Near-optimal Reinforcement Learning in Factored MDPs

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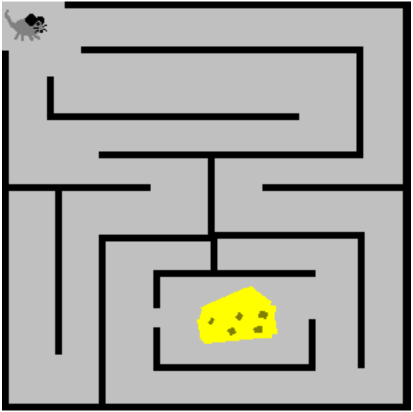
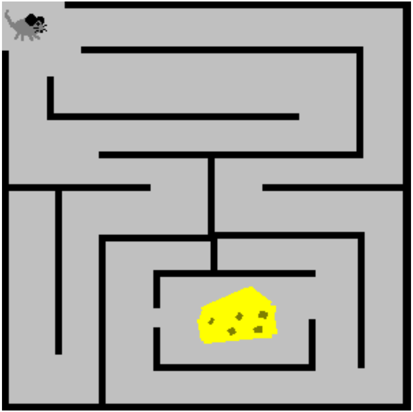
A mouse in a maze



- Simple model:
  "Mice love cheese".
- Put a mouse and some cheese together in a maze.
- How should the mouse get as much cheese as possible?

A mouse in a maze



- Simple model:
  "Mice love cheese".
- Put a mouse and some cheese together in a maze.
- How should the mouse get as much cheese as possible?
- Do **not** provide a map.

A mouse in a maze

- The mouse faces a sequential decision problem.
- At each timestep t the mouse must choose an **action**:
  $a_t \in \{\text{move up, down, left, right, eat}\}$.
- This choice of action will influence both:
  its immediate **reward** r_t (how much cheese it ate)
  its **state** at the following time step s_{t+1}.
- The mouse's goal is to maximize its cumulative rewards through time, not just the reward in any single timestep t.
- We can model this problem as a ***Markov Decision Process***.

Markov Decision Process

- An **agent** taking actions in an **enivronment** M (the MDP).
- **State** s_t encodes the relevant data on the environment.
- **Action** a_t is chosen by the agent.
- The agent receives a **reward** $r_t \sim R^M(s_t, a_t)$.
- The state **transitions** according to $s_{t+1} \sim P^M(s_t, a_t)$.

Maze as an MDP

- **Agent** $\leftrightarrow$ Mouse.
- **Environment** $\leftrightarrow$ Maze + Cheese.
- **State** $\leftrightarrow$ Position of the mouse.
- **Reward** $\leftrightarrow$ 1 if mouse eats cheese, 0 otherwise.
- **Transition** $\leftrightarrow$ Movement blocked by walls.

MDP notation

- Finite horizon MDP $M = (\mathcal{S}, \mathcal{A}, R^M, P^M, \tau, \rho)$.

- **Policy** μ is a function mapping each state $s \in \mathcal{S}$ and $i = 1, \ldots, \tau$ to an action $a \in \mathcal{A}$.

- For each MDP M and policy μ, we define a **value function**:

$$V^M_{\mu,i}(s) := \mathbb{E}_{M,\mu}\left[\sum_{j=i}^{\tau} \overline{R}^M(s_j, a_j) \middle| s_i = s\right].$$

- A policy μ is **optimal** for the MDP M if $V^M_{\mu,i}(s) = \max_{\mu'} V^M_{\mu',i}(s)$ for all $s \in \mathcal{S}$ and $i = 1, \ldots, \tau$.

- We write μ^M **as the optimal policy for** M.

Reinforcement learning

Reinforcement learning

- Agent interacts with an MDP just as before.
- **BUT** the agent is uncertain over dynamics R^M and P^M.
- The agent observes the outcomes of the states and actions it visits and so can learn about the MDP through time.
- Fundamental tradeoff:

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- Fundamental tradeoff: **exploration versus exploitation**.
- *The mouse does not know the maze the first time.*

Reinforcement learning

- Repeated episodes of length τ, initial distribution ρ.
  Episode k starts at $t_k := (k-1)\tau + 1$.

- **RL algorithm** is a sequence $\{\pi_k\}_{\mathbb{N}}$ of functions mapping H_{t_k} to a probability distribution $\pi_k(H_{t_k})$ over policies.

- We define the **regret** over episode k wrt the MDP M^*:

$$\Delta_k := \sum_{\mathcal{S}} \rho(s)(V^{M^*}_{\mu^*,1}(s) - V^{M^*}_{\mu_k,1}(s))$$

- And the regret to time T of algorithm π:

$$\mathrm{Regret}(T, \pi, M^*) := \sum_{k=1}^{\lceil T/\tau \rceil} \Delta_k.$$

Why do we care?

- ~~Mice need to get more cheese!~~
- MDPs are great models for sequential decision problems.
- **BUT** we rarely know the appropriate R^M, P^M exactly.
- We want algorithms that will give us performance close to that of the unknown optimal controller for the unknown system!

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- Examples: *healthcare, robotics, agriculture, finance and more.*

Algorithms for RL

- The **ϵ-greedy** approach:
  Maintain estimate $\hat{M}$ for M^*. With probability ϵ choose a random policy otherwise use $\mu^{\hat{M}}$ certainty equivalent.

- **Bayes-optimal** strategies:
  Mantain a posterior ϕ for M^*, choose $\mu \in \arg\max_\mu \mathbb{E}[V_\mu^{M^*}]$.

- **Optimism in the face of uncertainty**:
  Maintain a confidence set $\mathcal{M}_k$ that contains M^* with high probability. Choose $\mu_k \in \arg\max_\mu \max_{M \in \mathcal{M}_k} V_\mu^{M_k}$.

- **Posterior sampling**:
  Mantain a posterior ϕ for M^*. Every episode sample $M_k \sim \phi$ and choose μ^{M_k} which is optimal for that sample.

Existing regret bounds

- Naive exploration (ϵ-greedy, Boltzmann) generally take **exponentially** long in $|\mathcal{S}|, |\mathcal{A}|$ to learn the optimal policy.
- Bayes-optimal strategy usually computationally **intractable**.
- Optimism and posterior sampling are closely linked [1].
- **State of the art** regret bounds $\tilde{O}(|\mathcal{S}|\sqrt{|\mathcal{A}|T})$ attained by UCRL2 [2] (optimism) and PSRL [3] (sampling).
- Close to fundamental lower bounds $\Omega(\sqrt{|\mathcal{S}||\mathcal{A}|T})$.

Standard proof outline

Write $V^*_{*,1}$ for $V^{M^*}_{\mu^{M^*},1}$ and similarly k for M_k. The episode regret:

$$\Delta_k = V^*_{*1} - V^*_{k,1} = \left(V^*_1 * - V^k_{k,1}\right) + \left(V^k_{k,1} - V^*_{k,1}\right).$$

Using M_k chosen optimistically, the first term is ≤ 0 with high probability. For posterior sampling it is zero in expectation.

The remaining term can be **decomposed into the Bellman error**:

$$\left(V^k_{k,1} - V^*_{k,1}\right) = \sum_{i=1}^{\tau} \left(\mathcal{T}^k_{k,i} - \mathcal{T}^*_{k,i}\right) V^k_{k,i+1} + \sum_{i=1}^{\tau} d_{t_k+i}.$$

where d_i is a bounded martingale difference and $\mathcal{T}^M_\mu$ is the Bellman operator. The contribution from bounded martingale differences is zero in expectation and bounded $O(\sqrt{T})$ with high probability.

Standard proof outline (cont.)

The Bellman operator is defined

$$\mathcal{T}_{\mu}^{M} V(s) := \overline{R}^{M}(s, \mu(s)) + \sum_{s' \in \mathcal{S}} P^{M}(s'|s, \mu(s)) V(s').$$

Which, together with **Hölder's inequality** allows us to say:

$$\sum_{i=1}^{\tau} \left(\mathcal{T}_{k,i}^{k} - \mathcal{T}_{k,i}^{*} \right) V_{k,i+1}^{k} \leq \sum_{i=1}^{\tau} |\overline{R}^{k} - \overline{R}^{*}| + \frac{1}{2} \Psi_{k} \|P^{k} - P^{*}\|_{1}$$

Where $\Psi_k = max_{s,s'} V_{k,1}^k(s) - V_{k,1}^k(s')$ is the MDP span of M_k. Standard **concentration inequalities** [4] give the convergence of $R_k \to R^*$ and $P_k \to P^*$ at rate $\sqrt{\frac{1}{n}}$ and noting $\sum_{n=1}^{T} \sqrt{\frac{1}{T}} \leq 2\sqrt{T}$ completes the proof.

Problems with these bounds

- These bounds require $T = \Omega(|\mathcal{S}|^2|\mathcal{A}|)$ for guarantees.
- **But** many problems have **$|\mathcal{S}|$ and $|\mathcal{A}|$ large or infinite!**
- Mouse in maze $|\mathcal{S}| = 100, |\mathcal{A}| = 5 \implies |\mathcal{S}|^2|\mathcal{A}| = 50,000$.
- Factory line with 100 machines, each with 3 states, 3 actions:
  $|\mathcal{S}| = 3^{100}, |\mathcal{A}| = 3^{100} \implies |\mathcal{S}|^2|\mathcal{A}| = 3^{300} \simeq 10^{150}$
  Even lower bound $\sqrt{|\mathcal{S}||\mathcal{A}|T}$ requires $T = \Omega(|\mathcal{S}||\mathcal{A}|) \simeq 10^{100}$
- How do you even deal with continuous $\mathcal{S}, \mathcal{A}$?
  Discretisation $\rightarrow$ ***curse of dimensionality***.

Factored MDPs

A production line

At each step, the rewards and transition of each machine only depend upon its neighbours.

- 100 **distinct** machines, each with 3 states and 3 actions.
- Each machine only **directly** affected by its neighbours.
- How should you operate the production line?

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- 100 **distinct** machines, each with 3 states and 3 actions.
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- How should you operate the production line?
- **Goal:** Exploit some low-dimensional structure.

Exploiting low-dimensional structure

- We know that over all MDPs regret $\Omega(\sqrt{|\mathcal{S}||\mathcal{A}|T})$.
- However, if we know that M has some **low-dimensional structure** we can exploit this to improve guarantees.
- Previous works [5] showed loose sample complexity bounds for RL on factored MDPs. We prove the first regret bounds which are close to optimal.
- We can exploit the graphical structure of a factored MDP to obtain regret bounds that scale with the **parameters of the MDP**, which may be **exponentially smaller than $|\mathcal{S}|$ or $|\mathcal{A}|$**.

Factored MDPs

Let $\mathcal{S} \times \mathcal{A} = \mathcal{X} = \mathcal{X}_1 \times .. \times \mathcal{X}_n$, $Z \subseteq [n]$ and $\mathcal{X}[Z] := \bigotimes_{i \in Z} \mathcal{X}_i$

Definition (Factored transition functions $P \in \mathcal{P} \subseteq \mathcal{P}_{\mathcal{X},\mathcal{S}}$)

$\mathcal{P}$ is factored over $\mathcal{X} = \mathcal{X}_1 \times .. \times \mathcal{X}_n$ and $\mathcal{S} = \mathcal{S}_1 \times .. \times \mathcal{S}_m$ with scopes $Z_1, ..Z_m \iff$, for all $P \in \mathcal{P}, x \in \mathcal{X}, s \in \mathcal{S}$ there exist,

$$P(s|x) = \prod_{i=1}^{m} P_i\left(s[i] \,\middle|\, x[Z_i]\right) \leftarrow \textbf{\textit{(conditional independence)}}$$

Definition (Factored reward functions $R \in \mathcal{R} \subseteq \mathcal{P}^{C,\sigma}_{\mathcal{X},\mathbb{R}}$)

$\mathcal{R}$ is factored over $\mathcal{X} = \mathcal{X}_1 \times .. \times \mathcal{X}_n$ with scopes $Z_1, ..Z_l \iff$, for all $R \in \mathcal{R}, x \in \mathcal{X}$ there exist,

$$\mathbb{E}[R(x)] = \sum_{i=1}^{l} \mathbb{E}\big[R_i(x[Z_i])\big]$$

*with **each** $r_i \sim R_i(x[Z_i])$ **and individually observed**.*

Production line as a factored MDP

- **Agent** $\leftrightarrow$ Production manager.
- **Environment** $\leftrightarrow$ Production line and outputs.
- **State** $\leftrightarrow$ Machine states $s = (s_1, .., s_{100}) \in \{1, 2, 3\}^{100}$.
- **Reward** $\leftrightarrow$ Dollar output from each machine $r = \sum_{i=1}^{100} r_j$.
- **Transition** $\leftrightarrow$ Evolution of each machine state.

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- **Reward** $\leftrightarrow$ Dollar output from each machine $r = \sum_{i=1}^{100} r_j$.
- **Transition** $\leftrightarrow$ Evolution of each machine state.
- **Factored** since over one timestep s_i only depends on its neighbours' states and actions (s_k, a_k) for $k \in \{i-1, i, i+1\}$.

Main results

Posterior Sampling for Reinforcement Learning

Input: Prior ϕ encoding $\mathcal{G}$, $t = 1$
for episodes $k = 1, 2, ..$ **do**
    sample $M_k \sim \phi(\cdot | H_t)$
    compute near-optimal $\mu_k = \Gamma(M_k, \sqrt{\tau / k})$ $\leftarrow$(ADP planner)
    for timesteps $j = 1, .., \tau$ **do**
        sample and apply $a_t = \mu_k(s_t, j)$
        observe $r_t^1, .., r_t^l$ and $s_{t+1}^1, .., s_{t+1}^m$
        $t = t + 1$
    end for
end for

UCRL-Factored

Input: Graph structure $\mathcal{G}$, confidence δ, $t = 1$
for episodes $k = 1, 2, ..$ **do**
    $d_t^{R_i} = 4\sigma^2 \log\left(4l|\mathcal{X}[Z_i^R]|k/\delta\right)$ for $i = 1, .., l$
    $d_t^{P_j} = 4|\mathcal{S}_j| \log\left(4m|\mathcal{X}[Z_j^P]|k/\delta\right)$ for $j = 1, .., m$
    $\mathcal{M}_k = \{M \mid \mathcal{G}, \overline{R}_i \in \mathcal{R}_t^i(d_t^{R_i}), P_j \in \mathcal{P}_t^j(d_t^{P_j}) \ \forall i, j\}$ $\leftarrow$(Confidence sets)
    compute near-optimistic $\mu_k = \tilde{\Gamma}(\mathcal{M}_k, \sqrt{\tau/k})$ $\leftarrow$(Optim. ADP planner)
    for timesteps $u = 1, .., \tau$ **do**
        sample and apply $a_t = \mu_k(s_t, u)$
        observe $r_t^1, .., r_t^l$ and $s_{t+1}^1, .., s_{t+1}^m$
        $t = t + 1$
    end for
end for

Main results

Theorem (Expected regret for PSRL in factored MDPs)

If the prior ϕ is the distribution of M^* and Ψ is the span of the optimal value function:

$$\mathbb{E}\left[\mathrm{Regret}(T, \pi_\tau^{\mathrm{PS}}, M^*)\right] = \tilde{O}\left(\sigma \sum_{i=1}^{d_1} \sqrt{|\mathcal{X}[Z_i^R]| T} + \mathbb{E}[\Psi] \sum_{j=1}^{d_2} \sqrt{|\mathcal{X}[Z_j^P]||\mathcal{S}_j| T}\right) \quad (1)$$

Theorem (High probability regret for UCRL-Factored)

If D is the diameter of M^*, then for any M^* can bound the regret of UCRL-Factored:

$$\mathrm{Regret}(T, \pi_\tau^{\mathrm{UC}}, M^*) = \tilde{O}\left(\sigma \sum_{i=1}^{d_1} \sqrt{|\mathcal{X}[Z_i^R]| T} + CD \sum_{j=1}^{d_2} \sqrt{|\mathcal{X}[Z_j^P]||\mathcal{S}_j| T}\right) \quad (2)$$

with probability at least $1 - \delta$

Discussion of results

- Close link between posterior sampling and optimism [1].
- Bounds in expected regret versus high probability. Different MDP complexity measures, span $\Psi \leq CD$ (diameter) $\leq C\tau$.
- PSRL more **statistically and computationally** efficient [3].
- Known structure $\mathcal{G}$ **exponential** $\rightarrow$ **polynomial** regret.
- Both algorithms require approximate MDP planning.
- **Near optimal** as m independent MDPs $\rightarrow \tilde{O}(mS\sqrt{AT})$.

Clean bounds in the symmetric case

Let $\mathcal{Q}$ be shorthand for the structure $\mathcal{G}$ such that $l+1=m$, $C=\sigma=1$, $|\mathcal{S}_i|=|\mathcal{X}_i|=K$ and $|Z_i^R|=|Z_i^P|=\zeta$ for all suitable i and write $J=K^\zeta$. In this case $\Psi, D \leq \tau$ trivially.

Corollary (Clean bounds for PSRL)

$$\mathbb{E}\left[\mathrm{Regret}(T, \pi_\tau^{\mathrm{PS}}, M^*)\right] \leq 15 m\tau\sqrt{JKT\log(2mJT)} \qquad (3)$$

Corollary (Clean bounds for UCRL-Factored)

$$\mathrm{Regret}(T, \pi_\tau^{\mathrm{UC}}, M^*) \leq 15 m\tau\sqrt{JKT\log(12mJT/\delta)} \qquad (4)$$

with probability at least $1-\delta$.

Bounds for the production line

- 100 different machines, each with 3 states and 3 actions.
- Transitions only depend on neighbours $\to$ **factored MDP**.
- $\mathcal{G}$-naive bounds $|\mathcal{S}|\sqrt{|\mathcal{A}|T} = 3^{250}\sqrt{T} \simeq 10^{120}\sqrt{T}$.
- Using $\mathcal{G}$ we obtain $100\sqrt{(9)^3 3T} \simeq 10^3\sqrt{T}$.
- In general, **bounds exponentially tighter** than $\mathcal{G}$-naive.

Key lemma

Lemma (Bounding factored deviations)

Let the transition function class $\mathcal{P} \subseteq \mathcal{P}_{\mathcal{X},\mathcal{S}}$ be factored over $\mathcal{X} = \mathcal{X}_1 \times .. \times \mathcal{X}_n$ and $\mathcal{S} = \mathcal{S}_1 \times .. \times \mathcal{S}_m$ with scopes $Z_1, ..Z_m$. Then, for any $P, \tilde{P} \in \mathcal{P}$ we may bound their L1 distance:

$$\|P(x) - \tilde{P}(x)\|_1 \leq \sum_{i=1}^{m} \|P_i(x[Z_i]) - \tilde{P}_i(x[Z_i])\|_1$$

Proof:

We begin with the simple claim that for any $\alpha_1, \alpha_2, \beta_1, \beta_2 \in (0, 1]$:

$$\begin{aligned} |\alpha_1\alpha_2 - \beta_1\beta_2| &= \alpha_2 \left|\alpha_1 - \frac{\beta_1\beta_2}{\alpha_2}\right| \\ &\leq \alpha_2 \left(|\alpha_1 - \beta_1| + \left|\beta_1 - \frac{\beta_1\beta_2}{\alpha_2}\right|\right) \\ &\leq \alpha_2 |\alpha_1 - \beta_1| + \beta_1 |\alpha_2 - \beta_2| \end{aligned}$$

Key lemma continued

We now consider the probability distributions $p, \tilde{p}$ over $\{1, .., d_1\}$ and $q, \tilde{q}$ over $\{1, .., d_2\}$. We let $Q = pq^T, \tilde{Q} = \tilde{p}\tilde{q}^T$ be the joint probability distribution over $\{1, .., d_1\} \times \{1, .., d_2\}$. Using the claim above we bound the L1 deviation $\|Q - \tilde{Q}\|_1$ by the deviations of their factors:

$$
\begin{aligned}
\|Q - \tilde{Q}\|_1 &= \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} |p_i q_j - \tilde{p}_i \tilde{q}_j| \\
&\leq \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} q_j |p_i - \tilde{p}_i| + \tilde{p}_i |q_j - \tilde{q}_j| \\
&= \|p - \tilde{p}\|_1 + \|q - \tilde{q}\|_1
\end{aligned}
$$

We conclude the proof by applying this m times to the factored transitions P and $\tilde{P}$.

Conclusions

- **Regret polynomial in the parameters** encoding the factored MDP, which may be **exponentially smaller than $|\mathcal{S}|$ or $|\mathcal{A}|$**.
- Near-optimal regret bounds and simple algorithms.
- Two algorithms based on **posterior sampling** and **optimism**.

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- **Regret polynomial in the parameters** encoding the factored MDP, which may be **exponentially smaller than $|\mathcal{S}|$ or $|\mathcal{A}|$**.
- Near-optimal regret bounds and simple algorithms.
- Two algorithms based on **posterior sampling** and **optimism**.
- **BUT**:
  - Algorithms require access to approximate MDP planner.
  - You need to know $\mathcal{G}$ structure a priori.
  - How can you learn without episodic reset τ?
  - What about other large/continuous MDPs with different structure, for example linear-quadratic control? [6].

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