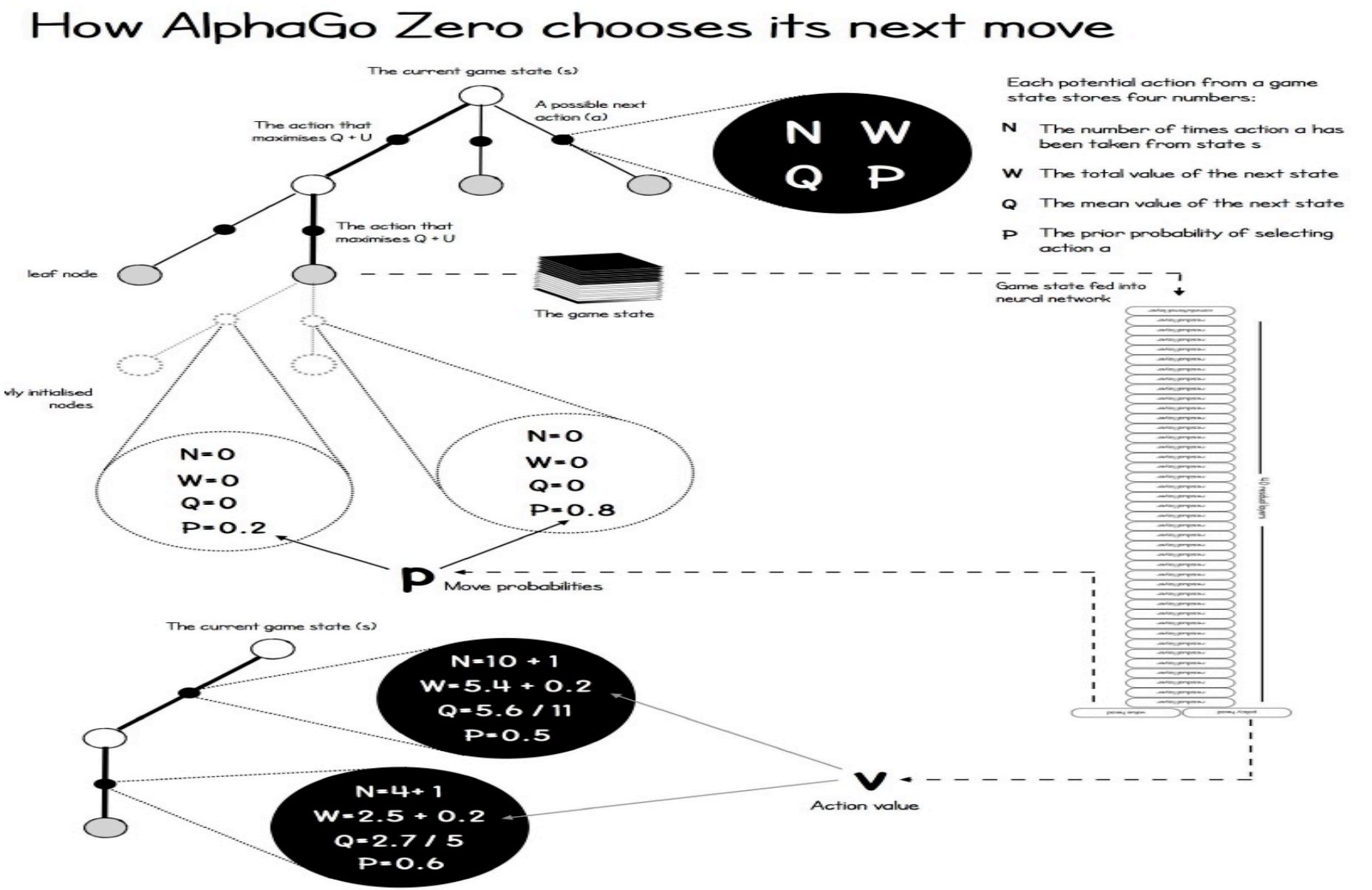
AlphaZero: Loss function

- The network is trained from self-play games.
- A game is played by repeatedly running MCTS from a state s_t and choosing a move $a_t \sim \pi_t$, until a terminal position s_T is encountered, which is then scored according to game rules as $z \in \{-1, 0, 1\}$.
- Finally, the network parameters are trained to minimize

$$L = (z - v)^2 + \pi^\top \log p + c\|\theta\|^2$$

  - a mean squared error between the predicted outcome v and the simulated outcome z
  - a crossentropy/KL divergence for the action distribution, i.e., the similarity of the policy vector p and the search probabilities π
  - L2 regularization

AlphaGo Zero



AlphaGo Zero

First, run the following simulation 1,600 times...

Start at the root node of the tree (the current game state)

1. Choose the action that maximises...

$$Q + U$$

- Q: The mean value of the next state
- U: A function of **P** and **N** that increases if an action hasn't been explored much, relative to the other actions, or if the prior probability of the action is high

Early on in the simulation, U dominates (more exploration), but later; Q is more important (less exploration)

2. Continue until a leaf node is reached

The game state of the leaf node is passed into the neural network, which outputs predictions about two things:

- **p** Move probabilities
- **v** Value of the state (for the current player)

The move probabilities p are attached to the new feasible actions from the leaf node

3. Backup previous edges

Each edge that was traversed to get to the leaf node is updated as follows:

$$N \rightarrow N + 1$$
$$W \rightarrow W + v$$
$$Q = W / N$$

AlphaGo Zero

...then select a move

After 1,600 simulations, the move can either be chosen:

Deterministically (for competitive play)

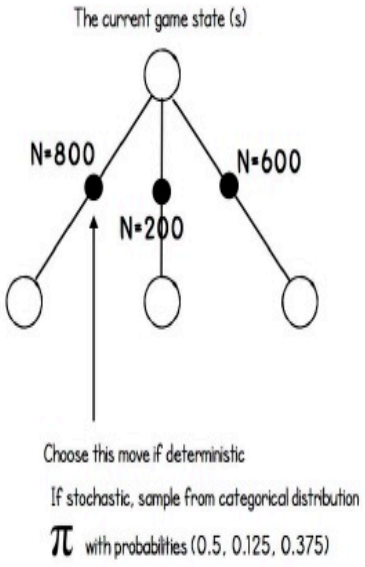
Choose the action from the current state with greatest N

Stochastically (for exploratory play)

Choose the action from the current state from the distribution

$$\pi \sim N^{1/\tau}$$

where τ is a temperature parameter, controlling exploration



Other points

- The sub-tree from the chosen move is retained for calculating subsequent moves
- The rest of the tree is discarded

AlphaGo Zero

SELF PLAY

Create a 'training set'

The best current player plays 25,000 games against itself

See MCTS section to understand how AlphaGo Zero selects each move

At each move, the following information is stored

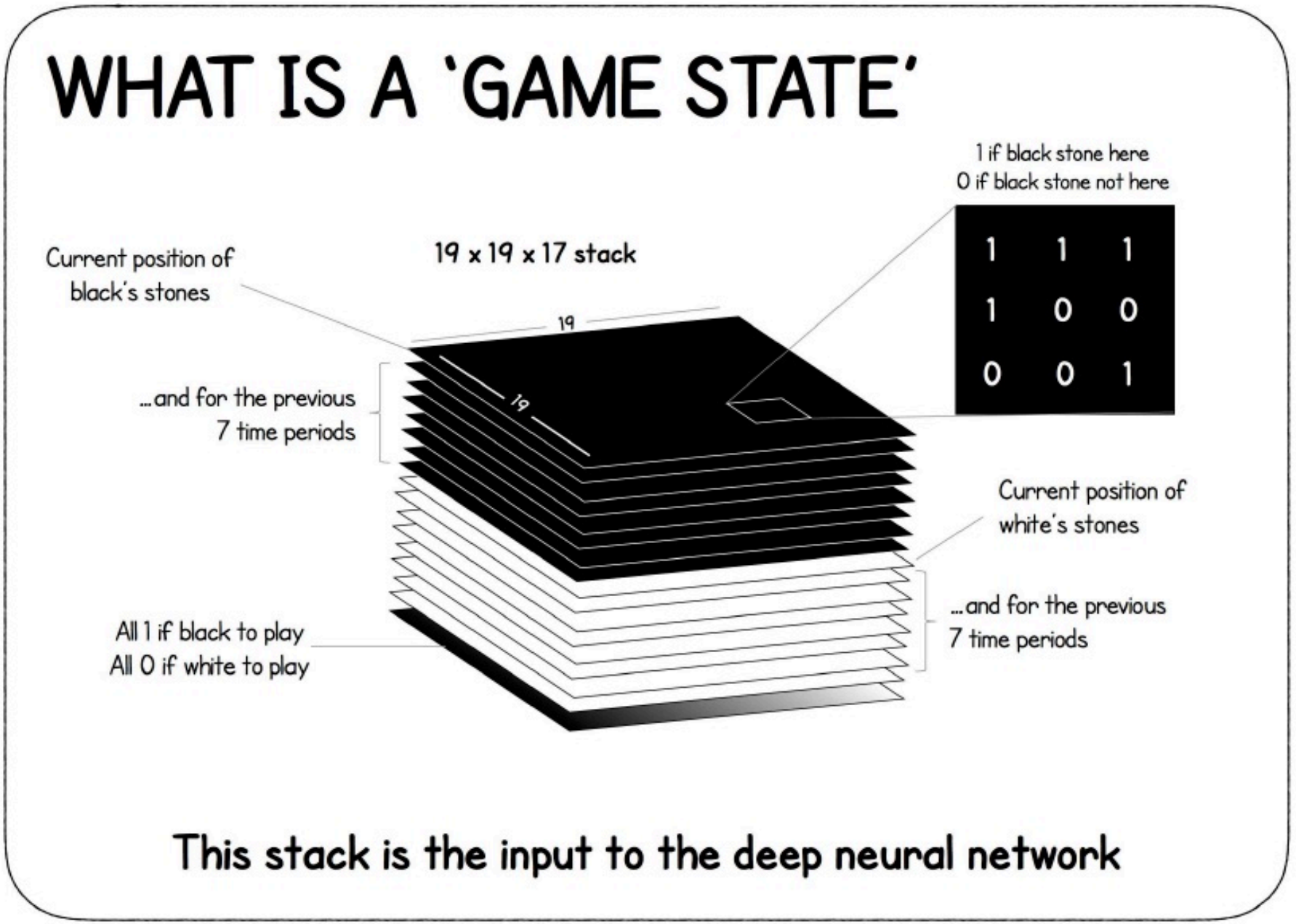
The game state
(see 'What is a Game State section')

π

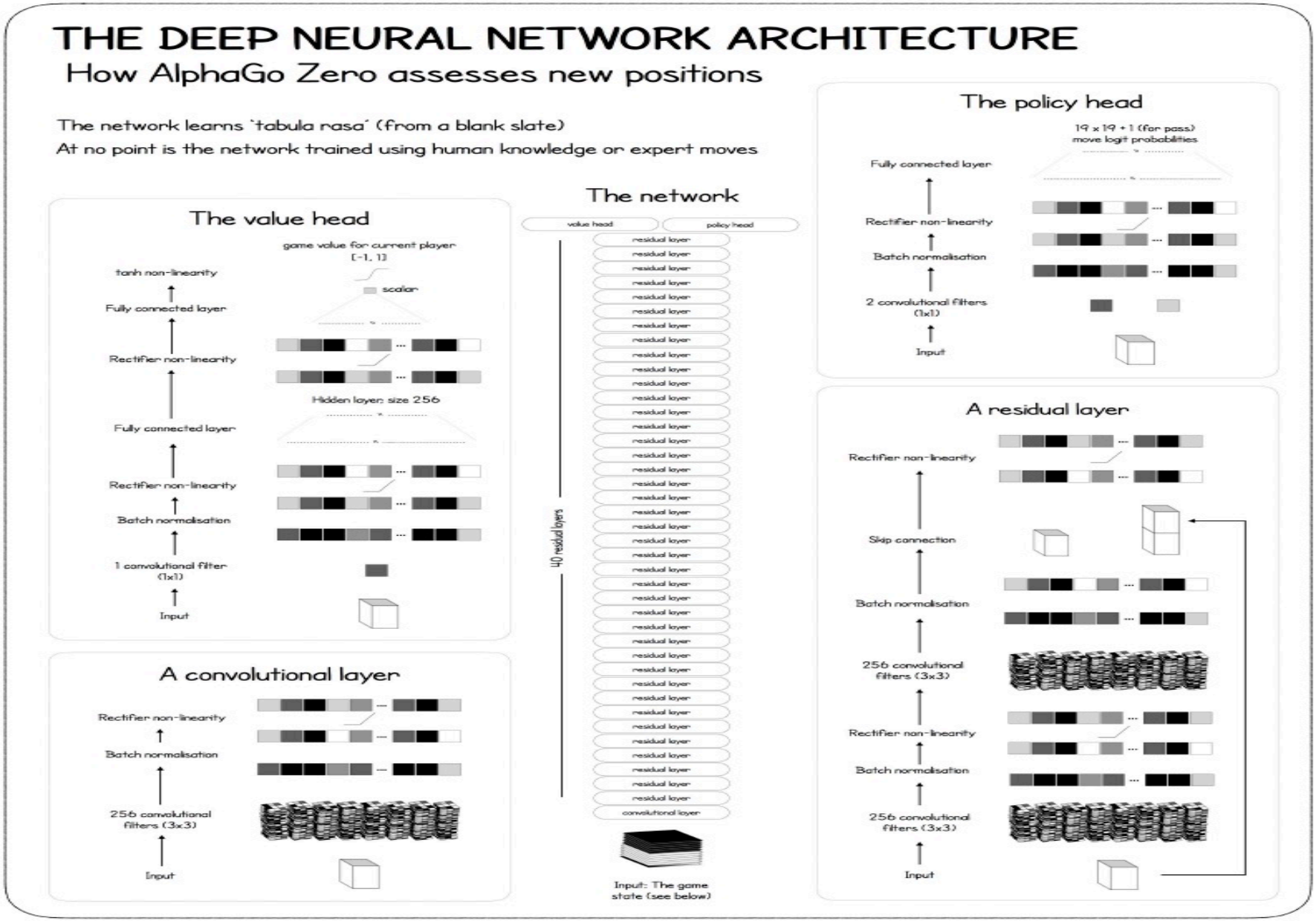
The search probabilities
(from the MCTS)

The winner
(+1 if this player won, -1 if this player lost - added once the game has finished)

AlphaGo Zero



AlphaGo Zero



RETRAIN NETWORK

Optimise the network weights

A TRAINING LOOP

Sample a mini-batch of 2048 positions from the last 500,000 games

Retrain the current neural network on these positions
- The game states are the input (see 'Deep Neural Network Architecture')

Loss function
Compares predictions from the neural network with the search probabilities and actual winner

PREDICTIONS **p** Cross-entropy π ACTUAL
+
v Mean-squared error 
+
Regularisation

After every 1,000 training loops, evaluate the network

AlphaGo Zero

EVALUATE NETWORK

Test to see if the new network is stronger

Play 400 games between the latest neural network and the current best neural network

Both players use MCTS to select their moves, with their respective neural networks to evaluate leaf nodes

Latest player must win 55% of games to be declared the new best player