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

Arizona State University
Course CSE 691, Spring 2023

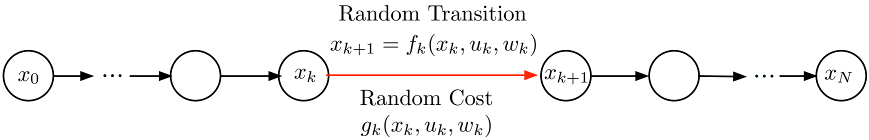
Links to Class Notes, Videolectures, and Slides at
http://web.mit.edu/dimitrib/www/RLbook.html

Dimitri P. Bertsekas
dbertsek@asu.edu

Lecture 5
Revisit Finite Horizon DP Problems - Deterministic Rollout

Outline

Review: The Generic Finite Horizon DP Problem



- 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.
- 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: $J_{\pi^*}(x_0) = J^*(x_0)$

We will be focusing on finite horizon: It's most convenient for our algorithmic purposes (e.g., rollout) ... but nearly everything applies to infinite horizon

Review: The 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 $k = 0, \dots, N-1$, 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 is to use the minimizing $u_k^* = \mu_k^*(x_k)$ above.

Approximation in Value Space - Use of $\tilde{J}_{k+1}$ in Place of J_{k+1}^*

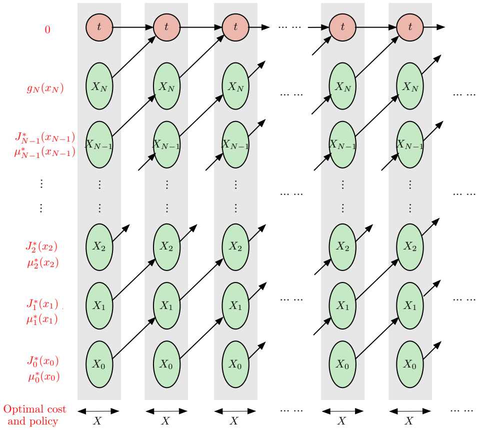
Sequentially, going forward, for $k = 0, 1, \dots, N-1$, observe x_k and apply

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

There is also a multistep version.

There are many different ways to compute $\tilde{J}_{k+1}$ (e.g., on-line rollout, off-line training, problem approximation, heuristics, etc)

An Important Conceptual Idea: Finite Horizon can be Transformed to Infinite Horizon



As a result:

- The Bellman equation of the infinite horizon problem is the DP algorithm for the finite horizon problem
- Policy iteration/Newton step ideas apply to finite horizon problems

At State x_k
DP minimization

First ℓ Steps — "Future"

$$\min_{u_k,\mu_{k+1},\ldots,\mu_{k+\ell-1}} E\left\{ g_k(x_k,u_k,w_k) + \sum_{i=k+1}^{k+\ell-1} g_i\big(x_i,\mu_i(x_i),w_i\big) + \tilde J_{k+\ell}(x_{k+\ell}) \right\}$$

Rollout Control $\tilde u_k$
Rollout Policy $\tilde \mu_k$

Lookahead Minimization

Base Policy Cost

$\tilde J_{k+\ell}(x_{k+\ell})$ 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 variants

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

Rollout is Important for this Course

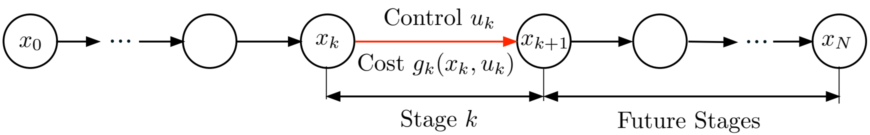
Role of Rollout

- It provides important options for cost function approximation in the context of value space methods (a “good" option because $J_k^* \leq \tilde{J}_k$, based on visualizations)
- 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 by far the most reliable
- 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
- Deals well with on-line replanning, and provides a useful alternative to reoptimization in adaptive control
- It relates to model predictive control, and can be used to improve the stability of MPC schemes
- Truncated rollout can be combined with many of the RL methods used in practice [including self-learning (approximate PI), Q-learning, aggregation, and others]

Review: Finite Horizon Deterministic Optimal Control Model



- 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:

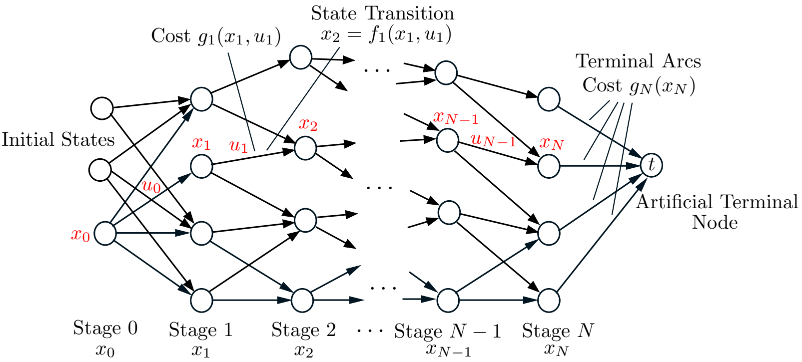
$$g_N(x_N) + \sum_{k=0}^{N-1} g_k(x_k, u_k)$$

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

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

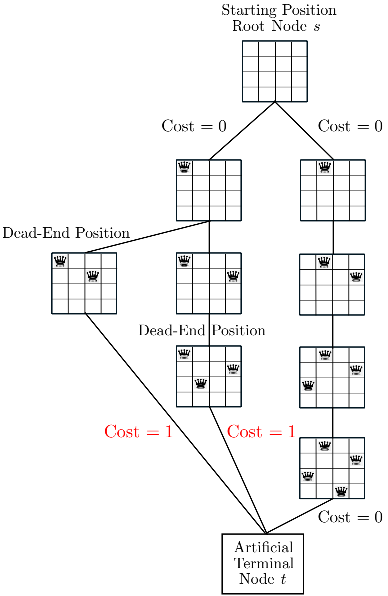
- Optimal cost function $J^*(x_0) = \min_{\substack{u_k \in U_k(x_k) \\ k=0,\ldots,N-1}} J(x_0; u_0, \ldots, u_{N-1})$

Review: Generic Finite-State Deterministic Finite Horizon Problem

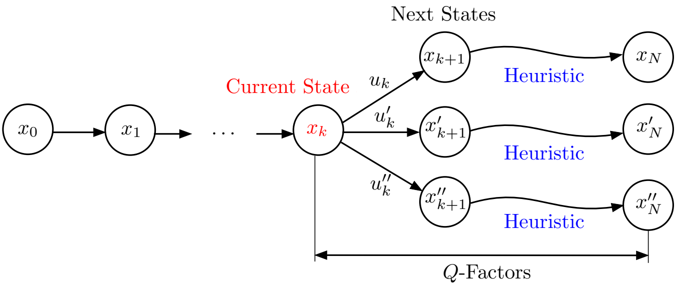


- Nodes correspond to states x_k
- Each arc corresponds to a state-control pair (x_k, u_k) (start node is x_k; end node is $x_{k+1} = f_k(x_k, u_k)$)
- An arc corresponding to (x_k, u_k) has a cost $g_k(x_k, u_k)$.
- The cost to optimize is the sum of the arc costs from the initial node/state x_0 to a terminal node t.
- The problem is equivalent to finding a minimum cost/shortest path from x_0 to t.

A Combinatorial Example: The N Queens Problem



General Structure of Deterministic Rollout with Some Base Heuristic

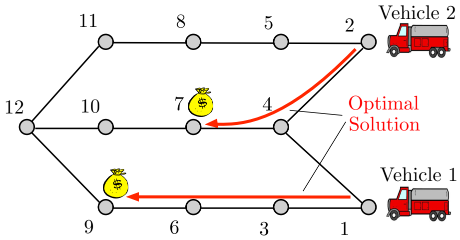


- At state x_k, for every pair (x_k, u_k), $u_k \in U_k(x_k)$, we generate a Q-factor

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

  using the base heuristic [$H_{k+1}(x_{k+1})$ is the heuristic cost starting from x_{k+1}]
- We select the control u_k with minimal Q-factor
- We move to next state x_{k+1}, and continue
- Multistep lookahead versions
- An important question: Is rollout cost improving? (Performs no worse than the base heuristic, from x_0)

A Multivehicle Routing Example



Base heuristic

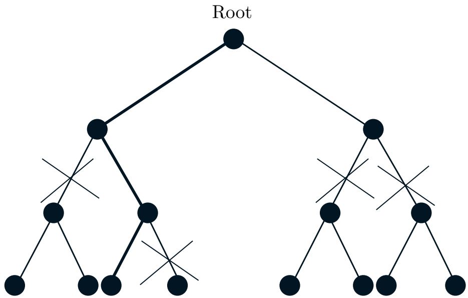
Move each vehicle one step towards its closest task

Base heuristic moves both vehicles to node 4 and moves them together after that

Rollout operation at each stage, given the current pair of vehicle positions

- Consider all the possible pairs of moves from the current position
- Run the base heuristic from each pair
- Select the move of min total vehicle moves
- Rollout finds the optimal solution (in this example). A total of 6 moves compared with 10 for the base heuristic.

An Example: Search for an N-Arc Breakthrough Path in a Tree (e.g., Search Through a Maze)



Greedy base heuristic: If one arc is free use it; if both arcs are free use the right arc

- Complexity of the DP algorithm is $O(N2^N)$ (size of tree grows exponentially)
- Complexity of the greedy and rollout algorithms is $O(N)$ and $O(N^2)$, respectively
- Assuming arcs are blocked with given probability, the rollout algorithm has $O(N)$ times higher probability of breakthrough; see the literature.
- This is qualitatively typical: Rollout improves performance of base heuristic substantially at the expense of polynomial amount of extra computation.

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

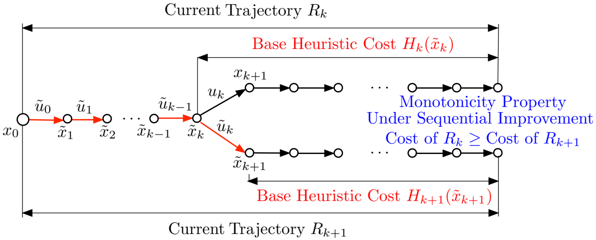
  $$\{x_k, x_{k+1}, \ldots, x_N\}$$

  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 $\{\mu_0, \ldots, \mu_{N-1}\}$
- "Greedy" heuristics are sequentially consistent (e.g., nearest neighbor for TSP)
- We will focus on a less restrictive condition: sequential improvement

Sequential Improvement Condition



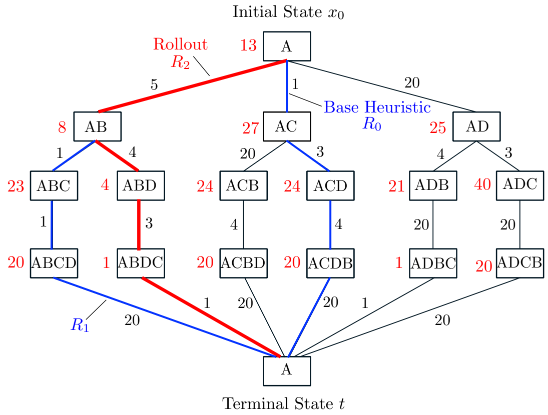
Implies cost improvement: (Cost of Rollout Policy) $\leq$ (Cost of Base Heuristic)

- Sequential improvement definition: Best heuristic Q-factor $\leq$ Heuristic cost, i.e.,

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

  where $H_k(x_k)$: cost of the trajectory generated by the heuristic starting from x_k
- Justification: Rollout, upon reaching $\tilde{x}_k$, has obtained a “current" trajectory R_k. Sequential improvement implies: Cost of $R_k \geq$ Cost of R_{k+1}
- Thus the current trajectory cannot get worse. Since R_0 corresponds to the base heuristic, R_N corresponds to the rollout, Cost of $R_0 \geq$ Cost of R_N
- Note that sequential consistency –> sequential improvement

Traveling Salesman Example: Rollout with a Nearest Neighbor Heuristic



Matrix of Intercity Travel Costs

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

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

Cost of $R_0 \geq$ Cost of $R_1 \geq$ Cost of R_2

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.

Simplified Rollout Algorithm - Assuming Sequential Improvement

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

- When at x_k, choose as rollout control any $\tilde{u}_k = \tilde{\mu}_k(x_k)$ such that

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

  where $H_k(x_k)$ is the cost of the trajectory generated by the heuristic from x_k.
- Can focus on a small subset of “promising" controls (save lots of computation)

Cost improvement for the simplified algorithm:

Let the rollout policy under the simplified algorithm be $\tilde{\pi} = \{\tilde{\mu}_0, \dots, \tilde{\mu}_{N-1}\}$, 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: Again, the current trajectory cannot get worse,

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

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

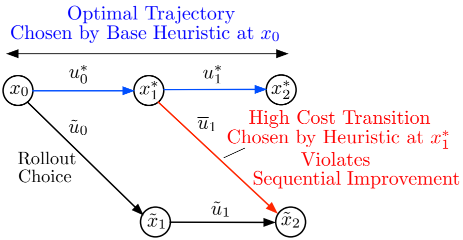
$$\min_{u_k \in U_k(x_k)} \tilde{Q}_k^m(x_k, u_k) \leq H_k^m(x_k), \qquad m = 1, \ldots, M,$$

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 mth heuristic. By taking minimum over m, and interchanging the order of the minimization $\min_{m=1,\ldots,M} \min_{u_k \in U_k(x_k)}$,

$$\min_{u_k \in U_k(x_k)} \underbrace{\min_{m=1,\ldots,M} \tilde{Q}_k^m(x_k, u_k)}_{\text{Superheuristic Q-factor}} \leq \underbrace{\min_{m=1,\ldots,M} H_k^m(x_k)}_{\text{Superheuristic cost}},$$

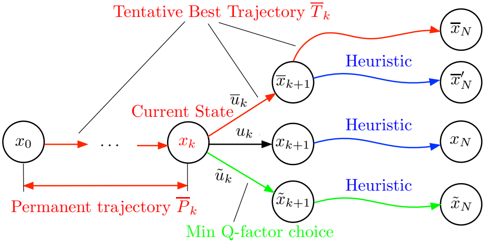
which is the sequential improvement condition for the superheuristic.

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



- The optimal trajectory $(x_0, u_0^*, x_1^*, u_1^*, x_2^*)$.
- Assume the heuristic produces (u_0^*, u_1^*) at x_0, and $\bar{u}_1$ at x_1^*.
- Rollout uses the base heuristic to construct a trajectory starting from x_1^* and $\tilde{x}_1$.
- Then (Q-factor of u_0^*)>(Q-factor of $\tilde{u}_0$). So the rollout algorithm selects $\tilde{u}_0$, and moves to a nonoptimal next state $\tilde{x}_1 = f_0(x_0, \tilde{u}_0)$.
- Thus 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



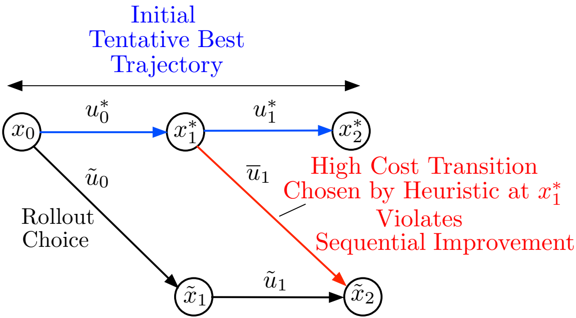
Idea: At each step, follow the best trajectory computed thus far

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

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

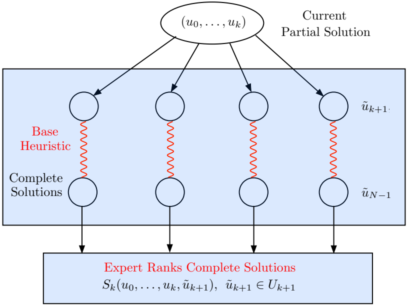
  $\overline{T}_k$ is the best end-to-end trajectory computed up to stage k
- We reject the minimum Q-factor choice $\tilde{u}_k$ if its complete trajectory is more costly than the current tentative best; otherwise we accept $\tilde{u}_k$, and update the tentative best trajectory.

Illustration of Fortified Algorithm



- At x_0, the fortified rollout stores as initial tentative best trajectory the unique optimal trajectory $(x_0, u_0^*, x_1^*, u_1^*, x_2^*)$ generated by the base heuristic.
- In the first rollout step, it computes the Q-factors of u_0^* and $\tilde{u}_0$ by running the heuristic from x_1^* and $\tilde{x}_1$.
- Even though the rollout prefers $\tilde{u}_0$ to u_0^*, it discards $\tilde{u}_0$ in favor of u_0^*, which is dictated by the tentative best trajectory.
- It then sets the permanent trajectory to (x_0, u_0^*, x_1^*) and keeps the tentative best trajectory unchanged to $(x_0, u_0^*, x_1^*, u_1^*, x_2^*)$.

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

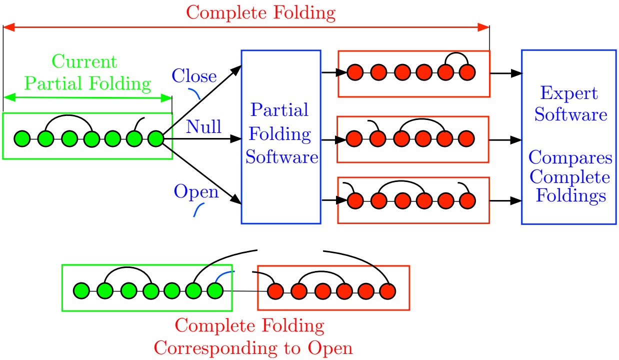


- Assume we do not know G, and/or the constraint sets U_k
- Instead we have a base heuristic, which given a partial solution $(u_0, \ldots, u_k)$, outputs all next controls $\tilde{u}_{k+1}$, and generates from each a complete solution

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

- 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.

Rollout with an Expert - RNA Folding Application (see [LPS21])



- Given a sequence of nucleotides (molecules of “types" A,C,G,U), “fold" it in an “interesting" way (introduce pairings that result in an “interesting" structure).
- Make a pairing decision at each nucleotide in sequence (open, close, do nothing).
- Base heuristic: Given a partial folding, generates a complete folding (this is the partial folding software).
- Two complete foldings can be compared by the expert software.
- There is no explicit cost function here (it is internal to the expert software).

About the Next Lecture

We will cover:

- Rollout with multistep lookahead
- Rollout for constrained problems
- Applications in integer programming

Homework (due in two weeks): Exercise 1.3