Topics in Reinforcement Learning: Lessons from AlphaZero for (Sub)Optimal Control and Discrete Optimization

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Links to Class Notes, Videolectures, and Slides at http://web.mit.edu/dimitrib/www/RLbook.html

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Lecture 5 Rollout for Deterministic and Stochastic Problems

# Outline

#### Rollout for Deterministic Finite-State Problems

- 2 Cost Improvement Property
- Oeterministic Rollout Variants and Extensions
  - Stochastic Rollout and Monte Carlo Tree Search
- Sollout for Deterministic Infinite Spaces Problems

# Rollout: A Special Case of Approximation in Value Space



 $\tilde{J}_{k+\ell}(x_{k+\ell})$  is the Cost Function of Some Policy or Heuristic

- The policy used for rollout is called base policy
- The policy obtained by lookahead minimization is called rollout policy

#### Approximate variant

- $\tilde{J}_{k+\ell}(x_{k+\ell})$  may also approximate the cost function of the base policy
- Possibility of truncated rollout

# Rollout is Important for this Course

#### Role of Rollout

- It provides important options for cost function approximation in the context of value space methods
- It is the basic building block of the fundamental PI algorithm (and approximate variants)

#### Reasons why it will be important:

- Rollout, in its pure form, is the RL method that is easiest to understand and apply
- Rollout is the most reliably successful (with "correct" implementation)
- It is very general: Applies to deterministic and stochastic problems, to finite horizon and infinite horizon
- As a special case of approximation in value space, it relates to Newton's method
- It provides a useful alternative to reoptimization in indirect adaptive control
- It relates to model predictive control, one of the most important control system design methods (it is used to bring *J* within the region of stability)
- It forms a building block for many of the RL methods used in practice [including Q-learning, self-learning (approximate PI), and others]

# General Structure of Deterministic Rollout with Some Base Heuristic



• At state  $x_k$ , for every pair  $(x_k, u_k)$ ,  $u_k \in U_k(x_k)$ , we generate a Q-factor

 $\tilde{Q}_k(x_k, u_k) = g_k(x_k, u_k) + H_{k+1}(f_k(x_k, u_k))$ 

using the base heuristic  $[H_{k+1}(x_{k+1})]$  is the heuristic cost starting from  $x_{k+1}$ 

- We select the control *u<sub>k</sub>* with minimal Q-factor
- We move to next state *x*<sub>*k*+1</sub>, and continue
- Multistep lookahead versions
- Is rollout cost improving? (Performs no worse than the base heuristic, from x<sub>0</sub>)

# Criteria for Cost Improvement of a Rollout Algorithm

- Cost improvement is not automatic: Special conditions must hold to guarantee that the rollout policy has no worse performance than the base heuristic
- Two such conditions are sequential consistency and sequential improvement.

The base heuristic is sequentially consistent if at a given state it chooses control that depends only on that state (and not on how we got to that state)

• If the heuristic generates the sequence

 $\{\mathbf{x}_k, \mathbf{x}_{k+1}, \ldots, \mathbf{x}_N\}$ 

starting from state  $x_k$ , it also generates the sequence

 $\{x_{k+1},\ldots,x_N\}$ 

starting from state  $x_{k+1}$ 

- The base heuristic is sequentially consistent if and only if it can be implemented with a legitimate DP policy {μ<sub>0</sub>,...,μ<sub>N-1</sub>}
- "Greedy" heuristics are sequentially consistent (e.g., nearest neighbor for TS)
- We will focus on a less restrictive condition: sequential improvement

# Sequential Improvement Condition



Implies cost improvement: (Cost of Rollout Policy)  $\leq$  (Cost of Base Heuristic)

• Definition: Best heuristic Q-factor  $\leq$  Heuristic cost, i.e.,

$$\min_{u_k\in U_k(x_k)}\left[g_k(x_k,u_k)+H_{k+1}(f_k(x_k,u_k))\right]\leq H_k(x_k),\quad\text{for all }x_k$$

where  $H_k(x_k)$ : cost of the trajectory generated by the heuristic starting from  $x_k$ 

- Justification: Rollout, upon reaching *x̃*<sub>k</sub>, has obtained a "current" trajectory *R*<sub>k</sub>.
   Sequential improvement implies monotonicity: Cost of *R*<sub>k</sub> ≥ Cost of *R*<sub>k+1</sub>
- $R_0$  is the cost of the base heuristic,  $R_N$  is the cost of the rollout, so  $R_0 \ge R_N$
- Note that Sequential consistency (i.e., heuristic is a DP policy) -> Sequential improvement

# Traveling Salesman Example: Rollout with a Nearest Neighbor Heuristic



Base heuristic: Nearest neighbor (sequentially consistent and sequentially improving)

#### Cost of $R_0 \ge$ Cost of $R_1 \ge$ Cost of $R_2$

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# Simplified Rollout Algorithm - Assuming Sequential Improvement

Simplified algorithm: Instead of control w/ minimal Q-factor, use any control with Q-factor  $\leq$  heuristic cost  $H_k(x_k)$ 

• At any  $x_k$ , choose as rollout control any  $\tilde{\mu}_k(x_k)$  such that

$$g_k(x_k, \tilde{\mu}_k(x_k)) + H_{k+1}(f_k(x_k, \tilde{\mu}_k(x_k))) \leq H_k(x_k),$$

where  $H_k(x_k)$  is the cost of the trajectory generated by the heuristic from  $x_k$ .

• May save lots of computation (case of multiagent rollout, where *u<sub>k</sub>* has multiple components)

#### Cost improvement for the simplified algorithm:

Let the rollout policy under the simplified algorithm be  $\tilde{\pi} = {\tilde{\mu}_0, ..., \tilde{\mu}_{N-1}}$ , and let  $J_{k,\tilde{\pi}}(x_k)$  denote its cost starting from  $x_k$ . Then for all  $x_k$  and k,  $J_{k,\tilde{\pi}}(x_k) \leq H_k(x_k)$ .

Proof: The monotonicity property

 $H_0(x_0) = \text{Cost of } R_0 \geq \cdots \geq \text{Cost of } R_k \geq \text{Cost of } R_{k+1} \geq \cdots \geq \text{Cost of } R_N = J_{0,\tilde{\pi}}(x_0)$ 

is maintained

#### Rollout with Superheuristic/Multiple Heuristics

#### Consider combining several heuristics in the context of rollout

- The idea is to construct a superheuristic, which runs all the heuristics at each state encountered, and selects the best out of the trajectories produced
- The superheuristic can be viewed as the base heuristic for a rollout algorithm
- It can be verified using the definitions, that if all the heuristics are sequentially improving, the same is true for the superheuristic

Proof: Write the sequential improvement condition for each of the *M* heuristics

$$\min_{u_k\in U_k(x_k)}\tilde{Q}_k^m(x_k,u_k)\leq H_k^m(x_k), \qquad m=1,\ldots,M,$$

and all  $x_k$  and k, where  $\tilde{Q}_k^m(x_k, u_k)$  and  $H_k^m(x_k)$  are Q-factors and heuristic costs that correspond to the *m*th heuristic. By taking minimum over *m*, and interchanging the order of the minimization min<sub>*m*=1,...,*M*</sub> min<sub>*u*\_k \in U\_k(x\_k)</sub>,

$$\min_{u_k \in U_k(x_k)} \min_{\substack{m=1,...,M\\ \text{Superheuristic Q-factor}}} \tilde{Q}_k^m(x_k, u_k) \le \min_{\substack{m=1,...,M\\ \text{Superheuristic cost}}} H_k^m(x_k),$$

which is the sequential improvement condition for the superheuristic.

# A Counterexample to Cost Improvement (w/out Sequential Improvement Condition)



- Suppose at  $x_0$  there is a unique optimal trajectory  $(x_0, u_0^*, x_1^*, u_1^*, x_2^*)$ .
- Suppose the base heuristic produces this optimal trajectory starting at *x*<sub>0</sub>.
- Rollout uses the base heuristic to construct a trajectory starting from x<sub>1</sub><sup>\*</sup> and x<sub>1</sub>.
- Suppose the heuristic's trajectory starting from  $x_1^*$  is "bad" (has high cost).
- Then (Q-factor of u<sub>0</sub><sup>\*</sup>)>(Q-factor of ũ<sub>0</sub>). So the rollout algorithm selects ũ<sub>0</sub>, and moves to a nonoptimal next state x<sub>1</sub> = f<sub>0</sub>(x<sub>0</sub>, ũ<sub>0</sub>).
- So in the absence of sequential improvement, the rollout can deviate from an already available good "current" trajectory.
- This suggests a possible remedy: Follow the best "current" trajectory found even if rollout suggests following a different (but inferior) trajectory.

# Fortified Rollout: Restores Cost Improvement for Base Heuristics that are not Sequentially Improving



Idea: At each step, follow the best trajectory computed thus far

• At state  $x_k$ : In addition to the permanent rollout trajectory  $\overline{P}_k = \{x_0, u_0, \dots, u_{k-1}, x_k\}$ , also store a tentative best trajectory

$$\overline{T}_k = \{x_0, \ldots, x_k, \overline{u}_k, \overline{x}_{k+1}, \overline{u}_{k+1}, \ldots, \overline{u}_{N-1}, \overline{x}_N\}$$

 $\overline{T}_k$  is the best end-to-end trajectory computed up to stage k

• We reject the minimum Q-factor choice  $\tilde{u}_k$  if its complete trajectory is more costly than the current tentative best; otherwise we accept  $\tilde{u}_k$ , and update the tentative best trajectory.

# Illustration of Fortified Algorithm



- At x<sub>0</sub>, the fortified rollout stores as initial tentative best trajectory the unique optimal trajectory (x<sub>0</sub>, u<sub>0</sub><sup>\*</sup>, x<sub>1</sub><sup>\*</sup>, u<sub>1</sub><sup>\*</sup>, x<sub>2</sub><sup>\*</sup>) generated by the base heuristic.
- In the first rollout step, it computes the Q-factors of u<sub>0</sub><sup>\*</sup> and ũ<sub>0</sub> by running the heuristic from x<sub>1</sub><sup>\*</sup> and x<sub>1</sub>.
- Even though the rollout prefers u
  <sub>0</sub> to u
  <sub>0</sub><sup>\*</sup>, it discards u
  <sub>0</sub> in favor of u
  <sub>0</sub><sup>\*</sup>, which is dictated by the tentative best trajectory.
- It then sets the permanent trajectory to (x<sub>0</sub>, u<sub>0</sub><sup>\*</sup>, x<sub>1</sub><sup>\*</sup>) and keeps the tentative best trajectory unchanged to (x<sub>0</sub>, u<sub>0</sub><sup>\*</sup>, x<sub>1</sub><sup>\*</sup>, u<sub>1</sub><sup>\*</sup>, x<sub>2</sub><sup>\*</sup>).

# Model-Free Rollout with an Expert for the General Discrete Optimization $\min_{u_0 \in U_0,...,u_{N-1} \in U_{N-1}} G(u_0,...,u_{N-1})$



- Assume we do not know G, and/or the constraint sets U<sub>k</sub>
- Instead we have a base heuristic, which given a partial solution (u<sub>0</sub>,..., u<sub>k</sub>), outputs all next controls ũ<sub>k+1</sub>, and generates from each a complete solution

$$S_k(u_0,\ldots,u_k,\tilde{u}_{k+1})=(u_0,\ldots,u_k,\tilde{u}_{k+1},\ldots,\tilde{u}_{N-1})$$

- Also, we have a human or software "expert" that can rank any two complete solutions without assigning numerical values to them.
- Deterministic rollout can be applied to this problem; we have all we need.

#### A Working Break with a Challenge Question



#### Consider deterministic rollout with multistep lookahead

- How would the rollout algorithm work?
- What is the main computational difficulty in applying multistep rollout?

# Stochastic Rollout with MC Simulation: Multistep Approximation in Value Space with $\tilde{J}_{k+\ell}(x_{k+\ell})$ the Cost Function of Some Policy



Consider the pure case (no truncation, no terminal cost approximation)

- Assume that the base heuristic is a legitimate policy  $\pi = {\mu_0, ..., \mu_{N-1}}$  (i.e., is sequentially consistent, in the context of deterministic problems)
- Let  $\tilde{\pi} = {\{\tilde{\mu}_0, \dots, \tilde{\mu}_{N-1}\}}$  be the rollout policy. Then cost improvement is obtained

 $J_{k,\tilde{\pi}}(x_k) \leq J_{k,\pi}(x_k),$  for all  $x_k$  and k

- A simple induction proof
- The big issue: How do we save in simulation effort?

# Backgammon Example of Rollout (Tesauro, 1996)



- Truncated rollout with cost function approximation provided by TD-Gammon (a 1992 program, involving a neural network trained by a form of approximate policy iteration that uses "Temporal Differences").
- The truncated rollout program (1996) plays better than TD-Gammon, and better than any human.
- It is slow due to excessive Monte Carlo simulation time.

# We assumed equal effort for evaluation of Q-factors of all controls at a state $x_k$

Drawbacks:

- Some controls may be clearly inferior to others and may not be worth as much sampling effort.
- Some controls that appear to be promising may be worth exploring better through multistep lookahead.

#### Monte Carlo tree search (MCTS) is a "randomized" form of lookahead

- MCTS involves adaptive simulation (simulation effort adapted to the perceived quality of different controls).
- Aims to balance exploitation (extra simulation effort on controls that look promising) and exploration (adequate exploration of the potential of all controls).
- MCTS does not directly improve performance; it just tries to save in simulation effort.

#### Monte Carlo Tree Search - Adaptive Simulation



MCTS provides an economical sampling policy to estimate the Q-factors

$$ilde{Q}_k(x_k,u_k) = E\Big\{g_k(x_k,u_k,w_k) + ilde{J}_{k+1}(f_k(x_k,u_k,w_k))\Big\}, \quad u_k \in U_k(x_k)$$

#### Assume that $U_k(x_k)$ contains a finite number of elements, say u = 1, ..., m

- After the *n*th sampling period we have Q<sub>u,n</sub>, the empirical mean of the Q-factor of each control u (total sample value divided by total number of samples corresponding to u). We view Q<sub>u,n</sub> as an exploitation index.
- How do we use the estimates  $Q_{u,n}$  to select the control to sample next?

## MCTS Based on Statistical Tests



MCTS balances exploitation (sample controls that seem most promising, i.e., a small  $Q_{u,n}$ ) and exploration (sample controls with small sample count).

- A popular strategy: Sample next the control *u* that minimizes the sum  $Q_{u,n} + R_{u,n}$  where  $R_{u,n}$  is an exploration index.
- $R_{u,n}$  is based on a confidence interval formula and depends on the sample count  $S_u$  of control u (which comes from analysis of multiarmed bandit problems).
- The UCB rule (upper confidence bound) sets  $R_{u,n} = -c\sqrt{\log n/S_u}$ , where *c* is a positive constant, selected empirically (values  $c \approx \sqrt{2}$  are suggested, assuming that  $Q_{u,n}$  is normalized to take values in the range [-1, 0]).
- MCTS with UCB rule has been extended to multistep lookahead ... but AlphaZero has used a different (semi-heuristic) rule.

# Classical Control Problems - Infinite Control Spaces



# On-Line Rollout for Deterministic Infinite-Spaces Problems



#### Suppose the control space is infinite (so the number of Q-factors is infinite)

- One possibility is discretization of  $U_k(x_k)$ ; but excessive number of Q-factors.
- Another possibility is to use optimization heuristics that look  $(\ell 1)$  steps ahead.
- Seemlessly combine the *k*th stage minimization and the optimization heuristic into a single *l*-stage deterministic optimization.
- Can solve it by nonlinear programming/optimal control methods (e.g., quadratic programming, gradient-based). Constraints can be readily accommodated.
- This is the idea underlying model predictive control (MPC).

#### We will cover:

- Model predictive control; relation to rollout
- Rollout for multiagent problems

Homework to be announced next week

#### Watch videolecture 6 from the 2021 ASU course offerings