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

Arizona State University
Course CSE 691, Spring 2022

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

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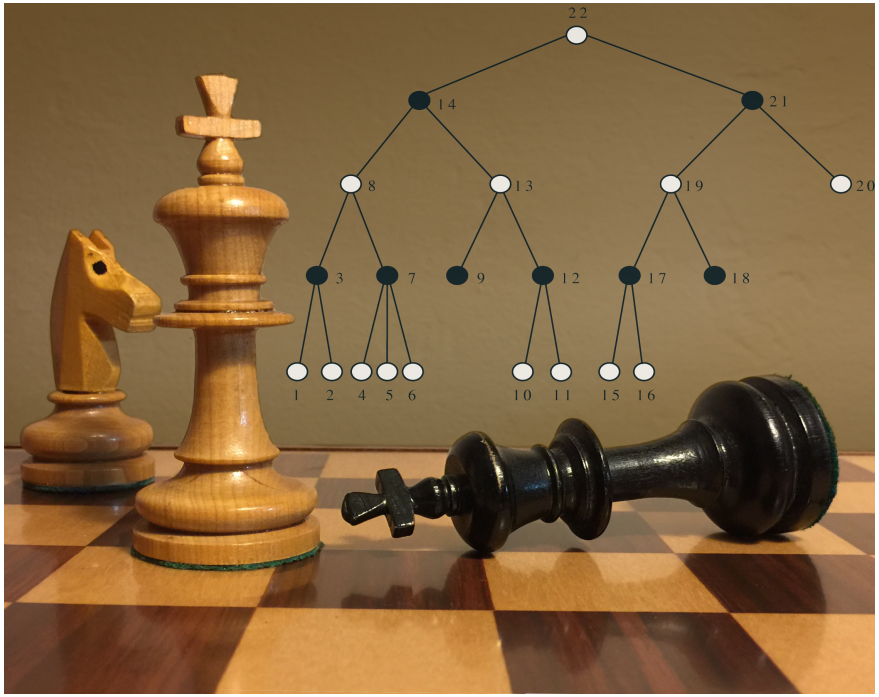
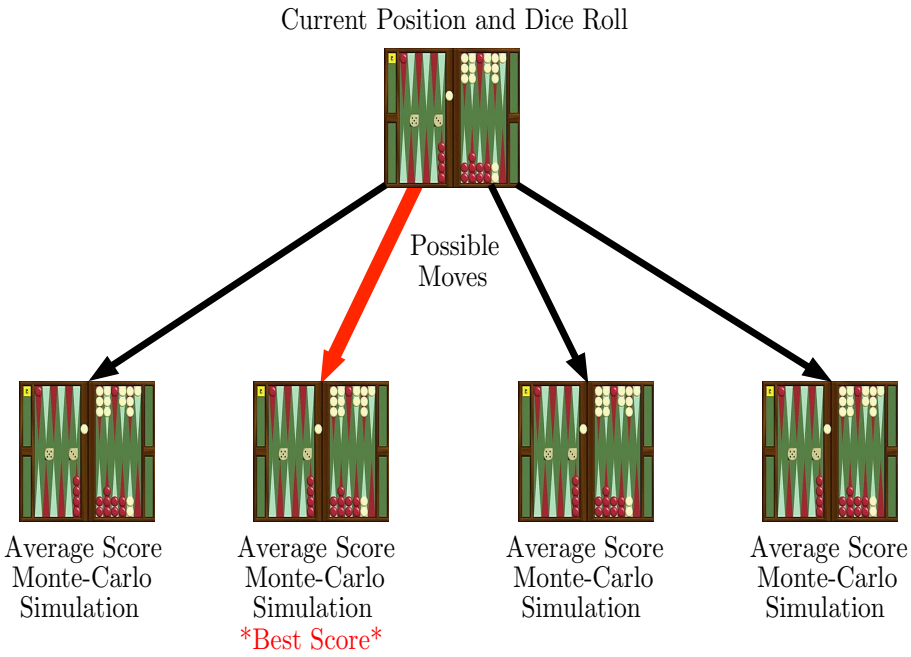
Lecture 1
Course Introduction and Overview

Outline

Chess and Backgammon - Off-Line Training and On-Line Play





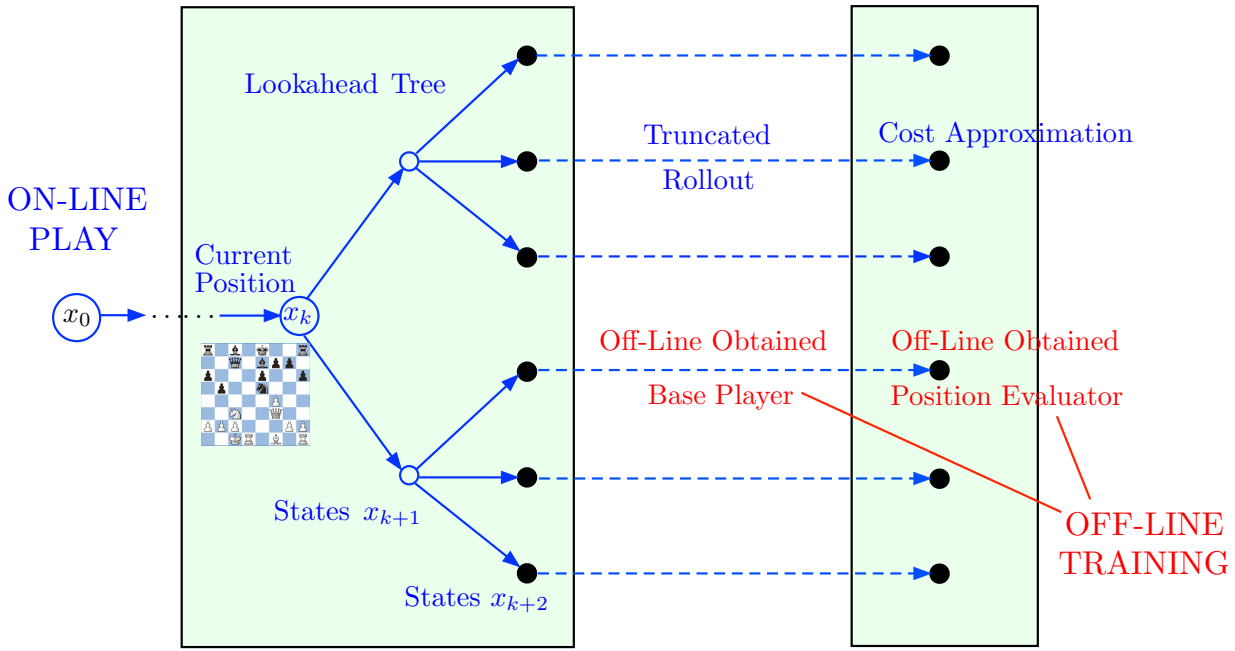
Both AlphaZero (2017) and TD-Gammon (1996) involve two algorithms:

- Off-line training of value and/or policy neural network approximations
- On-line play by multistep lookahead, rollout, and cost function approximation

Strong connections to DP, policy iteration, and RL-type methodology

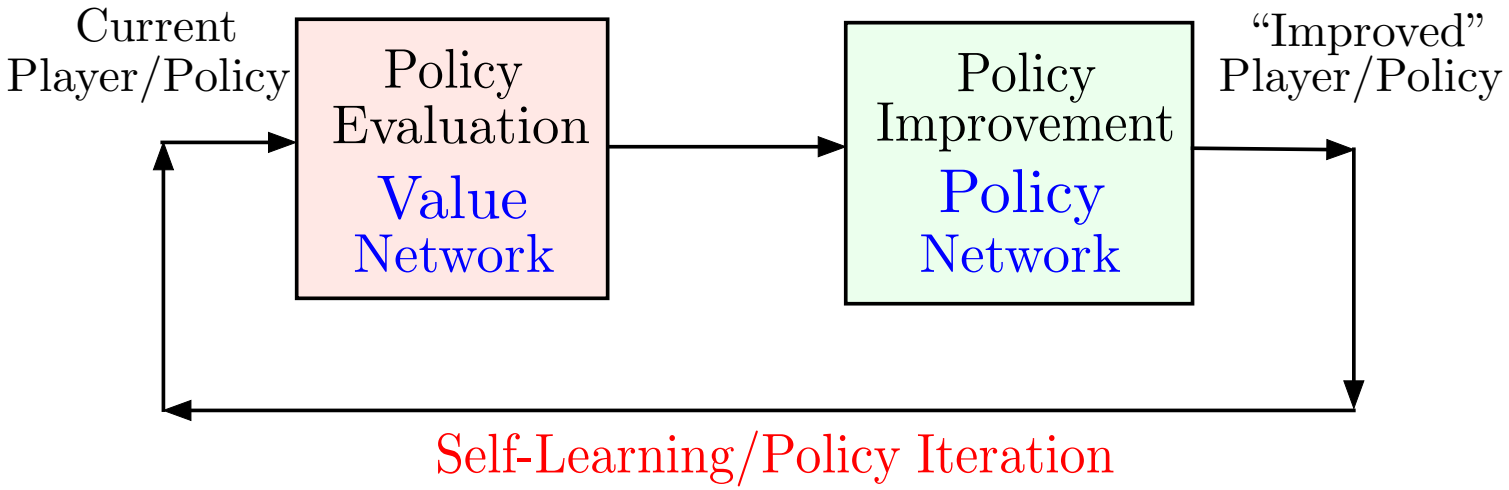
- We aim to understand this methodology, so it applies far more generally
- For example, in control system design (MPC and adaptive control), and discrete optimization by rollout

On-Line Play in AlphaZero/AlphaGo/TD-Gammon: Approximation in Value Space (Also Called “On-Line Tree Search")



- On-line play uses the results of off-line training, which are: A position evaluator and a base player
- It aims to improve the base player by:
  - Searching forward for several moves through the lookahead tree
  - Simulating the base player for some more moves at the tree leaves
  - Approximating the effect of future moves by using the terminal position evaluation
  - Calculating the “values" of the available moves at the root and playing the best move
- Similarities with Model Predictive Control (MPC) (which involves continuous spaces) and discrete optimization by rollout (which uses a heuristic as base player)

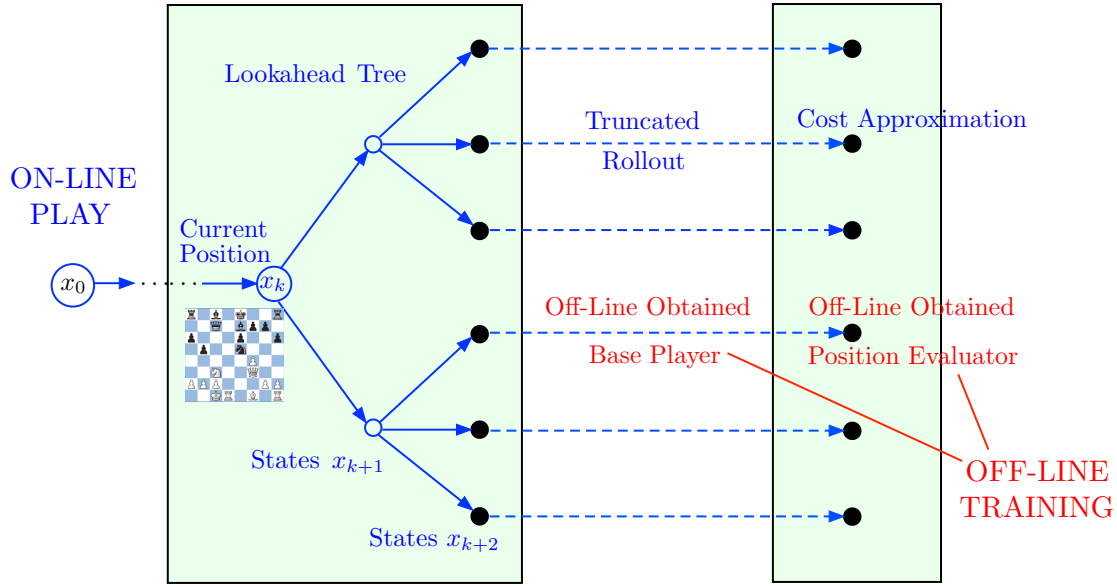
Off-Line Training in AlphaZero: Approximate Policy Iteration (PI) Using Self-Generated Data



- The current player is used to train an improved player, and the process is repeated
- The current player is "evaluated" by playing many games
- Its evaluation function is represented by a value neural net through training
- The current player is "improved" by using a form of approximate multistep lookahead minimization, called Monte-Carlo Tree Search (MCTS)
- The "improved player" is represented by a policy neural net through training
- TD-Gammon uses similar PI algorithm for off-line training of a value network (does not use MCTS and does not use a policy network)
- MPC and discrete optimization by rollout often use rudimentary forms of off-line training

A Major Empirical Observation

On-Line Play Improves on Off-Line Training



The AlphaZero on-line player plays much better than the off-line-trained player

TD-Gammon plays much better with truncated rollout than without rollout (Tesauro, 1996)

We will aim to explain these observations and use them within far more general contexts

Aims of the Course

Provide a unifying framework for several areas of large scale computation:

- Reinforcement learning (RL) as practiced by the AI community
- Approximate dynamic programming (DP) as practiced by parts of the optimization/OR community
- Model predictive and adaptive control as practiced by the control systems community
- Parts of discrete optimization as practiced by the algorithms/CS community

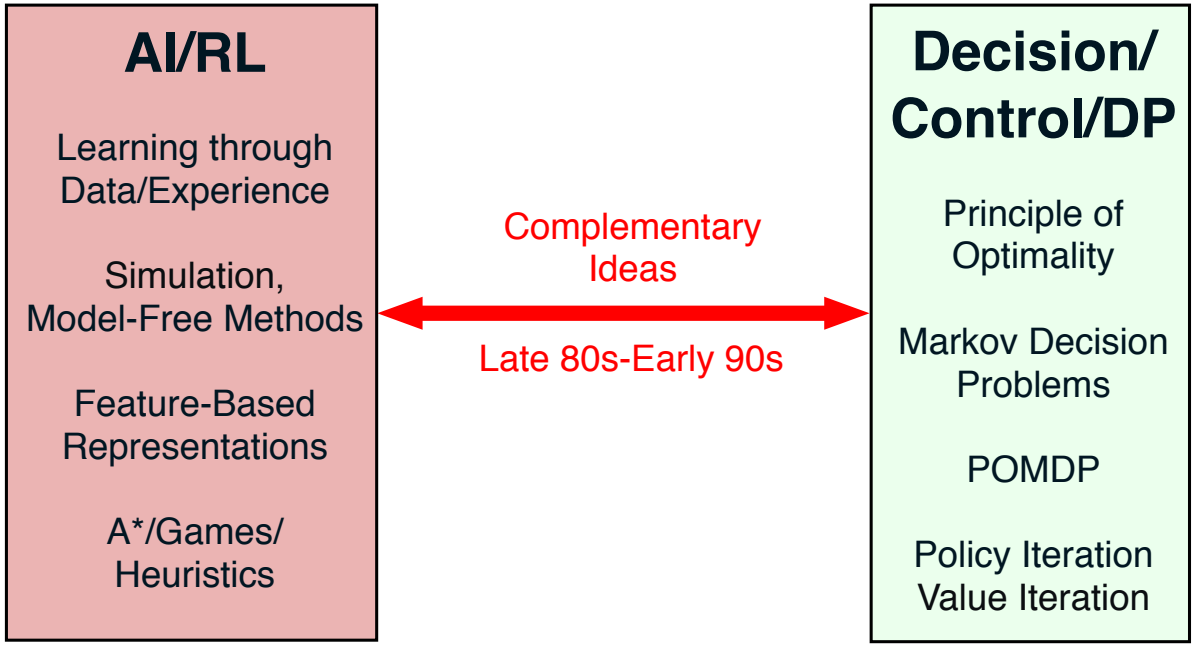
We rely on:

- The theory of exact, approximate, and abstract DP
- Intuitive visualization based on a Bellman operator formalism
- The paradigm of AlphaZero/TD-Gammon and similar design architectures
- Newton's method applied to Bellman's equation, which connects all of the above

We aim, through unification and abstraction, to:

- Bridge the gap between cultures of different communities
- Bring to bear the power of RL to a very broad range of applications

Evolution of Approximate DP/RL: A Fruitful Synergy



Historical highlights

- Exact DP, optimal control (Bellman, Shannon, and others 1950s ...)
- AI/RL and Decision/Control/DP ideas meet (late 80s-early 90s)
- First major successes: Backgammon programs (Tesauro, 1992, 1996)
- Algorithmic progress, analysis, applications, first books (mid 90s ...)
- Machine Learning, BIG Data, Robotics, Deep Neural Networks (mid 2000s ...)
- AlphaGo and AlphaZero (DeepMind, 2016, 2017)

Approximate DP/RL Methodology is now Ambitious and Universal

Exact DP applies (in principle) to a very broad range of optimization problems

- Deterministic <—-> Stochastic
- Combinatorial optimization <—-> Optimal control w/ infinite state/control spaces
- One decision maker <—-> Two player games
- ... BUT is plagued by the curse of dimensionality and need for a math model

Approximate DP/RL overcomes the difficulties of exact DP by:

- Approximation (use neural nets and other architectures to reduce dimension)
- Simulation (use a computer model in place of a math model)

State of the art:

- Broadly applicable methodology: Can address a very broad range of challenging problems. Deterministic-stochastic-dynamic, discrete-continuous, games, etc
- There are no methods that are guaranteed to work for all or even most problems
- There are enough methods to try with a reasonable chance of success for most types of optimization problems
- Role of the theory: Structure mathematically the methodology, guide the art, delineate the sound ideas

A Relevant Quotation from 25 Years Ago

From preface of Neuro-Dynamic Programming, Bertsekas and Tsitsiklis, 1996

A few years ago our curiosity was aroused by reports on new methods in reinforcement learning, a field that was developed primarily within the artificial intelligence community, starting a few decades ago. These methods were aiming to provide effective suboptimal solutions to complex problems of planning and sequential decision making under uncertainty, that for a long time were thought to be intractable.

Our first impression was that the new methods were ambitious, overly optimistic, and lacked firm foundation. Yet there were claims of impressive successes and indications of a solid core to the modern developments in reinforcement learning, suggesting that the correct approach to their understanding was through dynamic programming.

Three years later, after a lot of study, analysis, and experimentation, we believe that our initial impressions were largely correct. This is indeed an ambitious, often ad hoc, methodology, but for reasons that we now understand much better, it does have the potential of success with important and challenging problems.

This assessment still holds true!

References of this Course

This course is research-oriented. It aims:

- To explore the state of the art of approximate DP/RL at a graduate level
- To explore in depth some special research topics (rollout, policy iteration)
- To provide the opportunity for you to explore research in the area

Main references:

- Bertsekas, Reinforcement Learning and Optimal Control, 2019
- Bertsekas, Rollout, Policy Iteration, and Distributed Reinforcement Learning, 2020
- Bertsekas, Lessons from AlphaZero for Optimal, Model Predictive, and Adaptive Control, 2022
- Bertsekas: Class notes based on the above, and focused on our special RL topics.
- Slides, papers, and videos from the 2019-2021 ASU courses; check my web site

Supplementary references

- Exact DP: Bertsekas, Dynamic Programming and Optimal Control, Vol. I (2017), Vol. II (2012) (also contains approximate DP material), Abstract DP (2022)
- Bertsekas and Tsitsiklis, Neuro-Dynamic Programming, 1996
- Sutton and Barto, 1998, Reinforcement Learning (new edition 2018, on-line)

Terminology in RL/AI and DP/Control

RL uses Max/Value, DP uses Min/Cost

- Reward of a stage = (Opposite of) Cost of a stage.
- State value = (Opposite of) State cost.
- Value (or state-value) function = (Opposite of) Cost function.

Controlled system terminology

- Agent = Decision maker or controller.
- Action = Decision or control.
- Environment = Dynamic system.

Methods terminology

- Learning = Solving a DP-related problem using simulation.
- Self-learning (or self-play in the context of games) = Solving a DP problem using simulation-based policy iteration.
- Planning vs Learning distinction = Solving a DP problem with model-based vs model-free simulation.

Notation in RL/AI and DP/Control

- Reinforcement learning uses transition probability notation

$$p(s, a, s')$$

(s, s' are states, a is action), which is standard in finite-state problems (MDP)

- Control theory uses discrete-time system equation

$$x_{k+1} = f(x_k, u_k, w_k)$$

which is standard in continuous spaces problems

- Operations research uses both notations [typically $p_{ij}(u)$ for transition probabilities]

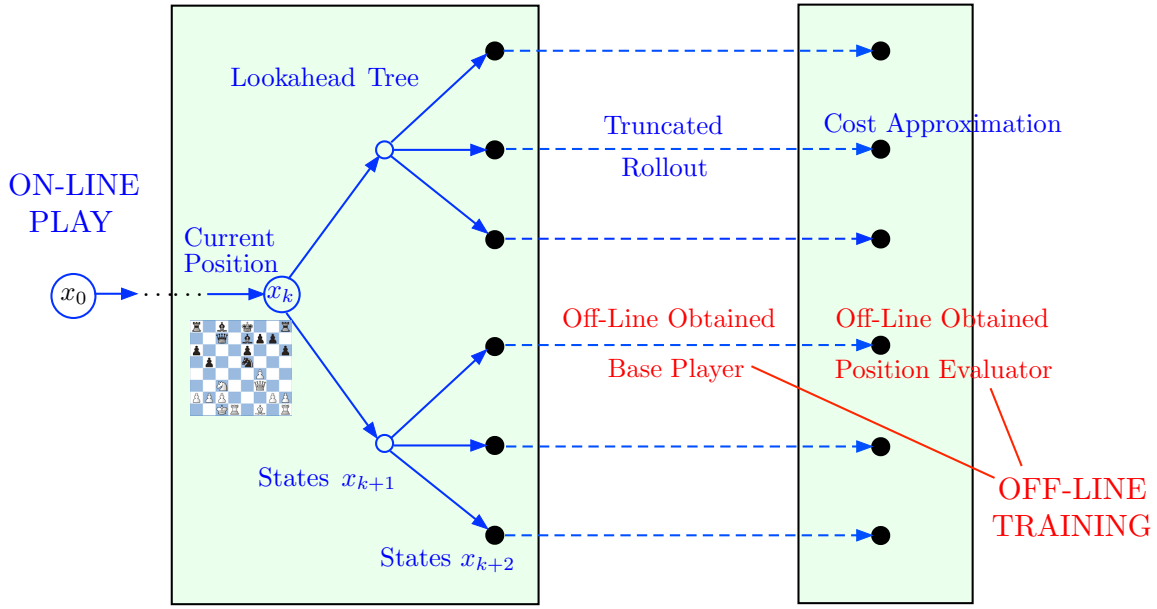
These two notational systems are mathematically equivalent but:

- Transition probabilities are cumbersome for deterministic problems and continuous spaces problems
- System equations are cumbersome for finite-state problems

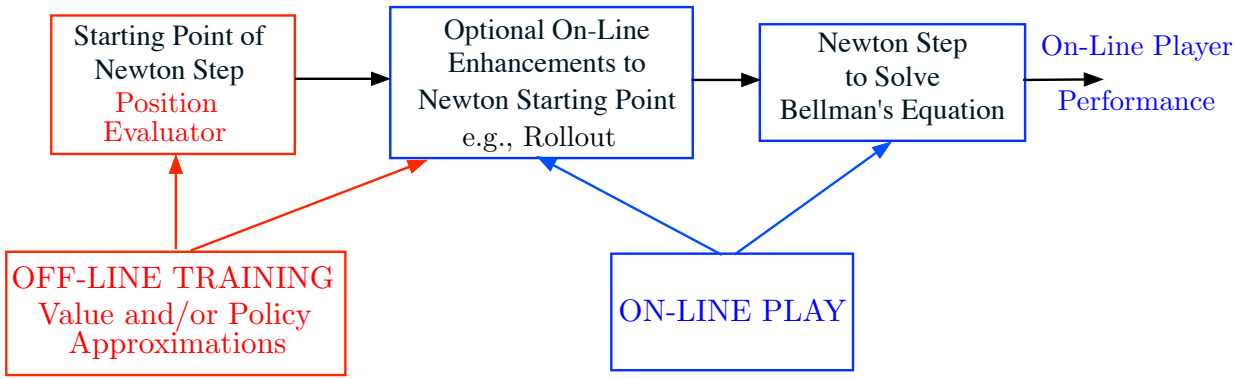
We use both notational systems:

- For the first 3/4 of the course we use system equations
- For the last 1/4 of the course we use transition probabilities

A Mathematical View: Newton Step to Solve Bellman's Equation



NEWTON STEP INTERPRETATION

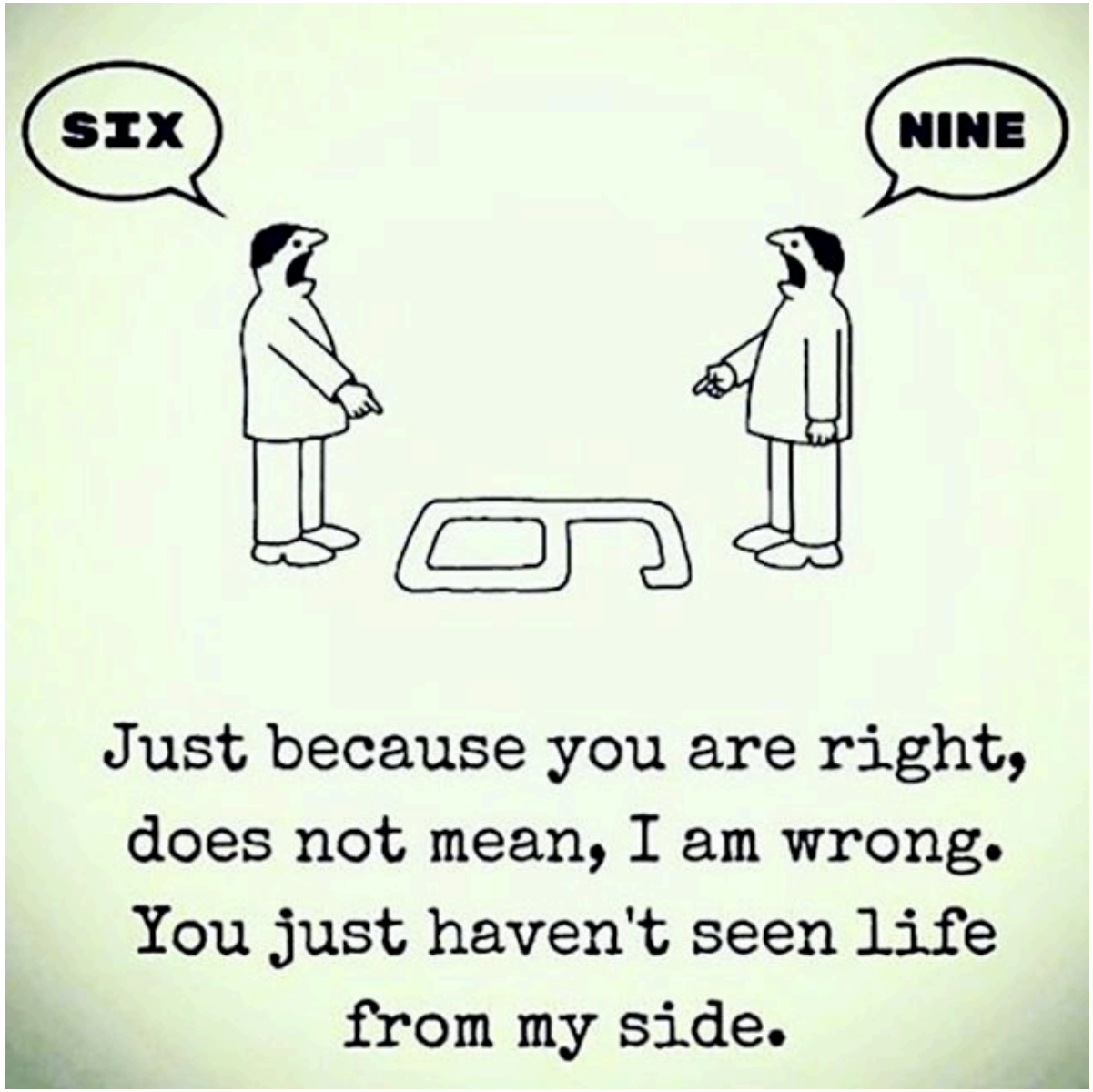


Explains why the AlphaZero on-line player is better than the off-line trained player

Our Principal Viewpoints

- On-line play is a step of Newton's method for solving the Bellman equation (the central DP equation that yields the optimal cost function)
- Off-line training provides the start point for the Newton step (a hot start)
- On-line play is the real workhorse ... off-line training plays a secondary role. A major reason: On-line play is an exact Newton step. It is not degraded by NN approximations
- Imperfections/differences in off-line training affect the start point, but are washed out by the (powerful) Newton step. (A hot algorithm within its "sweet spot" does not need a hot start.)
- A cultural difference that we will aim to bridge:
  - Reinforcement Learning/AI research is focused largely on off-line training issues (except in the special case of armed bandit problems)
  - Model Predictive and Adaptive Control research is focused largely on on-line play and stability issues
- Discrete optimization by rollout is also an exact Newton step
- All of this applies in great generality through the power of abstract DP (arbitrary state and control spaces, stochastic, deterministic, hybrid systems, multiagent systems, minimax, finite and infinite horizon, discrete optimization)

On Viewpoints and Objective Truth



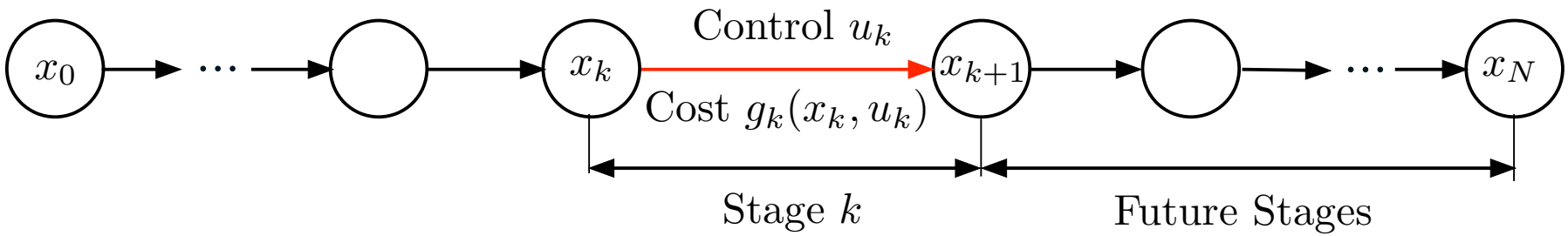
A Fifteen-Minute Break

All our lectures will have a 15-minute break, somewhere in the middle

Catch our breath and think about issues relating to the first half of the lecture.

A short discussion/questions/answers period will follow each break.

Finite Horizon Deterministic Problem



- System

$$x_{k+1} = f_k(x_k, u_k), \qquad k = 0, 1, \ldots, N-1$$

where x_k: State, u_k: Control chosen from some set $U_k(x_k)$

- Cost function:

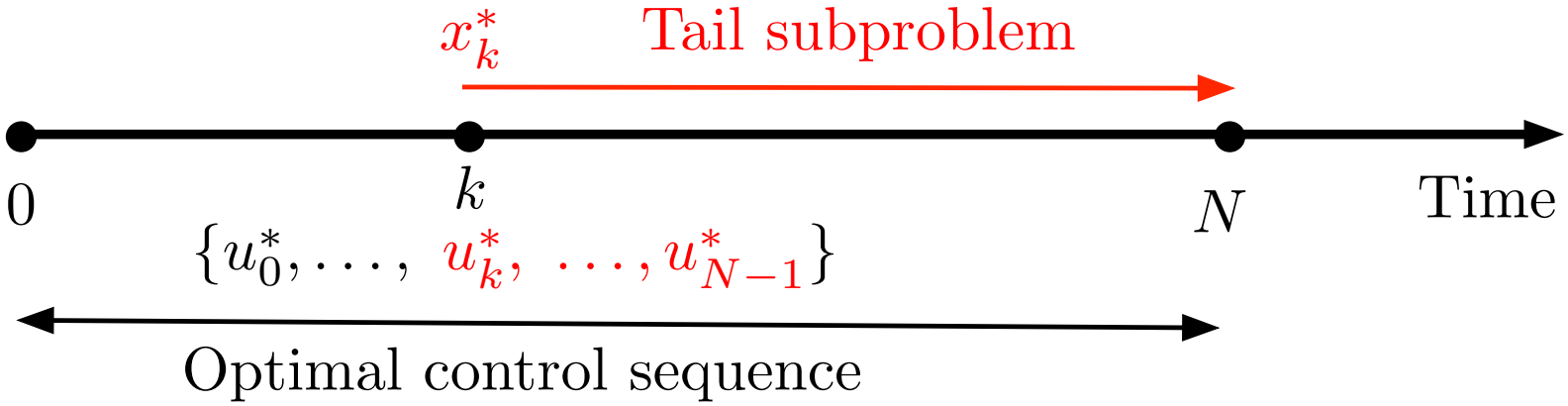
$$g_N(x_N) + \sum_{k=0}^{N-1} g_k(x_k, u_k)$$

- For given initial state x_0, minimize over control sequences $\{u_0, \ldots, u_{N-1}\}$

$$J(x_0; u_0, \ldots, u_{N-1}) = g_N(x_N) + \sum_{k=0}^{N-1} g_k(x_k, u_k)$$

- Optimal cost function $J^*(x_0) = \min_{\substack{u_k \in U_k(x_k) \\ k=0,\ldots,N-1}} J(x_0; u_0, \ldots, u_{N-1})$

Principle of Optimality: A Very Simple Idea



Principle of Optimality

THE TAIL OF AN OPTIMAL SEQUENCE IS OPTIMAL FOR THE TAIL SUBPROBLEM

Let $\{u_0^*, \ldots, u_{N-1}^*\}$ be an optimal control sequence with corresponding state sequence $\{x_1^*, \ldots, x_N^*\}$. Consider the tail subproblem that starts at x_k^* at time k and minimizes over $\{u_k, \ldots, u_{N-1}\}$ the "cost-to-go" from k to N,

$$g_k(x_k^*, u_k) + \sum_{m=k+1}^{N-1} g_m(x_m, u_m) + g_N(x_N).$$

Then the tail optimal control sequence $\{u_k^*, \ldots, u_{N-1}^*\}$ is optimal for the tail subproblem.

DP Algorithm: Solves All Tail Subproblems Using the Principle of Optimality

Idea of the DP algorithm

Solve all the tail subproblems of a given time length using the solution of all the tail subproblems of shorter time length

By the principle of optimality: To solve the tail subproblem that starts at x_k

- Consider every possible u_k and solve the tail subproblem that starts at next state $x_{k+1} = f_k(x_k, u_k)$. This gives the "cost of u_k"
- Optimize over all possible u_k

DP Algorithm: Produces the optimal costs $J_k^*(x_k)$ of the x_k-tail subproblems

Start with

$$J_N^*(x_N) = g_N(x_N), \qquad \text{for all } x_N,$$

and for $k = 0, \ldots, N-1$, let

$$J_k^*(x_k) = \min_{u_k \in U_k(x_k)} \Big[g_k(x_k, u_k) + J_{k+1}^*\big(f_k(x_k, u_k)\big) \Big], \qquad \text{for all } x_k.$$

The optimal cost $J^*(x_0)$ is obtained at the last step: $J_0(x_0) = J^*(x_0)$.

Construction of Optimal Control Sequence $\{u_0^*, \ldots, u_{N-1}^*\}$

Start with

$$u_0^* \in \arg \min_{u_0 \in U_0(x_0)} \Big[g_0(x_0, u_0) + J_1^* \big(f_0(x_0, u_0) \big) \Big]$$

This takes you to

$$x_1^* = f_0(x_0, u_0^*).$$

Sequentially, going forward, for $k = 1, 2, \ldots, N-1$, set

$$u_k^* \in \arg \min_{u_k \in U_k(x_k^*)} \Big[g_k(x_k^*, u_k) + J_{k+1}^* \big(f_k(x_k^*, u_k) \big) \Big], \qquad x_{k+1}^* = f_k(x_k^*, u_k^*).$$

Approximation in Value Space - Use Some $\tilde{J}_k$ in Place of J_k^* (off-line training)

Start with

$$\tilde{u}_0 \in \arg \min_{u_0 \in U_0(x_0)} \Big[g_0(x_0, u_0) + \tilde{J}_1 \big(f_0(x_0, u_0) \big) \Big]$$

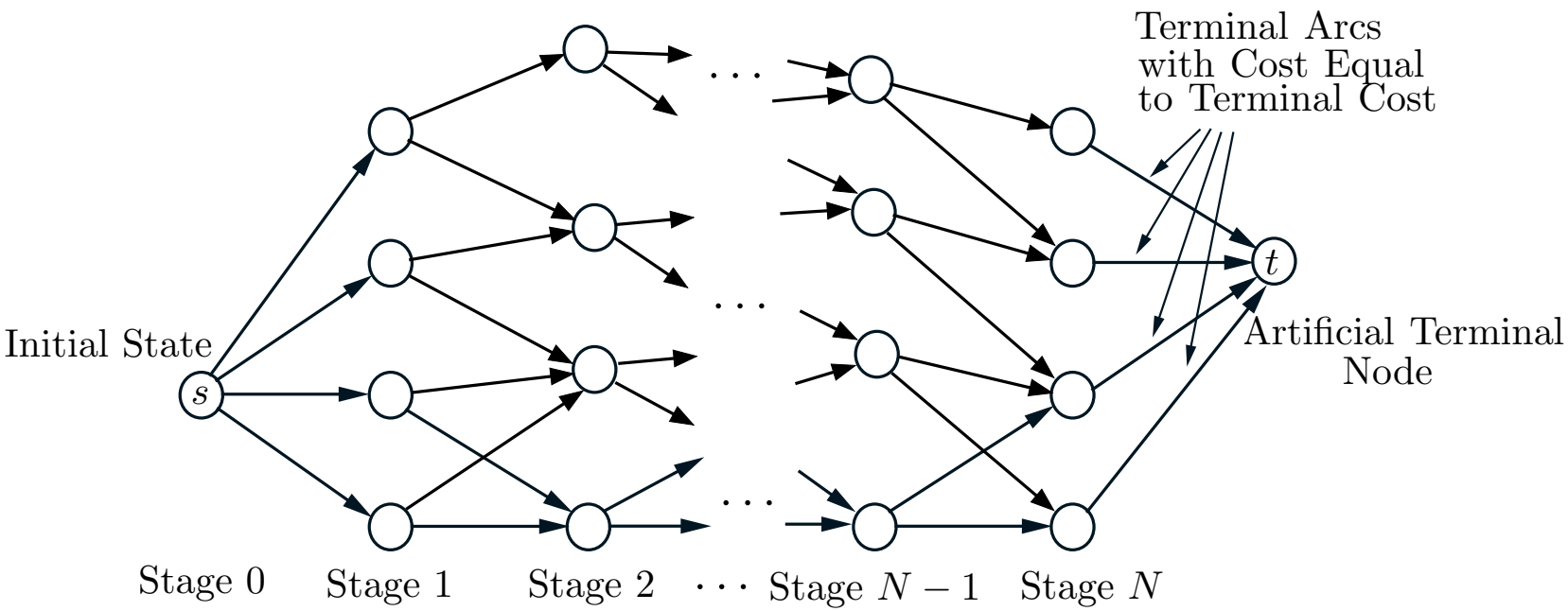
This takes you to

$$\tilde{x}_1 = f_0(x_0, \tilde{u}_0).$$

Sequentially, going forward, for $k = 1, 2, \ldots, N-1$, set (on-line play)

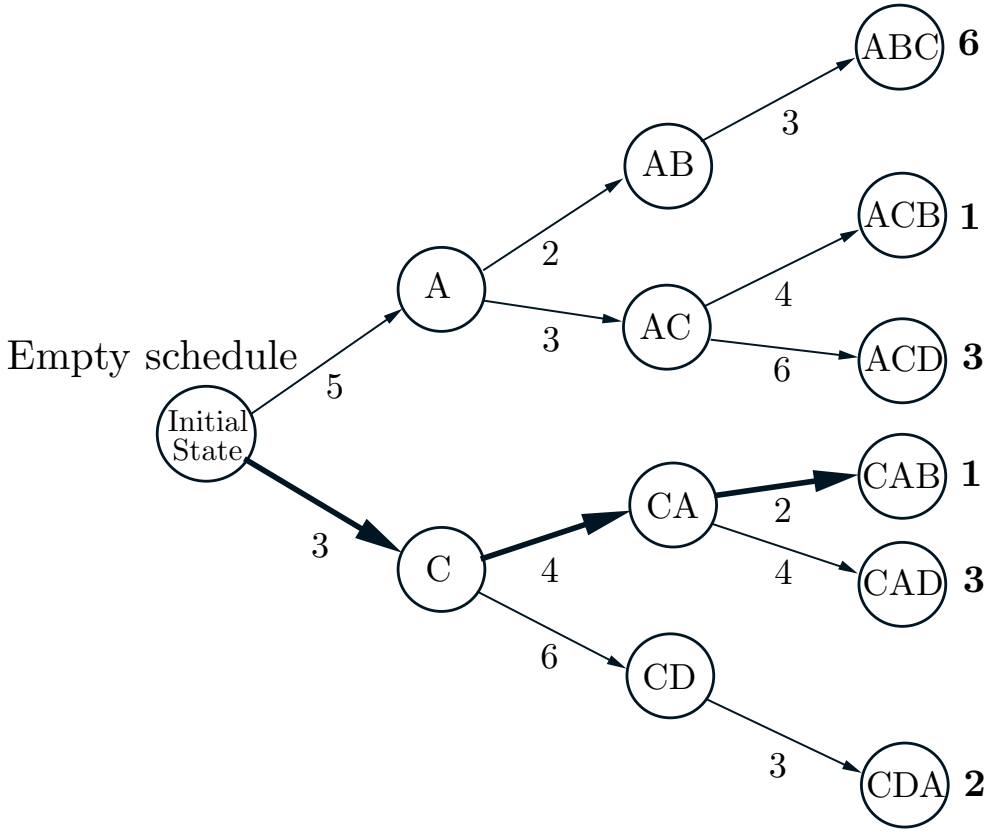
$$\tilde{u}_k \in \arg \min_{u_k \in U_k(\tilde{x}_k)} \Big[g_k(\tilde{x}_k, u_k) + \tilde{J}_{k+1} \big(f_k(\tilde{x}_k, u_k) \big) \Big], \qquad \tilde{x}_{k+1} = f_k(\tilde{x}_k, \tilde{u}_k).$$

Finite-State Problems: Shortest Path View



- Nodes correspond to states x_k
- Arcs correspond to state-control pairs (x_k, u_k)
- An arc (x_k, u_k) has start and end nodes x_k and $x_{k+1} = f_k(x_k, u_k)$
- An arc (x_k, u_k) has a cost $g_k(x_k, u_k)$. The cost to optimize is the sum of the arc costs from the initial node s to the terminal node t.
- The problem is equivalent to finding a minimum cost/shortest path from s to t.

Discrete-State Deterministic Scheduling Example

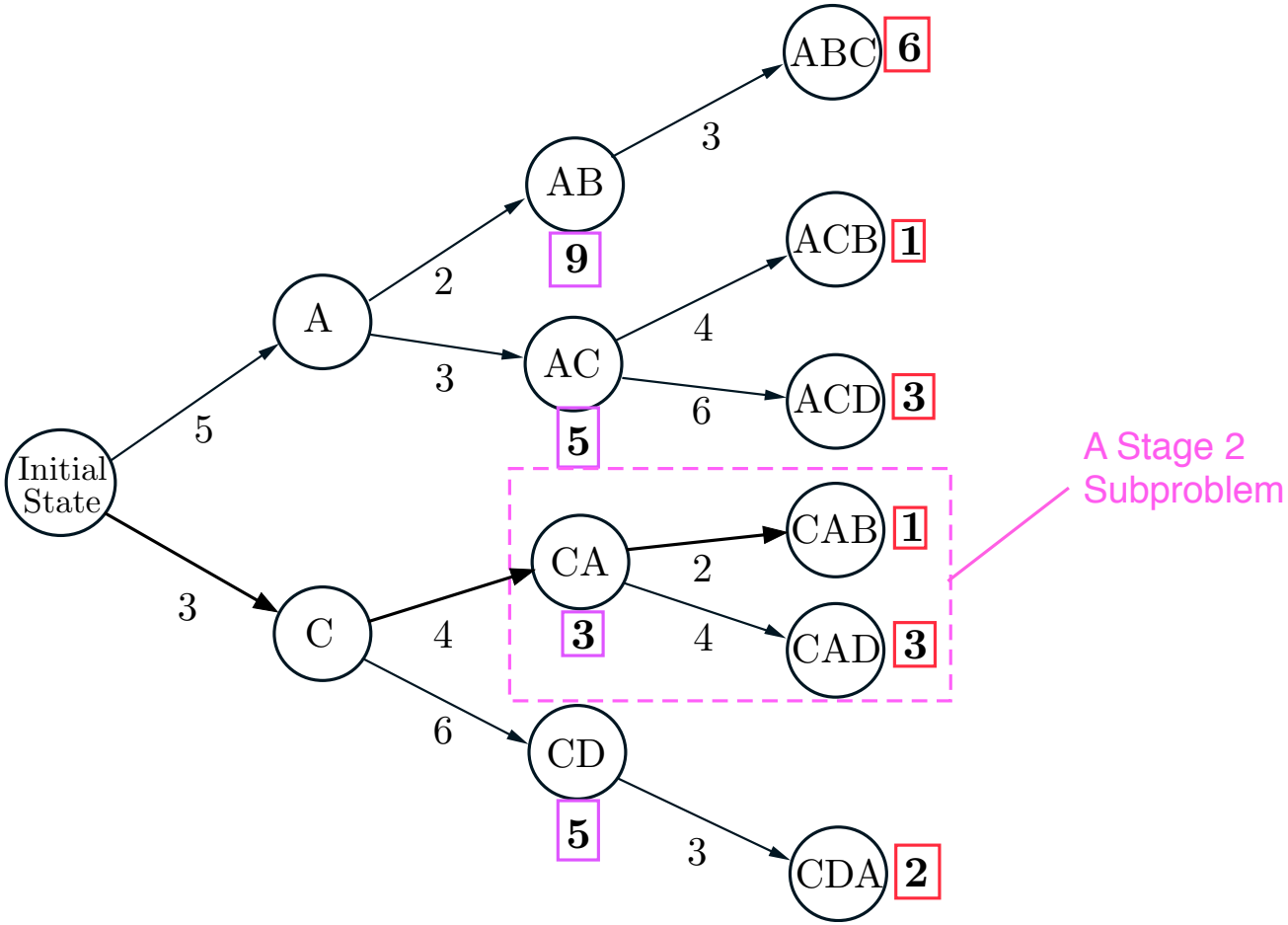


Find optimal sequence of operations A, B, C, D (A must precede B and C must precede D)

DP Problem Formulation

- States: Partial schedules; Controls: Stage 0, 1, and 2 decisions; Cost data shown along the arcs
- Recall the DP idea: Break down the problem into smaller pieces (tail subproblems)
- Start from the last decision and go backwards

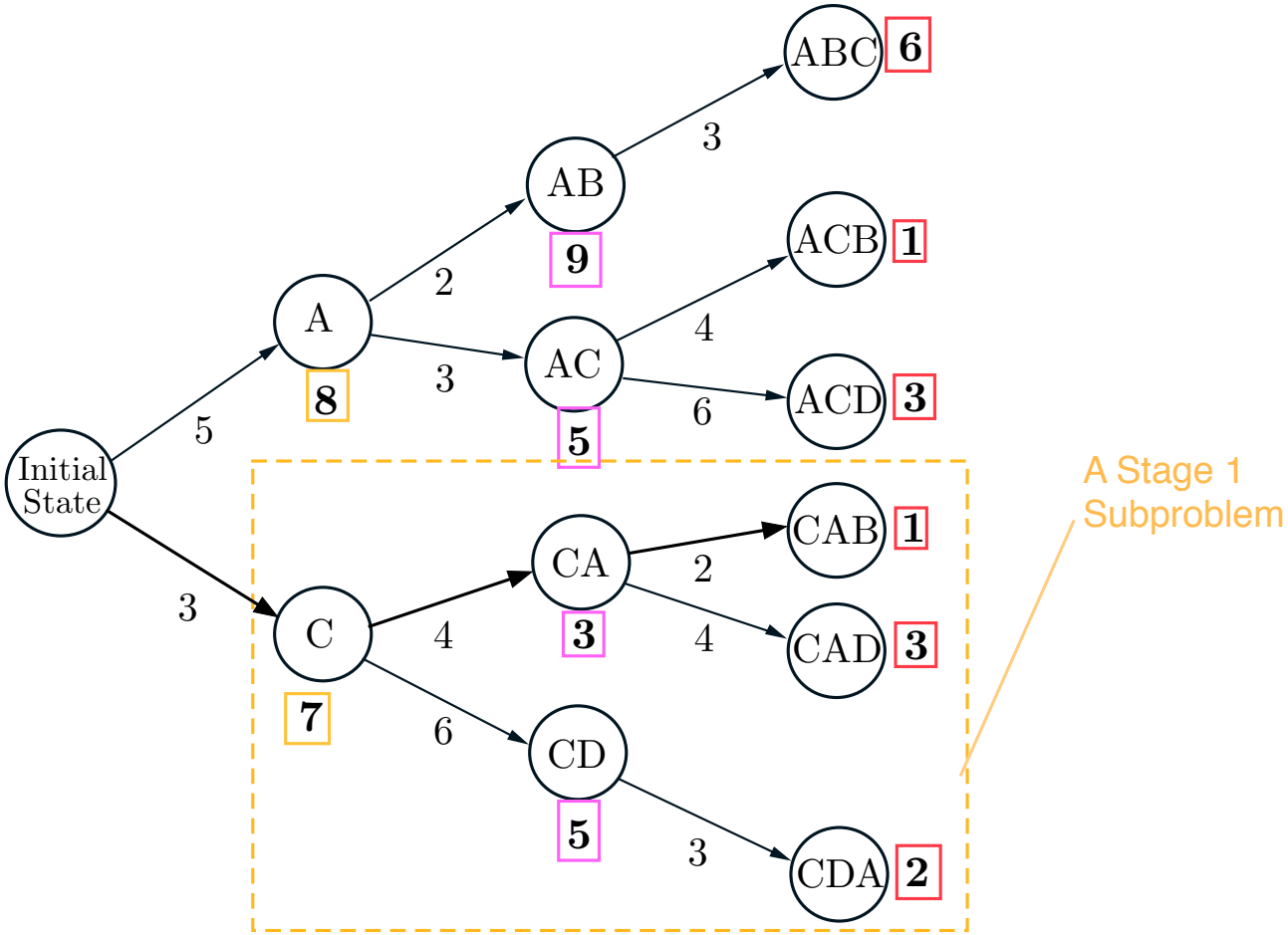
DP Algorithm: Stage 2 Tail Subproblems



Solve the stage 2 subproblems (using the terminal costs - in red)

At each state of stage 2, we record the optimal cost-to-go and the optimal decision

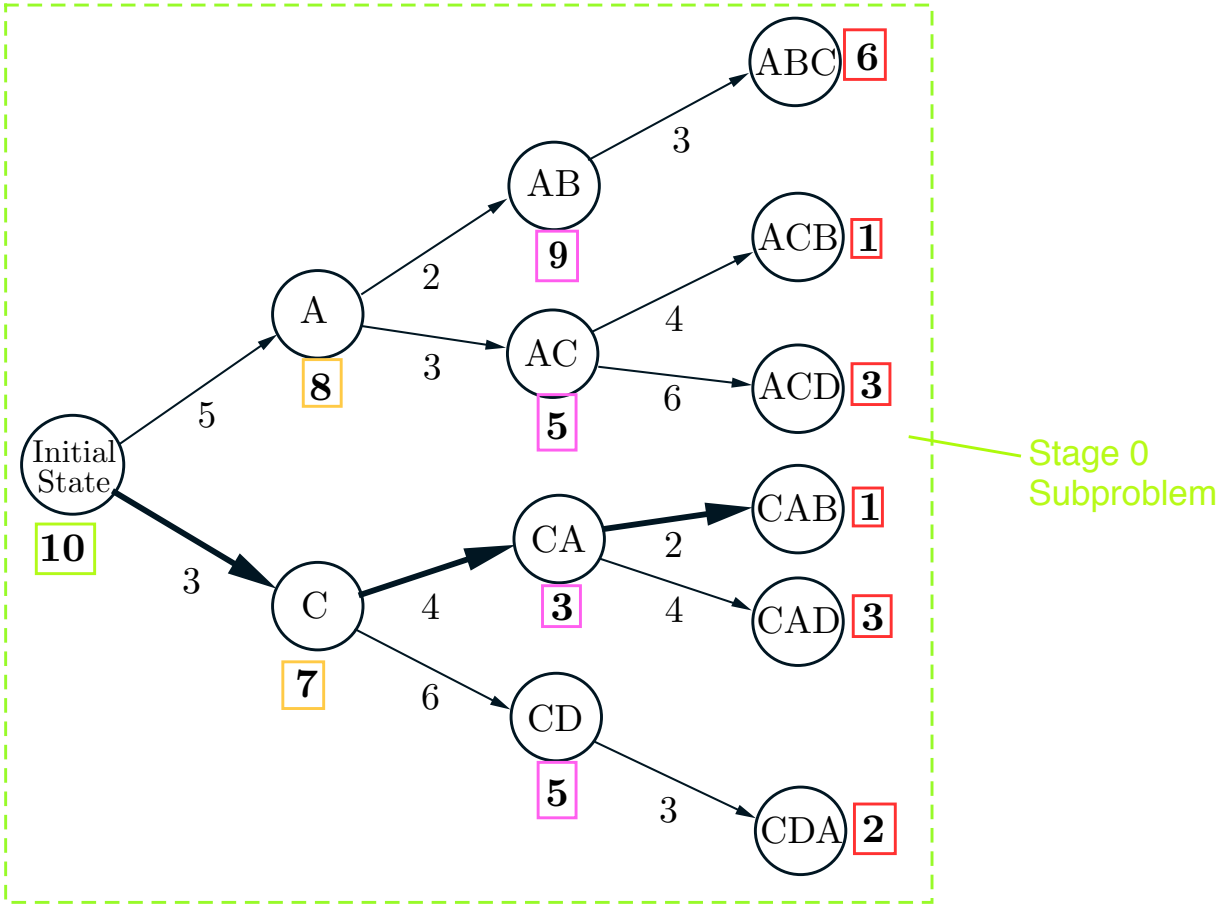
DP Algorithm: Stage 1 Tail Subproblems



Solve the stage 1 subproblems (using the optimal costs of stage 2 subproblems - in purple)

At each state of stage 1, we record the optimal cost-to-go and the optimal decision

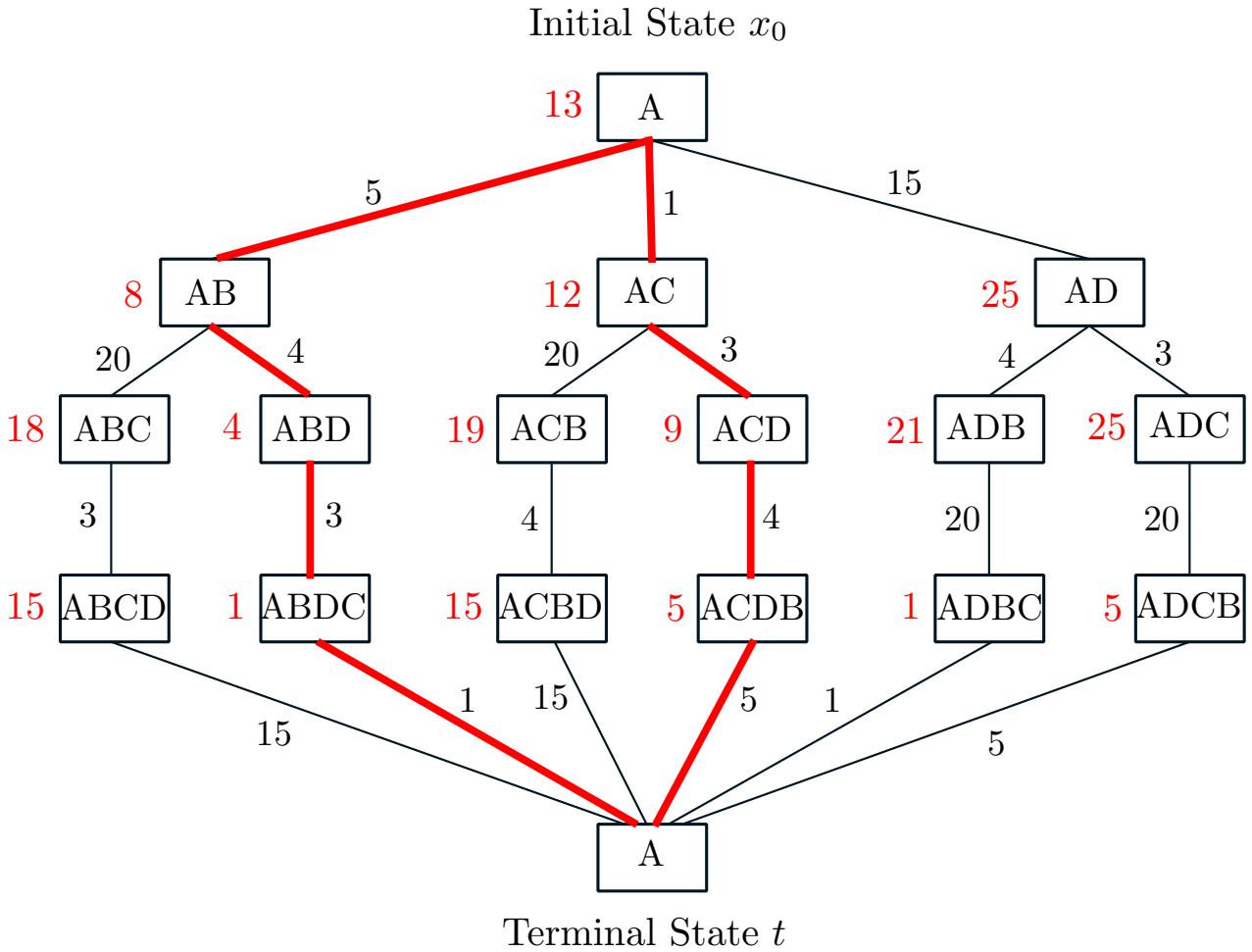
DP Algorithm: Stage 0 Tail Subproblems



Solve the stage 0 subproblem (using the optimal costs of stage 1 subproblems - in orange)

- The stage 0 subproblem is the entire problem
- The optimal value of the stage 0 subproblem is the optimal cost J^*(initial state)
- Construct the optimal sequence going forward

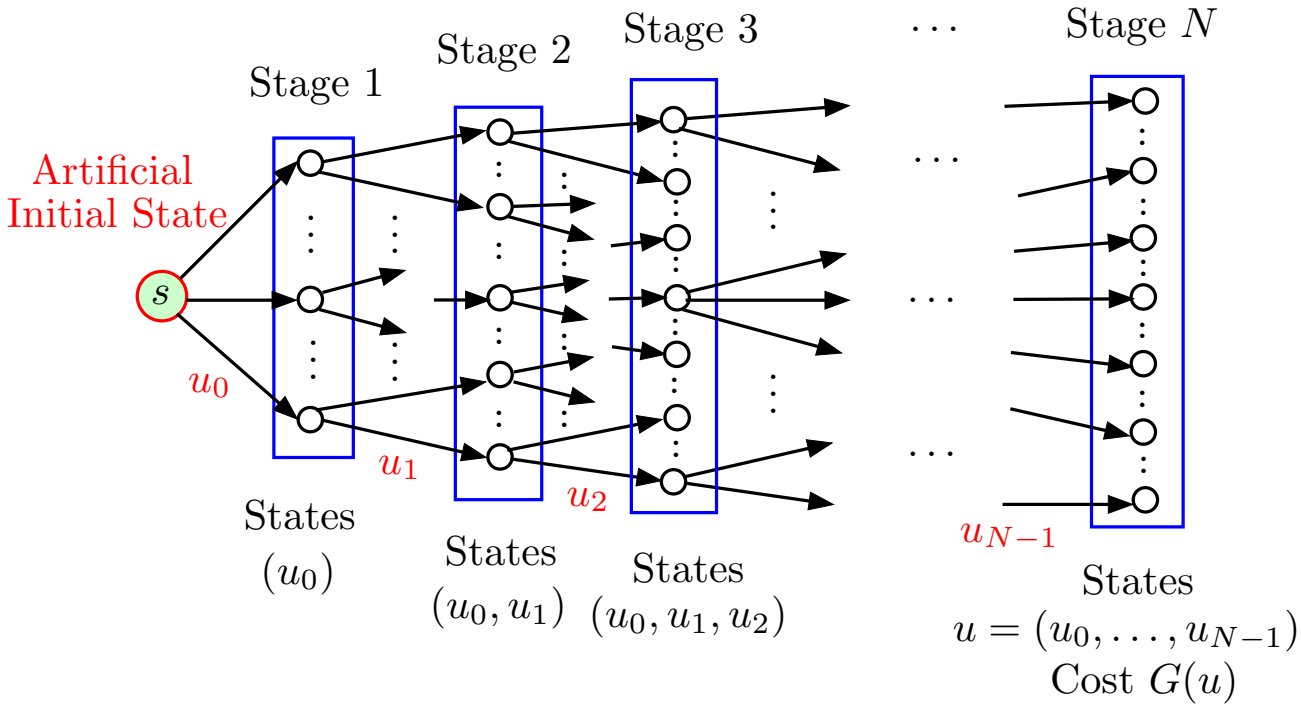
Discrete Optimization: Traveling Salesman Example; Cities A,B,C,D



Matrix of Intercity Travel Costs

	5	1	15
5		20	4
1	20		3
15	4	3	

General Discrete Optimization



Minimize $G(u)$ subject to $u \in U$

- Assume that each solution u has N components: $u = (u_0, \ldots, u_{N-1})$
- View the components as the controls of N stages
- Define $x_k = (u_0, \ldots, u_{k-1})$, $k = 1, \ldots, N$, and introduce artificial start state $x_0 = s$
- Define just terminal cost as $G(u)$; all other costs are 0

This formulation typically makes little sense for exact DP, but often makes a lot of sense for approximate DP/approximation in value space

Extensions

Stochastic finite horizon problems

The next state x_{k+1} is also affected by a random parameter (in addition to x_k and u_k). More difficult than deterministic (not equivalent to a shortest path problem).

Infinite horizon problems

The exact DP theory is mathematically more complex, but also more elegant.

Stochastic partial state information problems

We will convert them to problems of perfect state information, and then apply DP. Very hard to solve even approximately ... but offer great promise for applications.

Minimax/game problems

The exact DP theory is substantially more complex ... but the most spectacular successes of RL involve games. We will treat lightly.

Course Aims and Requirements

Our principal aim: To help you to think about how RL applies to your research interests

Requirements:

- Homework (30%): A total of 3-4
- Research-oriented term paper (70%). A choice of:
  - A mini-research project. You may work in teams of 1-3 persons. You are encouraged to try. Selected class presentations at the end.
  - A read-and-report term paper based on 2-3 research publications (chosen by you in consultation with me)

Notation: People in AI/RL, Control Theory, and Operations Research focus on different problems and use different notations

- AI/RL and OR focus on discrete/finite-state problems which are stochastic [Markovian Decision Problems (MDP)]. Use transition probabilities $p_{ij}(u)$ to describe the uncertainty.
- Control theorists use system equation notation $x_{k+1} = f_k(x_k, u_k, w_k)$. This notation is well-suited for continuous-state problems and deterministic problems.
- You are strongly encouraged to use the notation and terminology of the course.

Syllabus (Approximate)

- Lecture 1 (this lecture): Introduction, finite horizon deterministic exact DP
- Lecture 2: Stochastic exact DP, overview of infinite horizon methods
- Lecture 3: Linear quadratic problems, examples of problem formulation
- Lecture 4: Approximation in value space and the role of Newton's method
- Lecture 5: Rollout for deterministic problems
- Lecture 6: Rollout for stochastic problems
- Lecture 7: Model predictive and adaptive control
- Lecture 8: Multiagent systems and rollout
- Lecture 9: Combinatorial optimization and rollout
- Lecture 10: Parametric approximation architectures, feature-based architectures, (deep) neural nets, training with incremental/stochastic gradient methods
- Lecture 11: Infinite horizon problems, approximation in value space
- Lecture 12: Variants of policy iteration: Optimistic, multistep, multiagent, distributed asynchronous
- Lecture 13: Value and policy networks; use in approximate DP; perpetual rollout
- Lecture 14: Project presentations

About Machine Learning and Math

Math requirements for this course are modest

Calculus, elementary probability, minimal use of vector-matrix algebra. Our objective is to use math to the extent needed to develop insight into the mechanism of various methods, and to be able to start research.

However a math framework is critically important

Human insight can only develop within some structure of human thought ... math reasoning is most suitable for this purpose

On machine learning (from NY Times Article, Dec. 2018)

"What is frustrating about machine learning is that the algorithms can't articulate what they're thinking. We don't know why they work, so we don't know if they can be trusted ... As human beings, we want more than answers. We want insight. This is going to be a source of tension in our interactions with computers from now on."

About the Next Lecture

We will cover:

- Stochastic DP algorithm
- DP algorithm for Q-factors
- Approximation in value space
- Examples of discrete and continuous DP problems

PLEASE READ AS MUCH OF THE CLASS NOTES AS YOU CAN

Watch the video of Lecture 2 of the 2021 offering of the class at my web site
http://web.mit.edu/dimitrib/www/RLbook.html