# Bandits, Global Optimization, Active Learning, and Bayesian RL – understanding the common ground

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Autonomous Learning Summer School, Leipzig, Sep 2014

This does not focus on own work! It's really a lecture...

The goal is to understand sequential decision problems in which decisions equally influence the learning progress as well as rewards/states.

- Bandits, Global Optimization, Active Learning, and Bayesian RL are instances of this. The perspective taken is simple: All of these problems are eventually Markovian processes in belief space
- For instance, you'll learn what 'optimal optimization' is

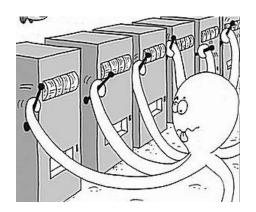
Disclaimer: Whenever I say "optimal" I mean "Bayes optimal" (we always assume having priors  $P(\theta)$ )

#### **Outline**

- Problems covered:
  - Bandits
  - Global optimization
  - Active learning
  - Bayesian RL
  - Monte Carlo Tree Search (MTCS)
- Methods covered (interweaved with the above):
  - Belief planning
  - Upper Confidence Bound (UCB)
  - Expected Improvement, probability of improvement
  - Predictive Entropy, Uncertainty Sampling, Shannon Information
  - Bayesian exploration bonus, Rmax
  - Monte Carlo Tree Search (MCTS; UCT)

## **Bandits**

### **Bandits**



- ullet There are n machines.
- Each machine i returns a reward  $y \sim P(y; \theta_i)$ The machine's parameter  $\theta_i$  is unknown

#### **Bandits**

- Let  $a_t \in \{1,..,n\}$  be the choice of machine at time tLet  $y_t \in \mathbb{R}$  be the outcome with mean  $\langle y_{a_t} \rangle$
- A policy or strategy maps all the history to a new choice:

$$\pi: [(a_1, y_1), (a_2, y_2), ..., (a_{t-1}, y_{t-1})] \mapsto a_t$$

• Problem: Find a policy  $\pi$  that

$$\max \left\langle \sum_{t=1}^{T} y_t \right\rangle$$

or

$$\max \langle y_T \rangle$$

or other objectives like discounted infinite horizon  $\max\left\langle \sum_{t=1}^{\infty} \gamma^t y_t \right\rangle$ 

## **Exploration, Exploitation**

- "Two effects" of choosing a machine:
  - You collect more data about the machine → knowledge
  - You collect reward
- For example
  - Exploration: Choose the next action  $a_t$  to  $\min \langle H(b_t) \rangle$
  - Exploitation: Choose the next action  $a_t$  to  $\max \langle y_t \rangle$

#### The Belief State

- "Knowledge" can be represented in two ways:
  - as the full history

$$h_t = [(a_1, y_1), (a_2, y_2), ..., (a_{t-1}, y_{t-1})]$$

- as the belief

$$b_t(\theta) = P(\theta|h_t)$$

where  $\theta$  are the unknown parameters  $\theta = (\theta_1,..,\theta_n)$  of all machines

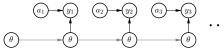
- In the bandit case:
  - The belief factorizes  $b_t(\theta) = P(\theta|h_t) = \prod_i b_t(\theta_i|h_t)$ 
    - e.g. for binary bandits,  $\theta_i = p_i$ , with prior Beta $(p_i | \alpha, \beta)$ :

$$b_t(p_i|h_t) = \text{Beta}(p_i|\alpha + a_{i,t}, \beta + b_{i,t})$$

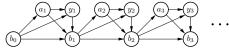
$$a_{i,t} = \sum_{s=1}^{t-1} [a_s = i][y_s = 0] , \quad b_{i,t} = \sum_{s=1}^{t-1} [a_s = i][y_s = 1]$$

#### The Belief MDP

• The process can be modelled as



or as Belief MDP



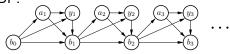
$$P(b'|y,a,b) = \begin{cases} 1 & \text{if } b' = b'_{[b,a,y]} \\ 0 & \text{otherwise} \end{cases}, \quad P(y|a,b) = \int_{\theta_a} b(\theta_a) \; P(y|\theta_a)$$

• The Belief MDP describes a *different* process: the interaction between the information available to the agent  $(b_t \text{ or } h_t)$  and its actions, where the agent uses his current belief to anticipate outcomes, P(y|a,b).

Optimality in the Belief MDP  $\Rightarrow$  optimality in the original problem

## Optimal policies via Dynamic Programming in Belief Space

The Belief MDP:



$$P(b'|y,a,b) = \begin{cases} 1 & \text{if } b' = b'_{[b,a,y]} \\ 0 & \text{otherwise} \end{cases}, \quad P(y|a,b) = \int_{\theta_a} b(\theta_a) \; P(y|\theta_a)$$

Belief Planning: Dynamic Programming on the value function

$$\forall_b: V_{t-1}(b) = \max_{\pi} \left\langle \sum_{t=t}^T y_t \right\rangle$$

$$= \max_{\pi} \left[ \left\langle y_t \right\rangle + \left\langle \sum_{t=t+1}^T y_t \right\rangle \right]$$

$$= \max_{a_t} \int_{y_t} P(y_t | a_t, b) \left[ y_t + V_t(b'_{[b, a_t, y_t]}) \right]$$

$$V_{t}^{*}(h) := \underset{\pi}{\operatorname{argmax}} \int_{\theta} P(\theta|h) V_{t}^{\pi,\theta}(h) \tag{1}$$

$$= \underset{\pi}{\operatorname{argmax}} \int_{\theta} P(\theta|h) \underset{a}{\operatorname{max}} \left[ R(a,h) + \int_{h'} P(h'|h,a,\theta) V_{t+1}^{\pi,\theta}(h') \right] \tag{2}$$

$$V_{t}^{*}(b) = \underset{\pi}{\operatorname{argmax}} \int_{\theta} b(\theta) \underset{a}{\operatorname{max}} \left[ R(a,b) + \int_{b'} P(b'|b,a,\theta) V_{t+1}^{\pi,\theta}(b') \right] \tag{3}$$

$$= \underset{\pi}{\operatorname{argmax}} \underset{a}{\operatorname{max}} \int_{\theta} \int_{b'} b(\theta) P(b'|b,a,\theta) \left[ R(a,b) + V_{t+1}^{\pi,\theta}(b') \right] \tag{4}$$

$$P(b'|b,a,\theta) = \int_{y} P(b',y|b,a,\theta) \tag{5}$$

$$= \int_{y} \frac{P(\theta|b,a,b',y) P(b',y|b,a)}{P(\theta|b,a)} \tag{6}$$

$$= \int_{y} \frac{b'(\theta) P(b',y|b,a)}{b(\theta)} \tag{7}$$

$$V_{t}^{*}(b) = \underset{\pi}{\operatorname{argmax}} \underset{a}{\operatorname{max}} \int_{\theta} \int_{b'} \int_{y} b(\theta) \frac{b'(\theta) P(b',y|b,a)}{b(\theta)} \left[ R(a,b) + V_{t+1}^{\pi,\theta}(b') \right] \tag{8}$$

$$= \underset{\pi}{\operatorname{argmax}} \underset{a}{\operatorname{max}} \int_{b'} \int_{y} P(b',y|b,a) \left[ R(a,b) + \int_{\theta} b'(\theta) V_{t+1}^{\pi,\theta}(b') \right] \tag{9}$$

$$= \underset{\pi}{\operatorname{argmax}} \underset{a}{\operatorname{max}} \int_{y} P(y|b,a) \left[ R(a,b) + V_{\theta}^{*}(b|b,a,y](\theta) V_{t+1}^{\pi,\theta}(b'|b,a,y]) \right] \tag{11}$$

$$= \underset{a}{\operatorname{max}} \int_{y} P(y|b,a) \left[ R(a,b) + V_{t+1}^{*}(b'|b,a,y](\theta) V_{t+1}^{\pi,\theta}(b'|b,a,y)(\theta) \right] \tag{11}$$

## **Optimal policies**

- The value function assigns a value (maximal achievable expected return) to a state of knowledge
- Optimal policies "navigate through belief space"
  - This automatically implies/combines "exploration" and "exploitation"
  - There is no need to explicitly address "exploration vs. exploitation" or decide for one against the other. Optimal policies will automatically do this.
- The optimal policy is greedy w.r.t. the value function (in the sense of the  $\max_{a_t}$  above)
- Computationally heavy:  $b_t$  is a probability distribution,  $V_t$  a function over probability distributions

• The term  $\int_{y_t} P(y_t|a_t,b_{t-1}) \left[ y_t + V_t(b_{t-1}[a_t,y_t]) \right]$  is related to the *Gittins Index*: it can be computed for each bandit separately.

- Consider 3 binary bandits for T = 10.
  - How "large" is the belief space? What numbers do you need to store a belief?

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The belief is 3 Beta distributions  $\mathrm{Beta}(p_i|\alpha+a_i,\beta+b_i) \to \mathbf{6}$  integers  $T=10 \to \mathbf{each}$  integer  $\leq 10$ 

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– How "large" is the value function  $V_t(b_t)$ ? How many numbers to store  $V_t(b_t)$ ?

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- How "large" is the value function  $V_t(b_t)$ ? How many numbers to store  $V_t(b_t)$ ?
  - $V_t(b_t)$  is a function over  $\{0,..,10\}^6 \to 1$  Mio. numbers  $\in \mathbb{R}$

- Consider 3 binary bandits for T = 10.
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- How "large" is the value function  $V_t(b_t)$ ? How many numbers to store  $V_t(b_t)$ ?  $V_t(b_t)$  is a function over  $\{0,..,10\}^6 \to 1$  Mio. numbers  $\in \mathbb{R}$  Many states cannot be visited (integers need to sum up) Only very few transitions are possible (incrementing integers)

## **Greedy heuristic: Upper Confidence Bound (UCB)**

- 1: Initializaiton: Play each machine once
- 2: repeat
- 3: Play the machine i that maximizes  $\hat{y}_i + \beta \sqrt{\frac{2 \ln n}{n_i}}$
- 4: until
- $\hat{y}_i$  is the average reward of machine i so far  $n_i$  is how often machine i has been played so far  $n=\sum_i n_i$  is the number of rounds so far  $\beta$  is often chosen as  $\beta=1$

See *Finite-time analysis of the multiarmed bandit problem*, Auer, Cesa-Bianchi & Fischer, Machine learning, 2002.

## **UCB** algorithms

UCB algorithms determine a confidence interval such that

$$\hat{y}_i - \sigma_i < \langle y_i \rangle < \hat{y}_i + \sigma_i$$

with high probability.

UCB chooses the upper bound of this confidence interval

- Optimism in the face of uncertainty
- Strong bounds on the regret (sub-optimality) of UCB (e.g. Auer et al.)

· Data so far:

Machine A: 8, 7, 12, 13, 11, 9

Machine B: 8, 12

Machine C: 5, 13

Which one do you choose next?

• Data so far:

Machine A: 8, 7, 12, 13, 11, 9

Machine B: 8, 12 Machine C: 5, 13

Which one do you choose next?

Machine A:  $10 \pm 2.16/\sqrt{6}$ Machine B:  $10 \pm 2/\sqrt{2}$ Machine C:  $9 \pm 4/\sqrt{2}$ 

#### **Conclusions**

- The bandit problem is an archetype for
  - Sequential decision making
  - Decisions that influence knowledge as well as rewards/states
  - Exploration/exploitation
- The same aspects are inherent also in global optimization, active learning & RL
- Belief Planning in principle gives the optimal solution
- Greedy Heuristics (UCB) are computationally much more efficient and guarantee bounded regret. MCTS is also applicable

## **Further reading**

- ICML 2011 Tutorial Introduction to Bandits: Algorithms and Theory,
   Jean-Yves Audibert, Rémi Munos
- Finite-time analysis of the multiarmed bandit problem, Auer,
   Cesa-Bianchi & Fischer, Machine learning, 2002.
- On the Gittins Index for Multiarmed Bandits, Richard Weber, Annals of Applied Probability, 1992.
  - Optimal Value function is submodular.

## **Global Optimization**

## **Global Optimization**

• Let  $x \in \mathbb{R}^n$ ,  $f: \mathbb{R}^n \to \mathbb{R}$ , find

$$\min_{x} f(x)$$

(I neglect constraints  $g(x) \le 0$  and h(x) = 0 here – but could be included.)

• Blackbox optimization: find optimium by sampling values  $y_t = f(x_t)$ No access to  $\nabla f$  or  $\nabla^2 f$ Observations may be noisy  $y \sim \mathcal{N}(y \,|\, f(x_t), \sigma)$ 

## Global Optimization = infinite bandits

- In global optimization f(x) defines a reward for every  $x \in \mathbb{R}^n$  Instead of a finite number of actions  $a_t$  we now have  $x_t$
- Optimal Optimization could be defined as: find  $\pi: h_t \mapsto x_t$  that

$$\min \left\langle \sum_{t=1}^{T} f(x_t) \right\rangle$$

or

$$\min \langle f(x_T) \rangle$$

#### Gaussian Processes as belief

- The unknown "world property" is the function  $\theta = f$
- Given a Gaussian Process prior  $GP(f|\mu,C)$  over f and a history

$$D_t = [(x_1, y_1), (x_2, y_2), ..., (x_{t-1}, y_{t-1})]$$

the belief is

$$\begin{split} b_t(f) &= P(f \,|\, D_t) = \mathsf{GP}(f|D_t,\mu,C) \\ \mathsf{Mean}(f(x)) &= \hat{f}(x) = \pmb{\kappa}(x)(\pmb{K} + \sigma^2\mathbf{I})^{\text{-}1}\pmb{y} & \textit{response surface} \\ \mathsf{Var}(f(x)) &= \hat{\sigma}(x) = k(x,x) - \pmb{\kappa}(x)(\pmb{K} + \sigma^2\mathbf{I}_n)^{\text{-}1}\pmb{\kappa}(x) & \textit{confidence interval} \end{split}$$

- Side notes:
  - Don't forget that  $Var(y^*|x^*, D) = \sigma^2 + Var(f(x^*)|D)$
  - We can also handle discrete-valued functions f using GP classification

## Optimal optimization via belief planning

As for bandits it holds

$$V_{t-1}(b_{t-1}) = \max_{\pi} \left\langle \sum_{t=t}^{T} y_{t} \right\rangle$$

$$= \max_{x_{t}} \int_{y_{t}} P(y_{t}|x_{t}, b_{t-1}) \left[ y_{t} + V_{t}(b_{t-1}[x_{t}, y_{t}]) \right]$$

 $V_{t-1}(b_{t-1})$  is a function over the GP-belief! If we could compute  $V_{t-1}(b_{t-1})$  we "optimally optimize"

I don't know of a minimalistic case where this might be feasible

## **Greedy 1-step heuristics**

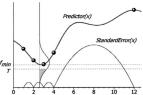


Figure 14. Using kriging, we can estimate the probability that sampling at a given point will 'improve' our solution, in the sense of yielding a value that is equal or better than some target

from Jones (2001)

Maximize Probability of Improvement (MPI)

$$x_t = \operatorname*{argmax} \int_{-\infty}^{y^*} \mathcal{N}(y|\hat{f}(x), \hat{\sigma}(x))$$

• Maximize Expected Improvement (EI)

$$x_t = \underset{x}{\operatorname{argmax}} \int_{-\infty}^{y^*} \mathcal{N}(y|\hat{f}(x), \hat{\sigma}(x)) (y^* - y)$$

Maximize UCB

$$x_t = \underset{\cdot}{\operatorname{argmin}} \hat{f}(x) - \beta_t \hat{\sigma}(x)$$

(Often,  $\beta_t=1$  is chosen. UCB theory allows for better choices. See Srinivas et al. citation below.)

#### From Srinivas et al., 2012:

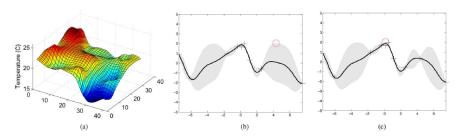


Fig. 2. (a) Example of temperature data collected by a network of 46 sensors at Intel Research Berkeley. (b) and (c) Two iterations of the GP-UCB algorithm. The dark curve indicates the current posterior mean, while the gray bands represent the upper and lower confidence bounds which contain the function with high probability. The "+" mark indicates points that have been sampled before, while the "o" mark shows the point chosen by the GP-UCB algorithm to sample next. It samples points that are either (b) uncertain or have (c) high posterior mean.

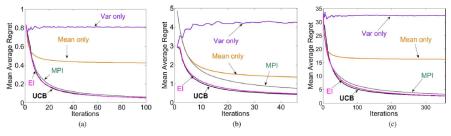


Fig. 6. Mean average regret: GP-UCB and various heuristics on (a) synthetic and (b, c) sensor network data.

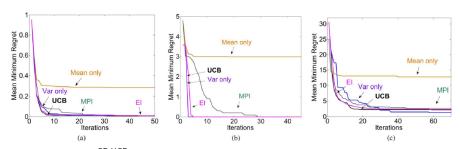


Fig. 7. Mean minimum regret: GP-UCB and various heuristics on (a) synthetic, and (b, c) sensor network data.

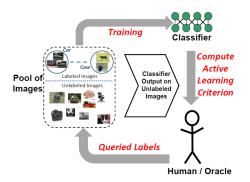
## **Further reading**

- Classically, such methods are known as Kriging
- Information-theoretic regret bounds for gaussian process optimization in the bandit setting Srinivas, Krause, Kakade & Seeger, Information Theory, 2012.
- Efficient global optimization of expensive black-box functions. Jones, Schonlau, & Welch, Journal of Global Optimization, 1998.
- A taxonomy of global optimization methods based on response surfaces Jones, Journal of Global Optimization, 2001.
- Explicit local models: Towards optimal optimization algorithms, Poland, Technical Report No. IDSIA-09-04, 2004.

## **Active Learning**

## **Example**

Active learning with gaussian processes for object categorization. Kapoor, Grauman, Urtasun & Darrell, ICCV 2007.



## **Active Learning**

- In standard ML, a data set  $D_t = \{(x_s,y_s)\}_{s=1}^{t-1}$  is given. In active learning, the learning agent sequencially decides on each  $x_t$  where to collect data
- Generally, the aim of the learner should be to learn as fast as possible, e.g. minimize predictive error
- Finite horizon T predictive error problem: Given  $P(x^*)$ , find a policy  $\pi: D_t \mapsto x_t$  that

$$\min \langle -\log P(y^*|x^*, D_T) \rangle_{y^*, x^*, D_T; \pi}$$

This also can be expressed as predictive entropy:

$$\langle -\log P(y^*|x^*, D_T) \rangle_{y^*, x^*} = \left\langle -\int_{y^*} P(y^*|x^*, D_T) \log P(y^*|x^*, D_T) \right\rangle_{x^*}$$
  
=  $\langle H(y^*|x^*, D_T) \rangle_{x^*} =: H(f|D_T)$ 

• Find a policy that  $\min \langle H(f|D_T) \rangle_{D_T:\pi}$ 

#### Gaussian Processes as belief

- Again, the unknown "world property" is the function  $\theta = f$
- · We can use a Gaussian Process to represent the belief

$$b_t(f) = P(f \mid D_t) = \mathsf{GP}(f \mid D_t, \mu, C)$$

## **Optimal Active Learning via belief planning**

- The only difference to global optimization is the reward.
   In active learning it is the predictive entropy: -H(f|D<sub>T</sub>)
- Dynamic Programming:

$$V_T(b_T) = -H(b_T) , \quad H(b) := \langle H(y^*|x^*, b) \rangle_{x^*}$$

$$V_{t-1}(b_{t-1}) = \max_{x_t} \int_{y_t} P(y_t|x_t, b_{t-1}) \ V_t(b_{t-1}[x_t, y_t])$$

Computationally intractable

#### **Greedy 1-step heuristic**

• The simplest greedy policy is 1-step Dynamic Programming: Directly maximize immediate expected reward, i.e., minimizes  $H(b_{t+1})$ .

$$\pi: b_t(f) \mapsto \underset{x}{\operatorname{argmin}} \int_{y_t} P(y_t|x_t, b_t) \ H(b_t[x_t, y_t])$$

• For GPs, you reduce the entropy most if you choose  $x_t$  where the current predictive variance is highest:

$$Var(f(x)) = k(x, x) - \kappa(x)(K + \sigma^{2}\mathbf{I}_{n})^{-1}\kappa(x)$$

This is referred to as uncertainty sampling

- Note, if we fix hyperparameters:
  - This variance is independent of the observations y<sub>t</sub>, only the set D<sub>t</sub> matters!
  - The order of data points also does not matter
  - You can pre-optimize a set of "grid-points" for the kernel and play them in any order

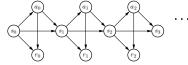
### Further reading

- Active learning literature survey. Settles, Computer Sciences Technical Report 1648, University of Wisconsin-Madison, 2009.
- Bayesian experimental design: A review. Chaloner & Verdinelli, Statistical Science, 1995.
- Active learning with statistical models. Cohn, Ghahramani & Jordan, JAIR 1996.
- ICML 2009 Tutorial on Active Learning, Sanjoy Dasgupta and John Langford http://hunch.net/~active\_learning/

# **Bayesian Reinforcement Learning**

#### **Markov Decision Process**

Other than the previous cases, actions now influence a world state



- initial state distribution  $P(s_0)$
- transition probabilities P(s'|s, a)
- reward probabilities P(r|s, a)
- agent's policy  $P(a|s;\pi)$
- Planning in MDPs: Given knowledge of P(s'|s,a), P(r|s,a) and P(y|s,a), find a policy  $\pi: s_t \mapsto a_t$  that maximizes the discounted infinite horizon return  $\langle \sum_{t=0}^{\infty} \gamma^t r_t \rangle$ :

$$V(s) = \max_{a} \left[ \mathsf{E}(r|s,a) + \gamma \sum_{s'} P(s'\,|\,s,a) \; V(s') \right]$$

#### Bayesian RL: The belief state

- In *Reinforcement Learning* we do not know the world Unknown MDP parameters  $\theta = (\theta_s, \theta_{s'sa}, \theta_{rsa})$  (for  $P(s_0), P(s'|s, a), P(r|s, a)$ )
- "Knowledge" can be represented in two ways:
  - as the full history

$$h_t = [(s_0, a_0, r_0), ..., (s_{t-1}, a_{t-1}, r_{t-1}), (s_t)]$$

- as the belief

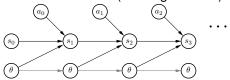
$$b_t(\theta) = P(\theta|h_t)$$

where  $\theta$  are all the unknown parameters

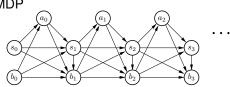
- In the case of discrete MDPs
  - $-\theta$  are CPTs (conditional probability tables)
  - Assuming Dirichlet priors over CPTs, the exact posterior is a Dirichlet
  - Amounts to counting transitions

### **Optimal policies**

• The process can be modelled as (omitting rewards)



or as Belief MDP



$$P(b'|s',s,a,b) = \begin{cases} 1 & \text{if } b' = b[s',s,a] \\ 0 & \text{otherwise} \end{cases}, \quad P(s'|s,a,b) = \int_{\theta} b(\theta) \; P(s'|s,a,\theta)$$

$$V(b,s) = \max_{a} \left[ \mathsf{E}(r|s,a,b) + \sum_{s'} P(s'|a,s,b) \; V(s',b') \right]$$

Dynamic programming can be approximated (Poupart et al.)

#### **Heuristics**

 As with UCB, choose estimators for R\*, P\* that are optimistic/over-confident

$$V_t(s) = \max_{a} \left[ R^* + \sum_{s'} P^*(s'|s, a) \ V_{t+1}(s') \right]$$

Rmax:

$$-\ R^*(s,a) = \begin{cases} R_{\max} & \text{if } \#_{s,a} < n \\ \hat{\theta}_{rsa} & \text{otherwise} \end{cases}, \quad P^*(s'|s,a) = \begin{cases} \delta_{s's^*} & \text{if } \#_{s,a} < n \\ \hat{\theta}_{s'sa} & \text{otherwise} \end{cases}$$

- Guarantees over-estimation of values, polynomial PAC results!
- Read about "KWIK-Rmax"! (Li, Littman, Walsh, Strehl, 2011)
- Bayesian Exploration Bonus (BEB), Kolter & Ng (ICML 2009)
  - Choose  $P^*(s'|s,a) = P(s'|s,a,b)$  integrating over the current belief  $b(\theta)$  (non-over-confident)
  - But choose  $R^*(s,a)=\hat{\theta}_{rsa}+\frac{\beta}{1+\alpha_0(s,a)}$  with a hyperparameter  $\alpha_0(s,a)$ , over-estimating return
- Confidence intervals for V-/Q-function (Kealbling '93, Dearden et al. '99)

# **Further reading**

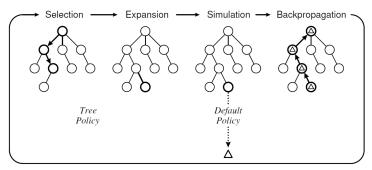
- ICML-07 Tutorial on Bayesian Methods for Reinforcement Learning
   https://cs.uwaterloo.ca/~ppoupart/ICML-07-tutorial-Bayes-RL.html
   Esp. part 3: Model-based Bayesian RL (Pascal Poupart); and the methods cited on slide 22
- Optimal learning: Computational procedures for Bayes-adaptive Markov decision processes. Duff, Doctoral dissertation, University of Massassachusetts Amherst, 2002.
- An analytic solution to discrete Bayesian reinforcement learning.
   Poupart, Vlassis, Hoey, & Regan (ICML 2006)
- KWIK-Rmax: *Knows what it knows: a framework for self-aware learning.* Li, Littman, Walsh & Strehl, Machine learning, 2011.
- Bayesian Exploration Bonus: Near-Bayesian exploration in polynomial time. Kolter & Ng, ICML 2009.
- The "interval exploration method" described in Reinforcement learning: A survey. Kaelbling, Littman & Moore, arXiv preprint cs/9605103, 1996.

# **Monte Carlo Tree Search (MCTS)**

## Monte Carlo Tree Search (MCTS)

- MCTS triggered a little revolution...
- MCTS is very successful on Computer Go and other games
- MCTS is rather simple to implement
- MCTS is very general: applicable on any discrete domain
- Key paper: Kocsis & Szepesvári: Bandit based Monte-Carlo Planning, ECML 2006.
- Survey paper:
   Browne et al.: A Survey of Monte Carlo Tree Search Methods, 2012.
- POMDPs:
  - Silver & Veness: Monte-Carlo Planning in Large POMDPs, NIPS 2010
- Tutorial presentation: http://web.engr.oregonstate.edu/~afern/icaps10-MCP-tutorial.ppt

#### **Basic MCTS scheme**



from Browne et al.

- 1: start tree  $V = \{v_0\}$
- 2: while within computational budget do
- 3:  $v_l \leftarrow \mathsf{TREEPolicy}(V)$  chooses a leaf of V
- 4: append  $v_l$  to V
- 5:  $\Delta \leftarrow \mathsf{ROLLOUTPOLICY}(V)$  rolls out a full simulation, with return  $\Delta$
- 6: BACKUP $(v_l, \Delta)$  updates the values of all parents of  $v_l$
- 7: end while
- 8: return best child of  $v_0$

### Growing the tree as a sequential decision problem

- We talk here about the internal planning process!
- Deciding to allocate resources to grow the tree in a certain direction (the TREEPOLICY) is a decision!
   Growing the full tree a sequential decision problem
- What would be the optimal way to make growing decisions?
  - → A problem of planning within the planning algorithm...
- The optimal solution is of course infeasible, but...

# **Upper Confidence Tree (UCT)**

- UCT uses UCB to realize the TREEPOLICY, i.e. to decide where to expand the tree
- BACKUP updates all parents of  $v_l$  as  $n(v) \leftarrow n(v) + 1$  (count how often has it been played)  $Q(v) \leftarrow Q(v) + \Delta$  (sum of rewards received)
- TREEPOLICY chooses child nodes based on UCB:

$$\underset{v' \in \partial(v)}{\operatorname{argmax}} \frac{Q(v')}{n(v')} + \beta \sqrt{\frac{2 \ln n(v)}{n(v')}}$$

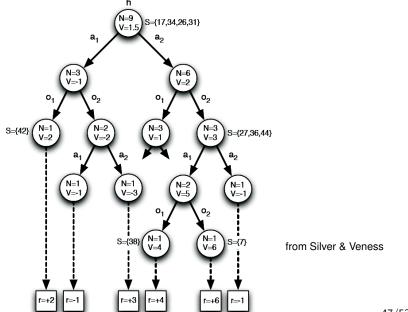
or choose v' if n(v') = 0

• In games use a "negamax" backup: While iterating upward, flip sign  $\Delta \leftarrow -\Delta$  in each iteration

# Issues when applying MCTS ideas to POMDPs

- · key paper:
  - Silver & Veness: Monte-Carlo Planning in Large POMDPs, NIPS 2010
- MCTS is based on generating rollouts using a simulator
  - Rollouts need to start at a specific state  $s_t$
  - ightarrow Nodes in our tree need to have states associated, to start rollouts from
- $\bullet$  At any point in time, the agent has only the history  $h_t=(y_{0:t},a_{0:t\text{--}1})$  to decide on an action
  - The agent wants to estimate the Q-funcion  $Q(h_t, a_t)$
  - → Nodes in our tree need to have a history associated
  - → Nodes in the search tree will
    - maintain n(v) and Q(v) as before
    - have a history h(v) attached
    - have a *set* of states S(v) attached

## MCTS applied to POMDPs



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### MCTS applied to POMDPs

- For each rollout:
  - Choose a *random* world state  $s_0 \sim S(v_0)$  from the set of states associated to the root  $v_0$ ; initialize the simulator with this  $s_0$
  - Use a TreePolicy to traverse the current tree; during this, update the state sets  $\mathbb{S}(v)$  to contain the world state simulated by the simulator
  - Use a ROLLOUTPOLICY to simulate a full rollout
  - Append a new leaf  $v_l$  with novel history  $h(v_l)$  and a single state  $\Im(v_l)$  associated

#### **Discussion**

3 points to make

#### Point 1: Common ground

What bandits, global optimization, active learning, Bayesian RL & POMDPs share

- Sequential decisions
- Markovian w.r.t. belief
- Decisions influence the knowledge as well as rewards/states
- Sometimes described as "exploration/exploitation problems"

### **Point 2: Optimality**

- In all cases, belief planning would yield optimal solutions
  - → Optimal Optimization, Optimal Active Learning, etc...
- Even if it may be computationally infeasible, it is important to know conceptually
- Optimal policies "navigate through belief space"
  - This automatically implies/combines "exploration" and "exploitation"
  - There is no need to explicitly address "exploration vs. exploitation" or decide for one against the other. Policies that maximize the single objective of future returns will automatically do this.

#### Point 3: Greedy (1-step) heuristics

- Also the optimal policy is greedy w.r.t. the value function!
- "Greedy heuristics" replace the value function by something simpler and more direct to compute, typically 1-step criteria
  - UCB
  - Probability of Improvement, Expected Improvement
  - Expected immediate reward, expected predictive entropy
- Typically they reflect optimism in the face of uncertainty
- Regret bounds for UCB on bandits and optimization (Auer et al.; Srinivas et al.)
- Theory on submodularity very stongly motivates greedy heuristics
- In RL: Optimism w.r.t.  $\theta$ , but planning w.r.t. s
  - Bayesian Exploration Bonus (BEB), Rmax, interval exploration method

#### **Thanks**

for your attention!