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

Arizona State University
Course CSE 691, Spring 2023

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

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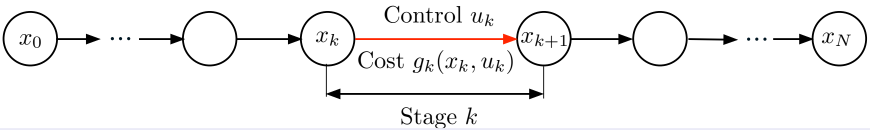
Lecture 2
Stochastic Finite and Infinite Horizon DP

Outline

Review - 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 $U_k(x_k)$

- Arbitrary state and control spaces
- 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 $J^*(x_0) = \min_{\substack{u_k \in U_k(x_k) \\ k=0,\ldots,N-1}} J(x_0; u_0, \ldots, u_{N-1})$

Review - DP Algorithm for Deterministic Problems

Go backward to compute the optimal costs $J_k^*(x_k)$ of the x_k-tail subproblems (off-line training - involves lots of computation)

Start with

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

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

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

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

Go forward to construct optimal control sequence $\{u_0^*, \ldots, u_{N-1}^*\}$ (on-line play)

Start with

$$u_0^* \in \arg \min_{u_0 \in U_0(x_0)} \Big[g_0(x_0, u_0) + J_1^*\big(f_0(x_0, u_0)\big) \Big], \qquad x_1^* = f_0(x_0, u_0^*).$$

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

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

Q-Factors for Deterministic Problems

An alternative (and equivalent) form of the DP algorithm

- Generates the optimal Q-factors, defined for all (x_k, u_k) and k by

$$Q_k^*(x_k, u_k) = g_k(x_k, u_k) + J_{k+1}^*\big(f_k(x_k, u_k)\big)$$

- The optimal cost function J_k^* can be recovered from the optimal Q-factor Q_k^*

$$J_k^*(x_k) = \min_{u_k \in U_k(x_k)} Q_k^*(x_k, u_k)$$

- The DP algorithm can be written in terms of Q-factors

$$Q_k^*(x_k, u_k) = g_k(x_k, u_k) + \min_{u_{k+1} \in U_{k+1}(f_k(x_k, u_k))} Q_{k+1}^*\big(f_k(x_k, u_k), u_{k+1}\big)$$

- Exact and approximate forms of this and other related algorithms, form an important class of RL methods known as Q-learning.

Approximation in Value Space

We replace J_k^* with an approximation $\tilde{J}_k$ during on-line play

- Start with

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

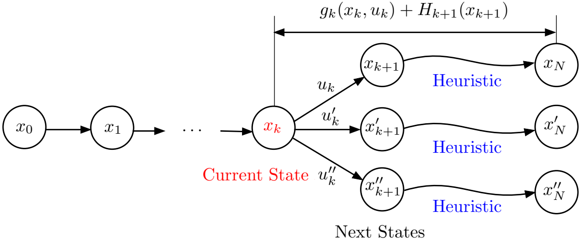
- Set $\tilde{x}_1 = f_0(x_0, \tilde{u}_0)$
- Sequentially, going forward, for $k = 1, 2, \ldots, N-1$, set

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

How do we compute $\tilde{J}_{k+1}(x_{k+1})$? This is one of the principal issues in RL

- Off-line problem approximation: Use as $\tilde{J}_{k+1}$ the optimal cost function of a simpler problem, computed off-line by exact DP
- On-line approximate optimization, e.g., solve on-line a shorter horizon problem by multistep lookahead minimization and simple terminal cost (often done in MPC)
- Parametric cost approximation: Obtain $\tilde{J}_{k+1}(x_{k+1})$ from a parametric class of functions $J(x_{k+1}, r)$, where r is a parameter, e.g., training using data and a NN.
- Rollout with a heuristic: We will focus on this for the moment.

Rollout for Finite-State Deterministic Problems



Cost approximation by running a heuristic from states of interest

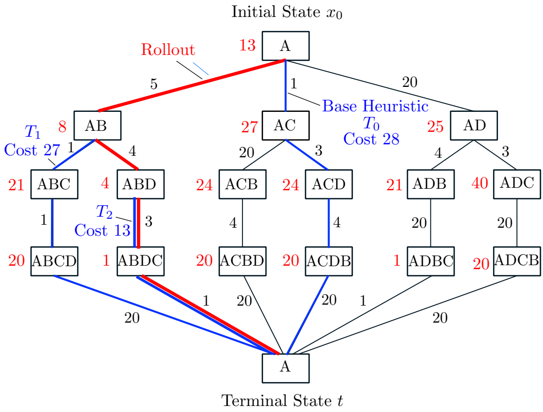
We generate a single system trajectory $\{x_0, x_1, \ldots, x_N\}$ by on-line play

- Upon reaching x_k, we compute for all $u_k \in U_k(x_k)$, the corresponding next states $x_{k+1} = f_k(x_k, u_k)$
- From each of the next states x_{k+1} we run the heuristic and compute the heuristic cost $H_{k+1}(x_{k+1})$
- We apply $\tilde{u}_k$ that minimizes over $u_k \in U_k(x_k)$, the (heuristic) Q-factor

$$g_k(x_k, u_k) + H_{k+1}(x_{k+1})$$

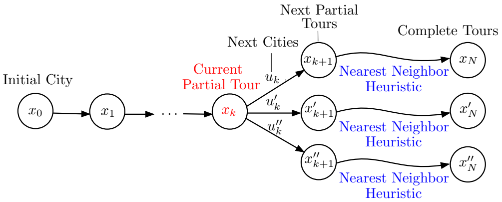
- We generate the next state $x_{k+1} = f_k(x_k, \tilde{u}_k)$ and repeat

Traveling Salesman Example

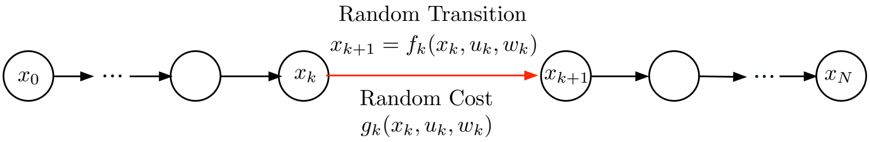


Matrix of Intercity Travel Costs

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



Stochastic DP Problems - Perfect State Observation (We Know x_k)



- System $x_{k+1} = f_k(x_k, u_k, w_k)$ with random "disturbance" w_k (e.g., physical noise, market uncertainties, demand for inventory, unpredictable breakdowns, etc)
- Cost function: $E\left\{g_N(x_N) + \sum_{k=0}^{N-1} g_k(x_k, u_k, w_k)\right\}$
- Policies $\pi = \{\mu_0, \ldots, \mu_{N-1}\}$, where μ_k is a "closed-loop control law" or "feedback policy"/a function of x_k. A "lookup table" for the control $u_k = \mu_k(x_k)$ to apply at x_k.
- An important point: Using feedback (i.e., choosing controls with knowledge of the state) is beneficial in view of the stochastic nature of the problem.
- For given initial state x_0, minimize over all $\pi = \{\mu_0, \ldots, \mu_{N-1}\}$ the cost

$$J_\pi(x_0) = E\left\{g_N(x_N) + \sum_{k=0}^{N-1} g_k\big(x_k, \mu_k(x_k), w_k\big)\right\}$$

- Optimal cost function: $J^*(x_0) = \min_\pi J_\pi(x_0)$. Optimal policy: $J_{\pi^*}(x_0) = J^*(x_0)$

The Stochastic DP Algorithm

Produces the optimal costs $J_k^*(x_k)$ of the tail subproblems that start at x_k

Start with $J_N^*(x_N) = g_N(x_N)$, and for $k = 0, \ldots, N-1$, let

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

- The optimal cost $J^*(x_0)$ is obtained at the last step: $J_0^*(x_0) = J^*(x_0)$.
- The optimal policy component μ_k^* can be constructed simultaneously with J_k^*, and consists of the minimizing $u_k^* = \mu_k^*(x_k)$ above.

Alternative on-line implementation of the optimal policy, given $J_1^*, \ldots, J_{N-1}^*$

Sequentially, going forward, for $k = 0, 1, \ldots, N-1$, observe x_k and apply

$$u_k^* \in \arg \min_{u_k \in U_k(x_k)} E_{w_k}\Big\{ g_k(x_k, u_k, w_k) + J_{k+1}^*\big(f_k(x_k, u_k, w_k)\big) \Big\}.$$

Issues: Need to know J_{k+1}^*, compute $E_{w_k}\{\cdot\}$ for each u_k, minimize over all u_k

A Very Favorable Case: Linear-Quadratic Problems

One-dimensional linear-quadratic problem

- System is $x_{k+1} = ax_k + bu_k + w_k$ (a and b are given scalars)
- Cost over N stages: $qx_N^2 + \sum_{k=0}^{N-1}(qx_k^2 + ru_k^2)$, where $q > 0$ and $r > 0$ are given scalars
- The DP algorithm starts with $J_N^*(x_N) = qx_N^2$, and generates J_k^* according to

$$J_k^*(x_k) = \min_{u_k} E_{w_k}\left\{qx_k^2 + ru_k^2 + J_{k+1}^*(ax_k + bu_k + w_k)\right\}, \quad k = 0, \ldots, N-1$$

- DP algorithm can be carried out in closed form to yield
  $J_k^*(x_k) = K_k x_k^2 + \text{const}, \ \mu_k^*(x_k) = L_k x_k$: K_k and L_k can be explicitly computed
- $\mu_k^*(x_k)$ does not depend on the distribution of w_k as long as it has 0 mean: Certainty Equivalence (a common approximation idea for other problems)

These results generalize to multidimensional linear-quadratic problems

$x_k \in \Re^n$, $u_k \in \Re^m$; the scalars a, b, q, r are replaced by matrices A, B, Q, R

Derivation - DP Algorithm starting from Terminal Cost $J_N^*(x_N) = qx_N^2$

$$
\begin{aligned}
J_{N-1}^*(x_{N-1}) &= \min_{u_{N-1}} E\big\{qx_{N-1}^2 + ru_{N-1}^2 + J_N^*(ax_{N-1} + bu_{N-1} + w_{N-1})\big\} \\
&= \min_{u_{N-1}} E\big\{qx_{N-1}^2 + ru_{N-1}^2 + q(ax_{N-1} + bu_{N-1} + w_{N-1})^2\big\} \\
&= \min_{u_{N-1}} \big[qx_{N-1}^2 + ru_{N-1}^2 + q(ax_{N-1} + bu_{N-1})^2 + 2q\,\underbrace{E\{w_{N-1}\}}_{=0}(ax_{N-1} + bu_{N-1}) + q\,\underbrace{E\{w_{N-1}^2}_{=\sigma^2} \\
&= qx_{N-1}^2 + \min_{u_{N-1}} \big[ru_{N-1}^2 + q(ax_{N-1} + bu_{N-1})^2\big] + q\sigma^2
\end{aligned}
$$

Minimize by setting to zero the derivative: $0 = 2ru_{N-1} + 2qb(ax_{N-1} + bu_{N-1})$, to obtain

$$\mu_{N-1}^*(x_{N-1}) = L_{N-1}x_{N-1} \quad \text{with} \quad L_{N-1} = -\frac{abq}{r + b^2q}$$

and by substitution, $J_{N-1}^*(x_{N-1}) = K_{N-1}x_{N-1}^2 + q\sigma^2$, where $K_{N-1} = \frac{a^2rq}{r+b^2q} + q$

Similarly, going backwards (starting with $K_N = q$), we obtain for all k:

$$J_k^*(x_k) = K_kx_k^2 + \sigma^2\sum_{m=k}^{N-1}K_{m+1}, \quad \mu_k^*(x_k) = L_kx_k, \quad K_k = \frac{a^2rK_{k+1}}{r + b^2K_{k+1}} + q, \quad L_k = -\frac{abK_{k+1}}{r + b^2K_{k+1}}$$

Linear-Quadratic Problems in General

Observations and generalizations

- The solution does not depend on the distribution of w_k, only on the mean (which is 0), i.e., we have certainty equivalence (the stochastic problem can be replaced by a deterministic problem)
- Generalization to multidimensional problems, nonzero mean disturbances, etc
- Generalization to infinite horizon
- Generalization to problems where the state is observed partially through linear measurements: Optimal policy involves an extended form of certainty equivalence

  $$L_k E\{x_k \mid \text{measurements}\}$$

  where $E\{x_k \mid \text{measurements}\}$ is provided by an estimator (e.g., Kalman filter)
- Linear systems and quadratic cost are a starting point for other lines of investigations and approximations:
  - Problems with safety/state constraints [Model Predictive Control (MPC)]
  - Problems with control constraints (MPC)
  - Unknown or changing system parameters (adaptive control)

Simplified minimization

First Step

"Future"

$$\text{At } x_k \longrightarrow \min_{u_k} E\Big\{ g_k(x_k, u_k, w_k) + \tilde{J}_{k+1}(x_{k+1}) \Big\}$$

"On-Line Play"

Expected value approximation **Cost-to-go approximation**

Important variants: Use multistep lookahead, use multiagent rollout (for multicomponent control problems)

Multistep lookahead (performance - computational overhead tradeoff)

At State x_k

DP minimization

First ℓ Steps

"Future"

$$\min_{u_k, \mu_{k+1}, \ldots, \mu_{k+\ell-1}} E\left\{ g_k(x_k, u_k, w_k) + \sum_{m=k+1}^{k+\ell-1} g_m\big(x_m, \mu_m(x_m), w_m\big) + \tilde{J}_{k+\ell}(x_{k+\ell}) \right\}$$

Lookahead Minimization

Cost-to-go Approximation

Approximate Min
Discretization
Selective Minimization

First Step "Future"

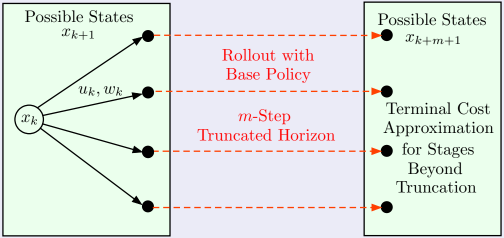
At x_k

$$\min_{u_k} E\Big\{ \underbrace{g_k(x_k, u_k, w_k)}_{\text{First Step}} + \underbrace{\tilde{J}_{k+1}(x_{k+1})}_{\text{"Future"}} \Big\}$$

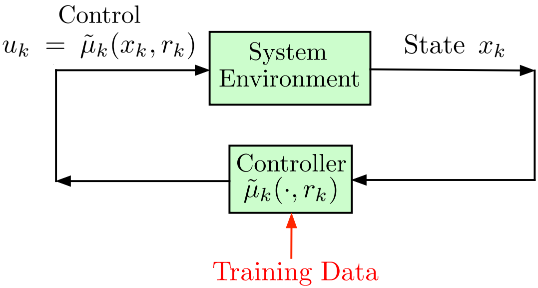
Approximate $E\{\cdot\}$
Adaptive simulation
Monte Carlo tree search

Approximate Cost-to-Go $\tilde{J}_{k+1}$
Certainty equivalence
Problem approximation
Rollout, Model Predictive Control
Parametric approximation
Neural nets
Aggregation

An example: Truncated rollout with base policy and terminal cost approximation (however obtained, e.g., off-line training)



Approximation in Policy Space: The Major Alternative to Approximation in Value Space



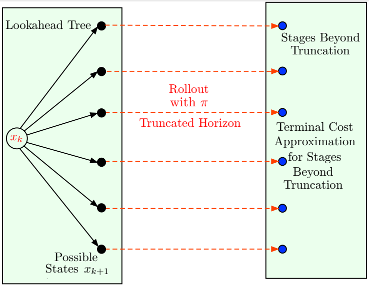
- Idea: Select the policy by optimization over a suitably restricted class of policies
- The restricted class is usually a parametric family of policies $\tilde{\mu}_k(x_k, r_k)$, $k = 0, \ldots, N-1$, of some form, where r_k is a parameter (e.g., a neural net)
- Methods used for optimization/off-line training: Random search, policy gradient, classification (to be discussed later)
- Important advantage once the parameters r_k are computed: The on-line computation of controls is often much faster ... at state x_k apply $u_k = \tilde{\mu}_k(x_k, r_k)$
- Important disadvantage: It does not allow for on-line replanning ... no Newton step

An Important Conceptual Difference Between Approximation in Value and in Policy Space

$$\boxed{\text{At } x_k} \longrightarrow \min_{u_k} E\Big\{ \overbrace{g_k(x_k,u_k,w_k)}^{\text{First Step}} + \overbrace{\tilde J_{k+1}(x_{k+1})}^{\text{“Future”}} \Big\}$$

Approximation in value space is primarily an “on-line play" method

with off-line training used optionally to construct cost function approximations for one-step or multistep lookahead



Approximation in policy space is primarily an “off-line training" method

which may be used optionally to provide a policy for on-line rollout

From Approximation in Value Space to Approximation in Policy Space

The approximate cost-to-go functions $\tilde{J}_{k+1}$ define a suboptimal policy $\tilde{\mu}_k$ through one-step or multistep lookahead minimization

- Given functions $\tilde{J}_{k+1}$, how do we simplify the computation of $\tilde{\mu}_k$?
- Idea: Use approximation in policy space to represent $\tilde{\mu}_k$: Approximate $\tilde{\mu}_k$ using a training set of a large number q of sample pairs (x_k^s, u_k^s), $s = 1, \ldots, q$, where $u_k^s = \tilde{\mu}_k(x_k^s)$:

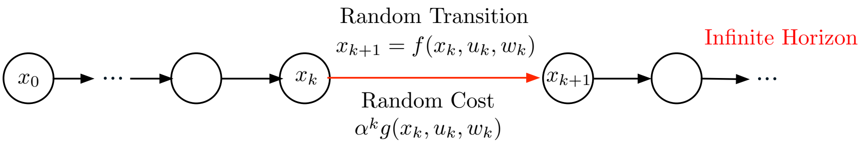
$$u_k^s \in \arg \min_{u \in U_k(x_k)} E\Big\{ g_k(x_k^s, u, w_k) + \tilde{J}_{k+1}\big(f_k(x_k^s, u, w_k)\big) \Big\}$$

- Example: Introduce a parametric family of randomized policies $\mu_k(x_k, r_k)$, $k = 0, \ldots, N-1$, of some form (e.g., a neural net), where r_k is a parameter. Then estimate the parameters r_k by least squares fit:

$$r_k \in \arg \min_r \sum_{s=1}^{q} \left\| u_k^s - \mu_k(x_k^s, r) \right\|^2$$

- Relation to classification methods ... policy <–> classifier; more on this later.

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.



Infinite number of stages, and stationary system and cost

- System $x_{k+1} = f(x_k, u_k, w_k)$ with state, control, and random disturbance.
- Policies $\pi = \{\mu_0, \mu_1, \ldots\}$ with $\mu_k(x) \in U(x)$ for all x and k.
- Cost of stage k: $\alpha^k g\big(x_k, \mu_k(x_k), w_k\big)$.
- $0 < \alpha \leq 1$ is the discount factor. If $\alpha < 1$ the problem is called discounted.
- Cost of a policy $\pi = \{\mu_0, \mu_1, \ldots\}$: The limit as $N \to \infty$ of the N-stage costs

$$J_\pi(x_0) = \lim_{N \to \infty} E_{w_k} \left\{ \sum_{k=0}^{N-1} \alpha^k g\big(x_k, \mu_k(x_k), w_k\big) \right\}$$

- Optimal cost function $J^*(x_0) = \min_\pi J_\pi(x_0)$.
- Problems with $\alpha = 1$ typically include a special cost-free termination state t. The objective is to reach (or approach) t at minimum expected cost.

k-stages opt. cost –> Infinite horizon opt. cost as $k \to \infty$

- We have $J^*(x) = \lim_{k\to\infty} J_k(x)$, for all x, where for any k, $J_k(x)$ = k-stages optimal cost starting from x, and is generated by

$$J_k(x) = \min_{u\in U(x)} E_w\Big\{g(x,u,w) + \alpha J_{k-1}\big(f(x,u,w)\big)\Big\}, \quad J_0(x) \equiv 0 \qquad \text{(VI)}$$

- Derivation using DP: Let $V_{N-k}(x)$ be the optimal cost-to-go starting at x with k stages to go,

$$V_{N-k}(x) = \min_{u\in U(x)} E_w\Big\{\alpha^{N-k} g(x,u,w) + V_{N-k+1}\big(f(x,u,w)\big)\Big\}, \quad V_N(x) \equiv 0$$

- Define $J_k(x) = V_{N-k}(x)/\alpha^{N-k}$ to obtain Eq. (VI)

J^* satisfies Bellman's equation: Take the limit in Eq. (VI)

$$J^*(x) = \min_{u\in U(x)} E_w\Big\{g(x,u,w) + \alpha J^*\big(f(x,u,w)\big)\Big\}, \qquad \text{for all } x$$

Optimality condition: Let $\mu^*(x)$ attain the min in the Bellman equation for all x

The policy $\{\mu^*, \mu^*, \ldots\}$ is optimal. (This type of policy is called stationary.)

Infinite Horizon Problems - The Two Algorithms

Value iteration (VI): Generates finite horizon opt. cost function sequence $\{J_k\}$

$$J_k(x) = \min_{u \in U(x)} E_w\Big\{g(x,u,w) + \alpha J_{k-1}\big(f(x,u,w)\big)\Big\}, \qquad J_0 \text{ is "arbitrary" (?)}$$

Policy Iteration (PI): Generates sequences of policies $\{\mu^k\}$ and their cost functions $\{J_{\mu^k}\}$; μ^0 is "arbitrary"

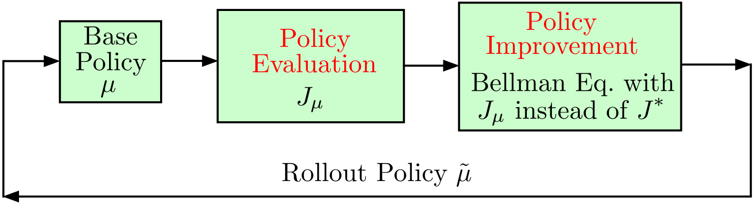
The typical iteration starts with a policy μ and generates a new policy $\tilde{\mu}$ in two steps:

- Policy evaluation step, which computes J_μ the cost function of the (base) policy μ
- Policy improvement step, which computes the improved (rollout) policy $\tilde{\mu}$ using the one-step lookahead minimization

$$\tilde{\mu}(x) \in \arg\min_{u \in U(x)} E_w\Big\{g(x,u,w) + \alpha J_\mu\big(f(x,u,w)\big)\Big\}$$

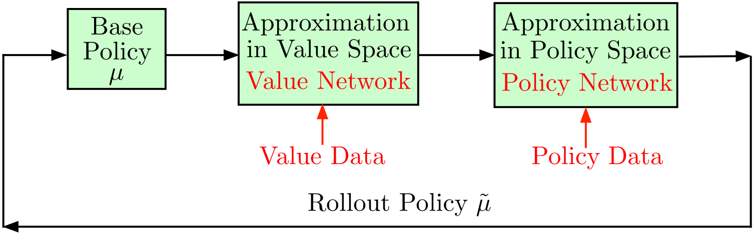
There are several options for policy evaluation to compute J_μ

- Solve Bellman's equation for μ [$J_\mu(x) = E\{g(x,\mu(x),w) + \alpha J_\mu(f(x,\mu(x),w))\}$] by using VI or other method (it is linear in J_μ)
- Use simulation (on-line Monte-Carlo, Temporal Difference (TD) methods)



Important facts (to be discussed later):

- PI yields in the limit an optimal policy (?)
- PI is faster than VI; can be viewed as Newton's method for solving Bellman's Eq.
- PI can be implemented approximately, with a value and (perhaps) a policy network



Deterministic Linear Quadratic Problem - Infinite Horizon, Undiscounted

Linear system $x_{k+1} = ax_k + bu_k$; quadratic cost per stage $g(x,u) = qx^2 + ru^2$

Bellman equation: $J(x) = \min_u \{qx^2 + ru^2 + J(ax+bu)\}$

Take the limit as $N \to \infty$ in the N-step horizon results: $K_k \to K^*$, $L_k \to L^*$

- $J^*(x) = K^* x^2$ where K^* is some positive scalar
- The optimal policy has the form $\mu^*(x) = L^* x$ where L^* is some scalar
- To characterize K^* and L^*, we plug $J(x) = Kx^2$ into the Bellman equation

$$Kx^2 = \min_u \{qx^2 + ru^2 + K(ax+bu)^2\} = \cdots = F(K)x^2$$

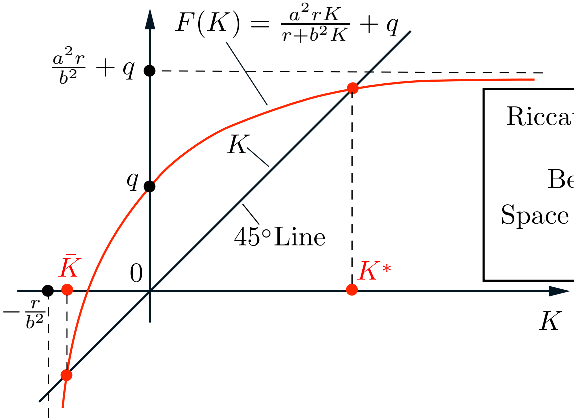
where $F(K) = \frac{a^2 rK}{r+b^2 K} + q$ with the minimizing u being equal to $-\frac{abK}{r+b^2 K} x$

- Thus the Bellman equation is solved by $J^*(x) = K^* x^2$, with K^* being a solution of the Riccati equation

$$K^* = F(K^*) = \frac{a^2 rK^*}{r + b^2 K^*} + q$$

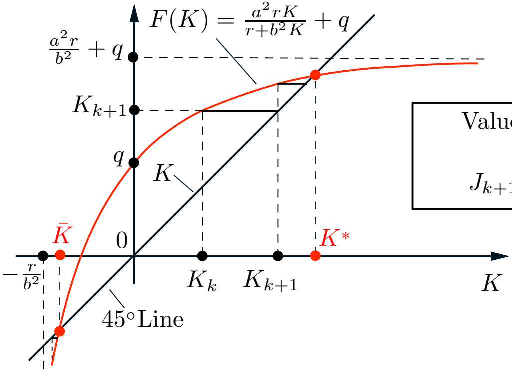
and the optimal policy is linear:

$$\mu^*(x) = L^* x \quad \text{with} \quad L^* = -\frac{abK^*}{r + b^2 K^*}$$



Riccati Equation: $K = F(K)$
from
Bellman Equation on
Space of Quadratic Functions
$J(x) = Kx^2$

Visualization of VI



Value Iteration: $K_{k+1} = F(K_k)$
from
$J_{k+1}(x) = K_{k+1} x^2 = F(K_k) x^2$

About the Next Lecture

Linear quadratic problems and Newton step interpretations

- Approximation in value space as a Newton step for solving the Riccati equation
- Rollout as a Newton step starting from the cost of the base policy
- Policy Iteration as repeated Newton steps

Problem formulations and reformulations

- How do we formulate DP models for practical problems?
- Problems involving a terminal state (stochastic shortest path problems)
- Problem reformulation by state augmentation (dealing with delays, correlations, forecasts, etc)
- Problems involving imperfect state observation (POMDP)
- Multiagent problems - Nonclassical information patterns
- Systems with unknown or changing parameters - Adaptive control

PLEASE READ SECTIONS 1.5-1.6 OF THE CLASS NOTES (as much as you can)

1ST HOMEWORK (DUE IN ONE WEEK): Exercise 1.1 of the Class Notes