MS-E2148 Dynamic optimization Lecture 7

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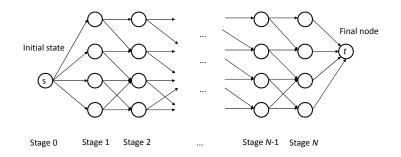
Recap

- ➤ The principle of optimality: if a-b-c is optimal route, then b-c is optimal subroute
- Cost-to-go: what is the cost starting from stage k to the last stage N
- ▶ DP-algorithm: compute the cost-to-go values backwards from N − 1 to the initial stage

- **Deterministic**: w_k get one value for each k
 - Problems that are truly deterministic
 - Problems that are stochastic but the noise can be assumed approximately constant
- **Finite state space**: S_k is *finite set* for all k
 - E.g. time table scheduling problems are finite
 - Are they finite in modeling altitude of 747 or the balance of bank account?
- At state x_k the control u_k means deterministic transition to state $f_k(x_k, u_k)$ with cost $g_k(x_k, u_k)$

- Special feature: feedback/closed-loop control does not give smaller cost (without stochastics, there is no benefit in observing the state)
- Minimizing cost over admissible controls $\{\mu_0, ..., \mu_{N-1}\} \in \Pi$ gives the same cost as minimizing cost over control vectors $\{u_0, ..., u_{N-1}\}$
- For some control law $\{\mu_0,...,\mu_{N-1}\}$ and initial state x_0 , the future states are perfectly predictable by the equation $x_{k+1} = f_k(x_k, \mu_k(x_k)), k = 0, 1, ..., N-1$, and the corresponding controls can be determined: $u_k = \mu_k(x_k)$
- This gives computational advantages

- ▶ These problems can be presented as *graphs*:
 - Nodes correspond states
 - Arcs correspond transition between consecutive states
 - The cost of moving from state to another is given by the length of the arc
- Initial state: initial node s that is attached to the states of stage 1
- Final state: artificial end node t that is attached to each final state x_N with arc that has cost $g_N(x_N)$
- Controls: paths that start from s and end to some x_N



Shortest path problem

- ► Transition cost $g_k(x_k, u_k)$ along the arc from state x_k to x_{k+1} is the length of the arc
- Let us denote: a_{ij} is the length of the arc from node i to j; if there is no arc then $a_{ij} = \infty$
- We want to find the **shortest path**, from every node i to the end node t
 - \Rightarrow we search for a sequence of controls that minimize the total cost of getting to t from each node 1, 2, ..., N

Shortest path problem

- ➤ The solution exists if we require that the length of the cycles are non-negative
- ► Cycle: $(i, j_1), (j_1, j_2), ..., (j_k, i)$
- ▶ The optimal path is at most N length: formulate the problem as N-length but allow degenerate transitions from node i to itself so that $a_{ii} = 0$

▶ We denote for all i = 1, ..., N and k = 0, ..., N - 1: $J_k(i) = \text{optimal cost with } N - k \text{ steps from node } i \text{ to end } t$

Shortest path problem

▶ The cost from *i* to *t* is then $J_0(i)$

DP algorithm for the shortest path problem: the optimal cost from i to t in N-k steps is

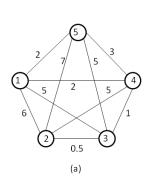
$$J_k(i) = \min_{j=1,...,N} [a_{ij} + J_{k+1}(j)], \quad k = 0, 1, ..., N-2,$$

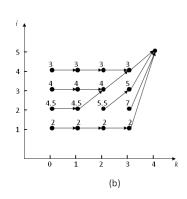
where
$$J_{N-1}(i) = a_{it}$$
, $i = 1, 2, ..., N$.

Note that the above $J_{k+1}(j) = \text{optimal cost from } j \text{ to } t \text{ in } N-k-1 \text{ steps}$

Shortest path problem: example

- ► The figure (a) is a graph where the costs a_{ij} are denoted on the arcs; figure (b) gives the cost-to-go $J_k(i)$ from each node i and stage k generated by DP
- Node 5 is the end node; N = 5, k = 0, 1, 2, 3, 4





Shortest path problem: example

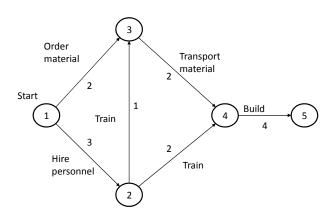
- The cost-to-go values are computed with DP in the following way in figure (b)
 - $J_2(2) = min\{5+3, 0.5+5, 6+2, ...\} = 5.5 \text{ (2 steps)}$
 - $J_0(4) = min\{0+0+0+3, 0+0+1+5, ...\} = 3$ (4 steps)
- Zero means staying in the node: a_{ii} = 0
- The optimal paths can be seen from the figure (b):

$$\begin{array}{c} 1\rightarrow 5,\\ 2\rightarrow 3\rightarrow 4\rightarrow 5,\\ 3\rightarrow 4\rightarrow 5,\\ 4\rightarrow 5\end{array}$$

Application: critical path analysis – general questions

- Project has various activities and some of them need to be finished before starting the next ones
- ▶ How to schedule the project?
- What are the critical activities, which cause the whole project to delay if they are delayed?
- How long does it take to complete the project (in minimal time)?

- Node in the graph represents the ending of a stage
- Arc (i, j) describes activity that starts when stage i is completed; arc length is the length of the activity t_{ij} > 0
- Stage j is done when all activities that end at node j (arcs (i, j)) are completed
- ▶ Nodes 1 and N are the start and end nodes
- Graph does not contain cycles



- ▶ $p = \{(1, j_1), (j_1, j_2), ..., (j_k, i)\}$ is path from start to node i
- ▶ D_p is the length of the path: $D_p = t_{1j_1} + t_{j_1j_2} + ... + t_{j_ki}$ ▶ E.g.: $D_{1\rightarrow 2\rightarrow 3} = 3 + 1 = 4$, $D_{1\rightarrow 3} = 2$
- Completion of stage i takes

$$T_i = \max_p D_p$$

- ► E.g.: completion of stage 3 takes max{4,2} = 4
- ▶ To find T_i we need to find the longest path from 1 to i
 - Does the longest path exist? Yes since there are no cycles

- ► The length of the project is the longest path from 1 to *N*; this is called the *critical* path
- Delay in any of the activities on the critical path will delay the whole project with that amount

Note: it is a shortest path problem if we multiply t_{ij} by -1

- ▶ Let S₁ be a group of stages (nodes) that do not depend on completion of any other stage
- Let S_k , when k = 1, 2, ..., be a set $S_k = \{i | \text{ all paths from 1 to } i \text{ have } \leq k \text{ arcs } \}$, where $S_0 = \{1\}$.
- ▶ The sets S_k are states of the DP, and DP-algorithm is $T_1 = 0$ and

$$T_i = \max_{(j,i)} [t_{ji} + T_j], \quad \forall i \in S_k, j \in S_{k-1}, i \notin S_{k-1}$$
 (1)

► This is "forward DP-algorithm" that starts from 1 and ends at N; computation does not change from the regular DP

► For the problem in the figure

$$\begin{split} S_0 &= \{1\}, \quad S_1 = \{1,2\}, \quad S_2 = \{1,2,3\} \\ S_3 &= \{1,2,3,4\}, \quad S_4 = \{1,2,3,4,5\} \end{split}$$

Using the algorithm (1) we get

$$T_1 = 0, T_2 = 3, T_3 = 4, T_4 = 6, T_5 = 10.$$

▶ Critical path is $1 \rightarrow 2 \rightarrow 3 \rightarrow 4 \rightarrow 5$

- The task is to compare two DNA sequences and find how similar they are
- Sequence consists of nucleotides that are named by their bases G(uanine), A(denine), C(ytosine), T(hymine)
- Sequence may contain (gaps)

Widely used Needleman-Wunsch algorithm is based on DP-algorithm in bioinformatics

Let us compare two sequences:

```
(1) G A A T T C A G T T A (2) G G A T C G A
```

They can be aligned in the following way:

```
(1) G A A T T C A G T T A
(2) G G A - T C - G - - A
```

- ► Sequence (2) has gaps
- Sequence (2) may develop to sequence (1) e.g. by mutation when one base G is transformed to A

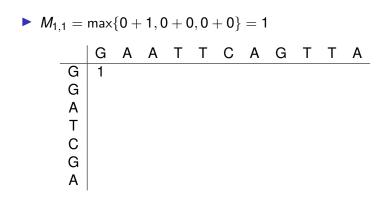
- ➤ To find out similarity of the sequences, we weight different alignments:
 - $S_{i,j} = 1$ if base in sequence 1 at place j matches the base of sequence 2 at place i; otherwise $S_{i,j} = 0$; w = 0 is a penalty for having a gap
- ► The alignment on previous slide gives:

$$S_{G,G} + S_{G,A} + S_{A,A} + w + S_{T,T} + S_{C,C} + w + S_{G,G} + 2w + S_{A,A} = 1 + 0 + 1 + 0 + 1 + 1 + 0 + 1 + 0 + 1$$

- ► The task is to find the alignment with highest score
- ▶ We design an alignment matrix whose elements are:

$$M_{i,j} = \max \left\{ egin{array}{ll} M_{i-1,j-1} + S_{i,j}, & ext{(match/no match)} \ M_{i,j-1} + w, & ext{(gap in sequence 2)} \ M_{i-1,j} + w, & ext{(gap in sequence 1)} \end{array}
ight\}$$

- ➤ This is recursion of "forward-DP", the text in the bracket gives the "control" how the sequence (2) is built
- ► Also assume that i, j = 1, 2, ... and $M_{0,0} = M_{i,0} = M_{0,j} = 0$



- $M_{1,2} = \max\{M_{0,1} + S_{1,2}, M_{1,1} + w, M_{0,2} + w\} = 1 + 0$
- $M_{1,3} = \max\{M_{0,2} + S_{1,3}, M_{1,2} + w, M_{0,3} + w\} = 1 + 0$
- $M_{2,1} = \max\{M_{1,0} + S_{2,1}, M_{2,0} + w, M_{1,1} + w\} = 0 + 1$

- $M_{2,2} = \max\{M_{1,1} + S_{2,2}, M_{2,1} + w, M_{1,2} + w\} = 1 + 0$
- $M_{3,2} = \max\{M_{2,1} + S_{3,2}, M_{3,1} + w, M_{2,2} + w\} = 1 + 1$

| | G | Α | Α | Т | Т | С | Α | G | Т | Т | Α |
|---|-------|---|---|---|---|---|---|---|---|---|---|
| G | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| G | 1 | 1 | | | | | | | | | |
| Α | 1 1 1 | 2 | | | | | | | | | |
| Τ | 1 | 2 | | | | | | | | | |
| С | 1 | 2 | | | | | | | | | |
| G | 1 | 2 | | | | | | | | | |
| Α | 1 | 2 | | | | | | | | | |

| | G | Α | Α | Т | Т | С | Α | G | Т | Т | Α |
|---|---|---|---|---|---|---|---|---|---|---|---|
| G | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| G | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 | 2 | 2 |
| Α | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 |
| Т | 1 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| С | 1 | 2 | 2 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 |
| G | 1 | 2 | 2 | 3 | 3 | 4 | 4 | 5 | 5 | 5 | 5 |
| Α | 1 | 2 | 3 | 3 | 3 | 4 | 5 | 5 | 5 | 5 | 6 |

► Maximum score is 6

- Now we find the alignment that gives score 6 by traceback-algorithm, where we move from the element of maximum score to the element M_{1,1}
- **► Traceback**: find the predecessor of *i*, *j*:
 - If M(i,j) = M(i,j-1), seq. (2) has gap at place i
 - If M(i,j) = M(i-1,j), seq. (1) has gap at place j
 - If M(i,j) > M(i-1,j), M(i,j-1), M(i-1,j-1), then element j of sequence (1) matches with element i of sequence (2)
 - If several of the above conditions hold at same time, we can move in any of the directions, i.e., there are several alignments that gives the score 6
- The example has many possible alignments

- Alignment and scoring matrix
- One possible alignment shown (notice that the sequences could be aligned in other ways, and we still get the score 6)
- (1) G A A T T C A G T T A
- (2) G G A T C G A

| | G | Α | Α | Τ | Τ | С | Α | G | Τ | Τ | Α |
|---|---|---|---|---|---|---|---|---|---|---|---|
| G | | | | | | | | | | | |
| G | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 2 | 2 | 2 | 2 |
| Α | 1 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 2 | 3 |
| Τ | 1 | 2 | 2 | 3 | 3 | 3 | 3 | 3 | 3 | 3 | 3 |
| С | 1 | 2 | 2 | 3 | 3 | 4 | 4 | 4 | 4 | 4 | 4 |
| G | 1 | 2 | 2 | 3 | 3 | 4 | 4 | 5 | 5 | 5 | 5 |
| Α | 1 | 2 | 3 | 3 | 3 | 4 | 5 | 5 | 5 | 5 | 6 |

Summary

- Deterministic problem
- Finite state space
- Shortest path problem
- DP-algorithm in shortest path problem
- Critical path analysis
- Comparison of DNA sequences