# Experiment design

## Bandit problems and Markov decision processes

Christos Dimitrakakis

UiO

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# Sequential problems: full observation

## Example 1

- $n$ meteorological stations $\{\mu_i \mid i = 1, \ldots, n\}$
- The $i$-th station gives a rain probability $x_{t,i} = P_{\mu_i}(y_t \mid y_1, \ldots, y_{t-1})$.

- Observation $\boldsymbol{x}_t = (x_{t,1}, \ldots, x_{t,n})$: the predictions of all stations.
- Decision $a_t$: Guess if it will rain
- Outcome $y_t$: Rain or not rain.
- Steps $t = 1, \ldots, T$.

## Linear utility function

Reward function is $\rho(y_t, a_t) = \mathbb{I}\{y_t = a_t\}$ simply rewarding correct predictions with utility being

$$U(y_1, y_2, \ldots, y_T, a_1, \ldots, a_T) = \sum_{t=1}^{T} \rho(y_t, a_t),$$

the total number of correct predictions.

The $n$ meteorologists problem is simple, as:

- You always see their predictions, as well as the weather, no matter whether you bike or take the tram (full information)
- Your actions do not influence their predictions (independence events)

In the remainder, we'll see two settings where decisions are made with either partial information or in a dynamical system. Both of these settings can be formalised with Markov decision processes.

# Experimental design and Markov decision processes

The following problems

- Shortest path problems.
- Optimal stopping problems.
- Reinforcement learning problems.
- Experiment design (clinical trial) problems
- Advertising.

can be all formalised as Markov decision processes.

## Applications

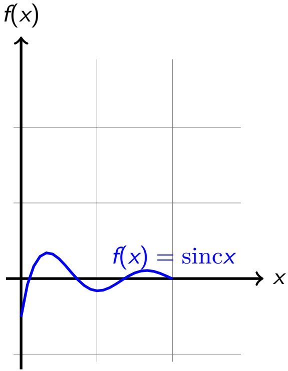
- Robotics.
- Economics.
- Automatic control.
- Resource allocation

# Bandit problems

# Bandit problems

## Applications

- Efficient optimisation.



# Bandit problems

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- Efficient optimisation.
- Online advertising.

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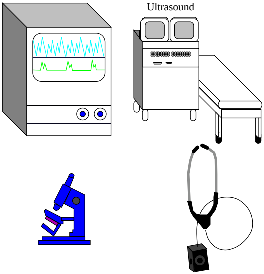

# Bandit problems

## Applications

- Efficient optimisation.
- Online advertising.
- Clinical trials.
- Robot scientist.

# The stochastic $n$-armed bandit problem

## Actions and rewards

- A set of actions $\mathcal{A} = \{1, \ldots, n\}$.
- Each action gives you a random reward with distribution $\mathbb{P}(r_t \mid a_t = i)$.
- The expected reward of the $i$-th arm is $\rho_i \triangleq \mathbb{E}(r_t \mid a_t = i)$.

## Interaction at time $t$

1. You choose an action $a_t \in \mathcal{A}$.
2. You observe a random reward $r_t$ drawn from the $i$-th arm.

## The utility is the sum of the rewards obtained

$$U \triangleq \sum_t r_t.$$

We must maximise the expected utility, without knowing the values $\rho_i$.

# Policy

### Definition 2 (Policies)

A policy $\pi$ is an algorithm for taking actions given the observed history $h_t \triangleq a_1, r_1, \ldots, a_t, r_t$

$$\mathbb{P}^\pi(a_{t+1} \mid h_t)$$

is the probability of the next action $a_{t+1}$.

### Exercise 1

Why should our action depend on the complete history?

A The next reward depends on all the actions we have taken.

B We don't know which arm gives the highest reward.

C The next reward depends on all the previous rewards.

D The next reward depends on the complete history.

E No idea.

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### Example 3 (The expected utility of a uniformly random policy)

If $\mathbb{P}^\pi(a_{t+1} \mid \cdot) = 1/n$ for all $t$, then

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If $\mathbb{P}^\pi(a_{t+1} \mid \cdot) = 1/n$ for all $t$, then

$$\mathbb{E}^\pi U = \mathbb{E}^\pi \left( \sum_{t=1}^T r_t \right) = \sum_{t=1}^T \mathbb{E}^\pi r_t = \sum_{t=1}^T \sum_{i=1}^n \frac{1}{n} \rho_i = \frac{T}{n} \sum_{i=1}^n \rho_i$$

# Policy

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## The expected utility of a general policy

$$\mathbb{E}^\pi U = \mathbb{E}^\pi \left( \sum_{t=1}^{T} r_t \right)$$

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## The expected utility of a general policy

$$\mathbb{E}^\pi U = \mathbb{E}^\pi \left( \sum_{t=1}^T r_t \right) = \sum_{t=1}^T \mathbb{E}^\pi (r_t) \tag{1.1}$$

# Policy

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A policy $\pi$ is an algorithm for taking actions given the observed history $h_t \triangleq a_1, r_1, \ldots, a_t, r_t$

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## The expected utility of a general policy

$$\begin{aligned}
\mathbb{E}^\pi U = \mathbb{E}^\pi \left(\sum_{t=1}^T r_t\right) &= \sum_{t=1}^T \mathbb{E}^\pi(r_t) \qquad (1.1)\\
&= \sum_{t=1}^T \sum_{a_t \in \mathcal{A}} \mathbb{E}(r_t \mid a_t) \sum_{h_{t-1}} \mathbb{P}^\pi(a_t \mid h_{t-1})\, \mathbb{P}^\pi(h_{t-1})
\end{aligned}$$

# A simple heuristic for the unknown reward case

Say you keep a running average of the reward obtained by each arm

$$\hat{\theta}_{t,i} = R_{t,i}/n_{t,i}$$

- $n_{t,i}$ the number of times you played arm $i$
- $R_{t,i}$ the total reward received from $i$.

Whenever you play $a_t = i$:

$$R_{t+1,i} = R_{t,i} + r_t, \qquad n_{t+1,i} = n_{t,i} + 1.$$

Greedy policy:

$$a_t = \arg\max_i \hat{\theta}_{t,i}.$$

What should the initial values $n_{0,i}$, $R_{0,i}$ be?

# Bernoulli bandits

## Decision-theoretic approach

- Assume $r_t \mid a_t = i \sim P_{\theta_i}$, with $\theta_i \in \Theta$.
- Define prior belief $\xi_1$ on $\Theta$.
- For each step $t$, find a policy $\pi$ selecting action $a_t \mid \xi_t \sim \pi(a \mid \xi_t)$ to

$$\max_\pi \mathbb{E}^\pi_{\xi_t}(U_t) = \max_\pi \mathbb{E}^\pi_{\xi_t} \sum_{a_t} \left( \sum_{k=1}^{T-t} r_{t+k} \,\middle|\, a_t \right) \pi(a_t \mid \xi_t).$$

- Obtain reward $r_t$.
- Calculate the next belief

$$\xi_{t+1} = \xi_t(\cdot \mid a_t, r_t)$$

How can we implement this?

## Bayesian inference on Bernoulli bandits

- Likelihood: $\mathbb{P}_\theta(r_t = 1) = \theta$.
- Prior: $\xi(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$ (i.e. $\mathcal{Beta}(\alpha, \beta)$).

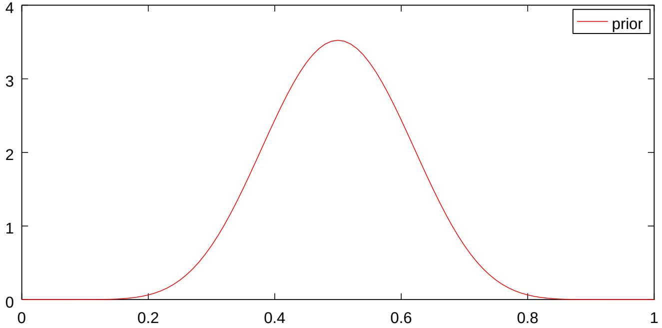



Figure: Prior belief $\xi$ about the mean reward $\theta$.

# Bayesian inference on Bernoulli bandits

For a sequence $r = r_1, \ldots, r_n, \Rightarrow P_\theta(r) \propto \theta_i^{\#1(\mathrm{r})}(1-\theta_i)^{\#0(\mathrm{r})}$

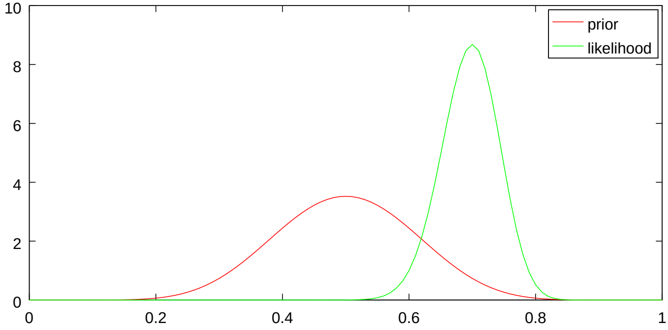



Figure: Prior belief $\xi$ about $\theta$ and likelihood of $\theta$ for 100 plays with 70 1s.

# Bayesian inference on Bernoulli bandits

Posterior: $\mathcal{Beta}(\alpha + \#1(\mathrm{r}), \beta + \#0(\mathrm{r}))$.

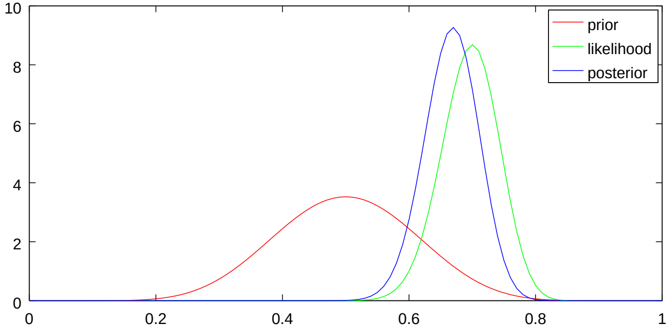



Figure: Prior belief $\xi(\theta)$ about $\theta$, likelihood of $\theta$ for the data $r$, and posterior belief $\xi(\theta \mid r)$

## Bernoulli example.

Consider $n$ Bernoulli distributions with unknown parameters $\theta_i$ ($i = 1, \ldots, n$) such that

$$r_t \mid a_t = i \sim \mathcal{B}ernoulli(\theta_i), \qquad \mathbb{E}(r_t \mid a_t = i) = \theta_i. \tag{1.2}$$

Our belief for each parameter $\theta_i$ is $\mathcal{B}eta(\alpha_i, \beta_i)$, with density $f(\theta \mid \alpha_i, \beta_i)$ so that

$$\xi(\theta_1, \ldots, \theta_n) = \prod_{i=1}^{n} f(\theta_i \mid \alpha_i, \beta_i). \qquad \text{(a priori independent)}$$

$$N_{t,i} \triangleq \sum_{k=1}^{t} \mathbb{I}\{a_k = i\}, \qquad \hat{r}_{t,i} \triangleq \frac{1}{N_{t,i}} \sum_{k=1}^{t} r_t \mathbb{I}\{a_k = i\}$$

Then, the posterior distribution for the parameter of arm $i$ is

$$\xi_t = \mathcal{B}eta(\alpha_i^t, \beta_i^t), \qquad \alpha_i^t = \alpha_i + N_{t,i}\hat{r}_{t,i}, \ \beta_i^t = \beta_i N_{t,i}(1 - \hat{r}_{t,i})).$$

Since $r_t \in \{0, 1\}$ there are $O((2n)^T)$ possible belief states for a $T$-step bandit problem.

# Belief states

- The state of the decision-theoretic bandit problem is the state of our belief.
- A sufficient statistic is the number of plays and total rewards.
- Our belief state $\xi_t$ is described by the priors $\alpha, \beta$ and the vectors

$$N_t = (N_{t,1}, \ldots, N_{t,i}) \tag{1.3}$$

$$\hat{r}_t = (\hat{r}_{t,1}, \ldots, \hat{r}_{t,i}). \tag{1.4}$$

- The next-state probabilities are defined as:

$$\mathbb{P}_{\xi_t}(r_t = 1 \mid a_t = i) = \frac{\alpha_i^t}{\alpha_i^t + \beta_i^t}$$

as $\xi_{t+1}$ is a deterministic function of $\xi_t$, $r_t$ and $a_t$
- Optimising this results in a Markov decision process.

# Markov process

$$s_{t-1} \longrightarrow s_t \longrightarrow s_{t+1}$$

### Definition 3 (Markov Process – or Markov Chain)

The sequence $\{s_t \mid t = 1, \ldots\}$ of random variables $s_t : \Theta \to \mathcal{S}$ is a Markov process if

$$\mathbb{P}(s_{t+1} \mid s_t, \ldots, s_1) = \mathbb{P}(s_{t+1} \mid s_t). \tag{1.5}$$

- $s_t$ is state of the Markov process at time $t$.
- $\mathbb{P}(s_{t+1} \mid s_t)$ is the transition kernel of the process.

### The state of an algorithm

Observe that the $\alpha, \beta$ form a Markov process. They also summarise our belief about which arm is the best.

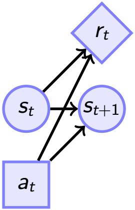
# Markov decision processes

In a Markov decision process (MDP), the state $s$ includes all the information we need to make predictions.

## Markov decision processes (MDP).

At each time step $t$:

- We observe state $s_t \in \mathcal{S}$.
- We take action $a_t \in \mathcal{A}$.
- We receive a reward $r_t \in \mathbb{R}$.

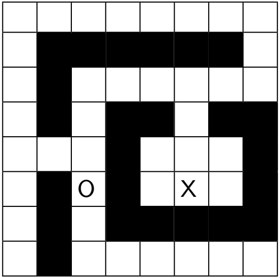



## Markov property of the reward and state distribution

$$\mathbb{P}_\mu(s_{t+1} \mid s_t, a_t) \qquad \text{(Transition distribution)}$$

$$\mathbb{P}_\mu(r_t \mid s_t, a_t) \qquad \text{(Reward distribution)}$$

# Stochastic shortest path problem with a pit




## Properties

- $T \to \infty$.
- $r_t = -1$, but $r_t = 0$ at X and $-100$ at O and the problem ends.
- $\mathbb{P}_\mu(s_{t+1} = X | s_t = X) = 1$.
- $\mathcal{A} = \{\mathrm{North}, \mathrm{South}, \mathrm{East}, \mathrm{West}\}$
- Moves to a random direction with probability $\omega$. Walls block.

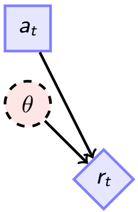



Figure: The basic bandit MDP. The decision maker selects $a_t$, while the parameter $\theta$ of the process is hidden. It then obtains reward $r_t$. The process repeats for $t = 1, \ldots, T$.

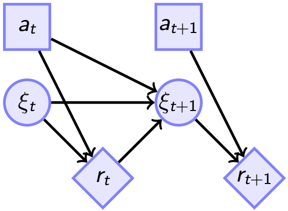


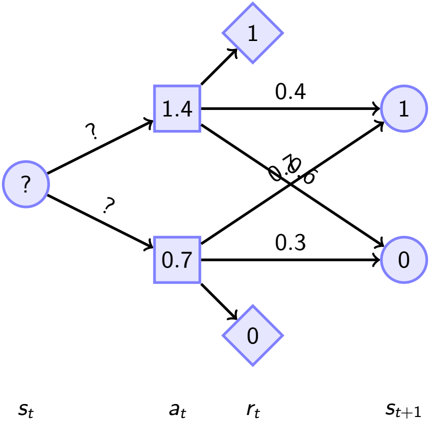

Figure: The decision-theoretic bandit MDP. While $\theta$ is not known, at each time step $t$ we maintain a belief $\xi_t$ on $\Theta$. The reward distribution is then defined through our belief.

## Backwards induction (Dynamic programming)

**for** $n = 1, 2, \ldots$ and $s \in \mathcal{S}$ **do**

$$\mathbb{E}(U_t \mid \xi_t) = \max_{a_t \in \mathcal{A}} \mathbb{E}(r_t \mid \xi_t, a_t) + \sum_{\xi_{t+1}} \mathbb{P}(\xi_{t+1} \mid \xi_t, a_t)\, \mathbb{E}(U_{t+1} \mid \xi_{t+1})$$

**end for**




### Exercise 1

What is the value $v_t(s_t)$ of the first state?

A 1.4

B 1.05

C 1.0

D 0.7

E 0

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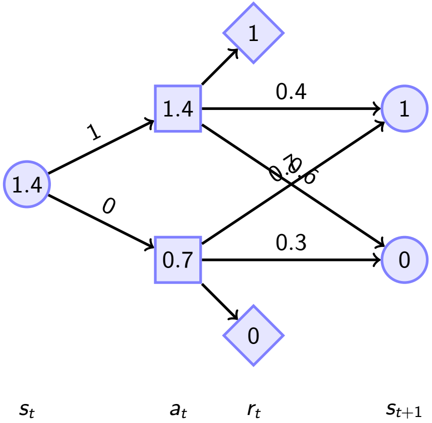


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What is the value $v_t(s_t)$ of the first state?

- A 1.4
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- C 1.0
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## Heuristic algorithms for the $n$-armed bandit problem

**Algorithm 1** UCB1

**Input** $\mathcal{A}$
$\hat{\theta}_{0,i} = 1, \forall i$
**for** $t = 1, \ldots$ **do**
  $a_t = \arg\max_{i \in \mathcal{A}} \left\{ \hat{\theta}_{t-1,i} + \sqrt{\frac{2 \ln t}{N_{t-1,i}}} \right\}$
  $r_t \sim P_\theta(r \mid a_t)$ `// play action and get reward // update model`
  $N_{t,a_t} = N_{t-1,a_t} + 1$
  $\hat{\theta}_{t,a_t} = [N_{t-1,a_t} \theta_{t-1,a_t} + r_t] / N_{t,a_t}$
  $\forall i \neq a_t,\ N_{t,i} = N_{t-1,i},\ \hat{\theta}_{t,i} = \hat{\theta}_{t-1,i}$
**end for**

**Algorithm 2** Thompson sampling

**Input** $\mathcal{A}, \xi_0$
**for** $t = 1, \ldots$ **do**
  $\hat{\theta} \sim \xi_{t-1}(\theta)$
  $a_t \in \arg\max_a \mathbb{E}_{\hat{\theta}}[r_t \mid a_t = a]$.
  $r_t \sim P_\theta(r \mid a_t)$ `// play action and get reward // update model`
  $\xi_t(\theta) = \xi_{t-1}(\theta \mid a_t, r_t)$.
**end for**

## Example 4 (Clinical trials)

Consider an example where we have some information $x_t$ about an individual patient $t$, and we wish to administer a treatment $a_t$. For whichever treatment we administer, we can observe an outcome $y_t$. Our goal is to maximise expected utility.

### Definition 5 (The contextual bandit problem.)

At time $t$,

- We observe $x_t \in \mathcal{X}$.
- We play $a_t \in \mathcal{A}$.
- We obtain $r_t \in \mathbb{R}$ with $r_t \mid a_t = a, x_t = x \sim P_\theta(r \mid a, x)$.

### Example 6 (The linear bandit problem)

- $\mathcal{A} = [n]$, $\mathcal{X} = \mathbb{R}^k$, $\theta = (\theta_1, \ldots, \theta_n)$, $\theta_i \in \mathbb{R}^k$, $r \in \mathbb{R}$.
- $r \sim \mathcal{N}(\theta_a^\top x), 1)$

### Example 7 (A clinical trial example)

- $\mathcal{A} = [n]$, $\mathcal{X} = \mathbb{R}^k$, $\theta = (\theta_1, \ldots, \theta_n)$, $\theta_i \in \mathbb{R}^k$, $y \in \{0, 1\}$.
- $y \sim \mathcal{Bernoulli}(1/(1 + exp[-(\theta_a^\top x)^2])$.
- $r = U(a, y)$.

Example 8 (One-stage problems)

- Initial belief $\xi_0$
- Side information $\boldsymbol{x}$
- Simultaneously takes actions $\boldsymbol{a}$.
- Observes outcomes $\boldsymbol{y}$.

$$\mathbb{E}^{\pi}_{\xi_0}(U \mid \boldsymbol{x}) = \sum_{\boldsymbol{x},\boldsymbol{y}} \mathbb{P}_{\xi_0}(\boldsymbol{y} \mid \boldsymbol{a}, \boldsymbol{x}) \pi(\boldsymbol{a} \mid \boldsymbol{x}) \underbrace{\mathbb{E}^{\pi}_{\xi_0}(U \mid \boldsymbol{x}, \boldsymbol{a}, \boldsymbol{y})}_{\text{post-hoc value}} \tag{4.1}$$

Example 8 (One-stage problems)

- Initial belief $\xi_0$
- Side information $\boldsymbol{x}$
- Simultaneously takes actions $\boldsymbol{a}$.
- Observes outcomes $\boldsymbol{y}$.

Definition 9 (Expected information gain)

$$\mathbb{E}^{\pi}_{\xi_0}\left(\mathbb{D}\left(\xi_1 \| \xi_0\right) \mid \boldsymbol{x}\right) = \sum_{\boldsymbol{x},\boldsymbol{y}} \mathbb{P}_{\xi_0}(\boldsymbol{y} \mid \boldsymbol{a}, \boldsymbol{x}) \pi(\boldsymbol{a} \mid \boldsymbol{x}) \mathbb{D}\left(\xi_0(\cdot \mid \boldsymbol{x}, \boldsymbol{a}, \boldsymbol{y}) \| \xi_0\right) \tag{4.1}$$

## Example 8 (One-stage problems)

- Initial belief $\xi_0$
- Side information $\boldsymbol{x}$
- Simultaneously takes actions $\boldsymbol{a}$.
- Observes outcomes $\boldsymbol{y}$.

## Definition 9 (Expected utility of final policy)

$$\mathbb{E}^{\pi}_{\xi_0}\left(\max_{\pi_1} \mathbb{E}^{\pi_1}_{\xi_1} \rho \middle| \boldsymbol{x}\right) = \sum_{\boldsymbol{x},\boldsymbol{y}} \mathbb{P}_{\xi_0}(\boldsymbol{y} \mid \boldsymbol{a}, \boldsymbol{x}) \pi(\boldsymbol{a} \mid \boldsymbol{x}) \max_{\pi_1} \mathbb{E}^{\pi_1}_{\xi_0}(\rho \mid \boldsymbol{a}, \boldsymbol{x}, \boldsymbol{y}) \tag{4.1}$$

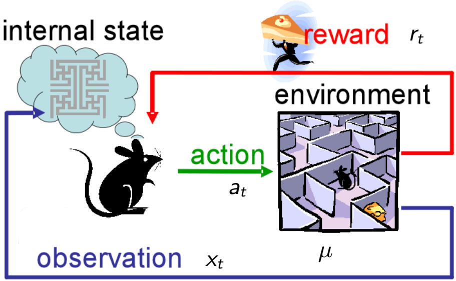
$$\mathbb{E}^{\pi_1}_{\xi_0}(\rho \mid \boldsymbol{a}, \boldsymbol{x}, \boldsymbol{y}) = \sum_{a,x,y} \rho(a, y) \mathbb{P}_{\xi_1}(y \mid x, a) \pi_1(a \mid x) \mathbb{P}_{\xi_1}(x) \tag{4.2}$$

## Experiment design for a one-stage problem

- Select some model $\mathbb{P}$ for generating data.
- Select an inference and/or decision making algorithm $\lambda$ for the task.
- Select a performance measure $U$.
- Generate data $D$ from $\mathbb{P}$ and measure the performance of $\lambda$ on $D$.

## The reinforcement learning problem

Learning to act in an unknown world, by interaction and reinforcement.




Learning by interaction

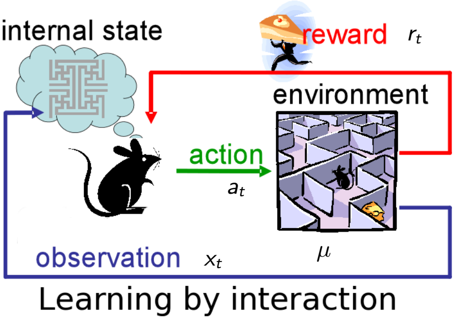
## The reinforcement learning problem

Learning to act in an unknown world, by interaction and reinforcement.

Expected total reward

...when using policy $\pi$ in $\mu$:

$$U(\mu, \pi)$$



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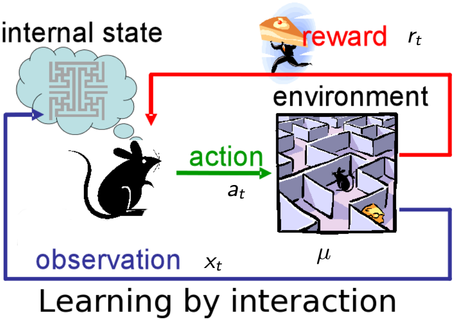


Expected total reward

...when using policy $\pi$ in $\mu$:

$$U(\mu, \pi)$$

Can't we just $\max_\pi U(\mu, \pi)$?

## The reinforcement learning problem

Learning to act in an unknown world, by interaction and reinforcement.

Expected total reward

...when using policy $\pi$ in $\mu$:

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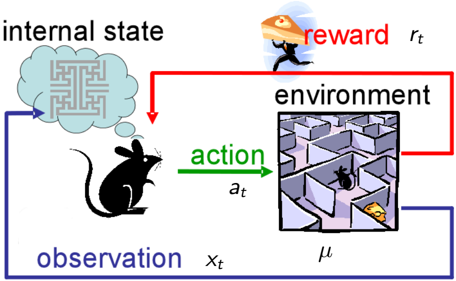



Learning by interaction

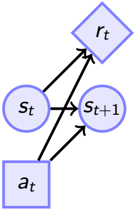
Knowing $\mu$ contradicts the problem definition

# Solving a given MDP

## Markov decision processes (MDP).

At each time step $t$:

- We observe state $s_t \in \mathcal{S}$.
- We take action $a_t \in \mathcal{A}$.
- We receive a reward $r_t \in \mathbb{R}$ with $r_t \sim P_\mu(r_t \mid s_t, a_t)$
- We go to the next state $s_{t+1} \in \mathcal{S}$ with $s_{t+1} \sim P_\mu(s_{t+1} \mid s_t, a_t)$




## Backwards induction (Value iteration)

**for** $n = 1, 2, \ldots$ and $s \in \mathcal{S}$ **do**

$$\mathbb{E}_\mu^{\pi^*}(U_t \mid s_t) = \max_{a_t \in \mathcal{A}} \mathbb{E}_\mu(r_t \mid s_t, a_t) + \sum_{s_{t+1}} \mathbb{P}_\mu(s_{t+1} \mid s_t, a_t)\, \mathbb{E}_\mu^{\pi^*}(U_{t+1} \mid s_{t+1})$$

**end for**

# The discounted setting

$$U_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k}, \qquad \gamma \in (0, 1)$$

## Value functions

$$V_\mu^\pi(s) \triangleq \mathbb{E}(U_t \mid s_t = s), \qquad Q_\mu^\pi(s, a) \triangleq \mathbb{E}(U_t \mid s_t = s, a_t = a)$$

# The discounted setting

$$U_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k}, \qquad \gamma \in (0,1)$$

## Value functions

$$V^{\pi}_{\mu}(s) \triangleq \mathbb{E}(U_t \mid s_t = s), \qquad Q^{\pi}_{\mu}(s,a) \triangleq \mathbb{E}(U_t \mid s_t = s, a_t = a)$$

## Bellman equation

$$V^{\pi}_{\mu}(s) = \mathbb{E}^{\pi}_{\mu}(r_t \mid s_t = s) + \gamma \sum_{s_{t+1}} V^{\pi}_{\mu}(s_{t+1})\, \mathbb{P}^{\pi}_{\mu}(s_{t+1} \mid s_t)$$

$$Q^{\pi}_{\mu}(s,a) = \mathbb{E}_{\mu}(r_t \mid s_t = s, a_t = a) + \gamma \sum_{s_{t+1}} Q^{\pi}_{\mu}(s_{t+1}, \pi(s_{t+1})) P_{\mu}(s_{t+1} \mid s_t, a_t = a)$$

# The discounted setting

$$U_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k}, \qquad \gamma \in (0, 1)$$

## Value functions

$$V_\mu^\pi(s) \triangleq \mathbb{E}(U_t \mid s_t = s), \qquad Q_\mu^\pi(s, a) \triangleq \mathbb{E}(U_t \mid s_t = s, a_t = a)$$

## Bellman equation

$$V_\mu^\pi(s) = \mathbb{E}_\mu^\pi(r_t \mid s_t = s) + \gamma \sum_{s_{t+1}} V_\mu^\pi(s_{t+1}) \, \mathbb{P}_\mu^\pi(s_{t+1} \mid s_t)$$

$$Q_\mu^\pi(s, a) = \mathbb{E}_\mu(r_t \mid s_t = s, a_t = a) + \gamma \sum_{s_{t+1}} Q_\mu^\pi(s_{t+1}, \pi(s_{t+1})) P_\mu(s_{t+1} \mid s_t, a_t = a)$$

## Optimality condition

$$V_\mu^*(s) \geq V_\mu^\pi(s) \forall s$$

## $Q$-learning and induction

### $Q$-Value iteration

$$Q_{n+1}(s, a) = r(s, a) + \gamma \sum_{s_{t+1}} P_{\mu}(s_{t+1} \mid s_t, a_t = a) \max_{a'} Q_n(s_{t+1}, a')$$

### $Q$-learning

$$\hat{R}_t = r_t + \gamma \max_{a'} \hat{Q}_t(s_{t+1}, a')$$

$$\hat{Q}_{t+1}(s, a) = (1 - \alpha) \hat{Q}_n(s, a) + \alpha(\hat{R}_t)$$

# Summary

### Markov decision processes

- Formalise experiment design
- Formalise environments in reinforcement learning

### Solving MDPs

- Discrete case: dynamic programming.
- General case: approximations, gradient methods, etc.

### Reinforcement learning and experiment design

- Formal but intractable Bayesian solution.
- Convergent algorithms in simple settings.