CSE 548: (Design and) Analysis of Algorithms

Dynamic Programming

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Another approach for *optimization problems*, more general and versatile than greedy algorithms.

*Optimal substructure* The optimal solution contains optimal solutions to subproblems.

*Overlapping subproblems*. Typically, the same subproblems are solved repeatedly.

Solve subproblems in *a certain order*, and *remember solutions* for later reuse.
## Topics

1. **Intro**
   - Overview
   - Topological Sort
   - DAGs and Dynamic Programming

2. **LIS**
   - DAG Formulation
   - Algorithm

3. **LCS**
   - Defn
   - Towards Soln.
   - Variations
   - Seq. Alignment

4. **Knapsack**
   - Knapsack w/ Repetition
   - 0-1 Knapsack

5. **Chain MM**
   - Memoization

6. **Fixpoints & Shortest Paths**
   - Iterative Solving
   - Shortest Path
   - SSP
   - ASP I
   - ASP II

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UNIX apps
Topological Sort

A way to linearize DAGs while ensuring that for every vertex, all its ancestors appear before itself.

Applications: Instruction scheduling, spreadsheet recomputation of formulas, Make (and other compile/build systems) and Task scheduling/project management.

Captures dependencies, and hence arises frequently in all types of programming tasks, and of course, dynamic programming!
Topological Sort

\textit{topoSort}(V, E)

\textbf{while} |V| \# 0

\textbf{if} there is a vertex v in V with in-degree of 0

\textbf{output} v

V = V \setminus \{v\}; E = E \setminus \{e \in E | e \text{ is incident on } v\}

\textbf{else output} “graph is cyclic”; \textbf{break}

\textbf{return}

![Diagram of a directed acyclic graph (DAG) with nodes labeled S, C, A, B, D, E and edges labeled with weights.](image)
Topological Sort

topoSort(V, E)

while |V| \neq 0

    if there is a vertex v in V with in-degree of 0

    output v

    V = V - \{v\}; E = E - \{e \in E | e \ text{ is incident on } v\}

else output “graph is cyclic”; break

return

Correctness:
- If there is no vertex with in-degree 0, it is not a DAG
- When the algorithm outputs v, it has already output v’s ancestors

Performance: What is the runtime? Can it be improved?
Shortest paths in DAGs

**SSPDag**\((V, E, w, s)\)

```plaintext
for u in V do
  dist(u) = \infty

dist(s) = 0

for v \in V - \{s\} in topological order do
  dist(v) = \min_{(u,v) \in E}(dist(u) + w(u, v))
```

That's all!
DAGs and Dynamic Programming

- **Canonical way to represent dynamic programming**
  - Nodes in the DAG represent subproblems
  - Edges capture dependencies between subproblems
  - Topological sorting solves subproblems in the right order
  - Remember subproblem solutions to avoid recomputation

- Many bottom-up computations on trees/dags are instances of dynamic programming
  - Applies to trees of recursive calls (w/ duplication), e.g., Fib

- For problems in other domains, DAGs are implicit, and topological sort is also done implicitly
  - Can you think of a way to do topological sorting implicitly, without modifying the dag at all?
Longest Increasing Subsequence

Definition
Given a sequence \( a_1, a_2, \ldots, a_n \), its LIS is a sequence \( a_{i_1}, a_{i_2}, \ldots, a_{i_k} \) that maximizes \( k \) subject to \( i_j < i_{j+1} \) and \( a_{i_j} \leq a_{i_{j+1}} \).

In this example, the arrows denote transitions between consecutive elements of the optimal solution. More generally, to better understand the solution space, let's create a graph of all permissible transitions: establish a node \( i \) for each element \( a_i \), and add directed edges \((i, j)\) whenever it is possible for \( a_i \) and \( a_j \) to be consecutive elements in an increasing subsequence, that is, whenever \( i < j \) and \( a_i < a_j \).
Casting LIS problem using a DAG

Nodes: represent elements in the sequence

Edges: connect an element to all followers that are larger

Topological sorting: sequence already topologically sorted

Remember: Using an array $L[1..n]$
Algorithm for LIS

\[ \textbf{LIS}(E) \]

\begin{verbatim}
for \( j = 1 \) to \( n \) do
    \( L[j] = 1 + \max_{(i,j) \in E} L[i] \)
\end{verbatim}

\textbf{return} \( \max_{j=1}^{n} L[j] \)

\textbf{Correctness:} Straight-forward

\textbf{Complexity:} What is it? Can it be improved?
Key step in Dyn. Prog.: Identifying subproblems

i. The input is $x_1, x_2, \ldots, x_n$ and a subproblem is $x_1, x_2, \ldots, x_i$.

$$
\begin{array}{cccccccc}
  x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 & x_9 & x_{10} \\
\end{array}
$$

The number of subproblems is therefore linear.

ii. The input is $x_1, \ldots, x_n$, and $y_1, \ldots, y_m$. A subproblem is $x_1, \ldots, x_i$ and $y_1, \ldots, y_j$.

$$
\begin{array}{cccccccc}
  x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 & x_9 & x_{10} \\
  y_1 & y_2 & y_3 & y_4 & y_5 & y_6 & y_7 & y_8 \\
\end{array}
$$

The number of subproblems is $O(mn)$.

iii. The input is $x_1, \ldots, x_n$ and a subproblem is $x_i, x_{i+1}, \ldots, x_j$.

$$
\begin{array}{cccccccc}
  x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & x_7 & x_8 & x_9 & x_{10} \\
\end{array}
$$

The number of subproblems is $O(n^2)$.

iv. The input is a rooted tree. A subproblem is a rooted subtree.
Definition

A sequence $a[1..m]$ is a subsequence of $b[1..n]$ occurring at position $r$ if there exist $i_1, ..., i_k$ such that $a[r..(r+l-1)] = b[i_1]b[i_2] \cdots b[i_l]$, where $i_j < i_{j+1}$

The relative order of elements is preserved in a subsequence, but unlike a substring, the elements need not be contiguous.

Example: $BDEFHJ$ is a subsequence of $ABCDEFGHIJK$
Longest Common Subsequence

Definition (LCS)

The LCS of two sequences $x[1..m]$ and $y[1..n]$ is the longest sequence $z[1..k]$ that is a subsequence of both $x$ and $y$.

*Example:* BEHJ is a common subsequence of \textit{ABCDEFGHIJKLMNOP}\textit{LM} and \textit{AABBXEHJHZ}

By aligning elements of $z$ with the corresponding elements of $x$ and $y$, we can compare $x$ and $y$

$x: \ P \ R \ O \ F \quad - \quad E \ S \ S \quad O \ R$

$z: \ P \ R \ O \ F \quad - \quad E \ S \quad - \quad - \quad R$

$y: \ P \ R \ O \ F \ \text{F}_{\text{ins}} \ E \ S \quad -_{\text{del}} \ U_{\text{sub}} \ R$

To identify the \textit{edit} operations (insert, delete, substitute) operations needed to map $x$ to $y$
Edit (Levenshtein) distance

Definition (ED)

Given sequences $x$ and $y$ and functions $I$, $D$ and $S$ that associate costs with each insert, delete and substitute operations, what is the minimum cost of any the edit sequence that transforms $x$ into $y$.

Applications

- Spell correction (Levenshtein automata)
- diff
- In the context of version control, reconcile/merge concurrent updates by different users.
- DNA sequence alignment, evolutionary trees and other applications in computational biology
Towards a dynamic programming solution (1)

What subproblems to consider?

- Just like the LIS problem, we proceed from left to right, i.e., compute $L[j]$ as $j$ goes from 1 to $n$.

- But there are two strings $x$ and $y$ for LCS, so the subproblems correspond to prefixes of both $x$ and $y$ — there are $O(mn)$ such prefixes.

E X P O N E N T I A L

P O L Y N O M I A L

The subproblem above can be represented as $E[7, 5]$. $E[i, j]$ represents the edit distance of $x[1..i]$ and $y[1..j]$. 
Towards a dynamic programming solution (2)

For $E[k, l]$, consider the following possibilities:

- $x[k] = y[l]$: in this case, $E[k, l] = E[k - 1, l - 1]$ — the edit distance has not increased as we extend the string by one character, since these characters match

- $x[k] \neq y[l]$: Three possibilities
  - extend $E[k - 1, l]$ by deleting $x[k]$: $E[k, l] = E[k - 1, l] + DC(x[k])$
  - extend $E[k, l - 1]$ by inserting $y[l]$: $E[k, l] = E[k, l - 1] + IC(y[l])$
  - extend $E[k - 1, l - 1]$ by substituting $x[k]$ with $y[l]$: $E[k, l] = E[k - 1, l - 1] + SC(x[k], y[l])$
Towards a dynamic programming solution (3)

\[ E[k, l] = \min( E[k - 1, l] + DC(x[k]), \quad \text{// ↓} \]
\[ E[k, l - 1] + IC(y[l]), \quad \text{// →} \]
\[ E[k - 1, l - 1] + SC(x[k], y[l])) \quad \text{// \↓} \]

\[ E[0, l] = \sum_{i=1}^{l} IC(y[i]) \]
\[ E[k, 0] = \sum_{i=1}^{k} DC(x[i]) \]

Edit distance = \( E[m, n] \)

(Recall: \( m \) and \( n \) are lengths of strings \( x \) and \( y \))
Towards a dynamic programming solution (4)

Figure 6.4(a) The table of subproblems. Entries $E(i-1, j-1)$, $E(i-1, j)$, and $E(i, j-1)$ are needed to fill in $E(i, j)$. (b) The final table of values found by dynamic programming.

For $i = 0, 1, 2, \ldots, m$:

$$E(i, 0) = i$$

For $j = 1, 2, \ldots, n$:

$$E(0, j) = j$$

For $i = 1, 2, \ldots, m$:

$$E(i, j) = \min\{E(i-1, j) + 1, E(i, j-1) + 1, E(i-1, j-1) + \text{diff}(i, j)\}$$

This procedure fills in the table row by row, and left to right within each row. Each entry takes constant time to fill in, so the overall running time is just the size of the table, $O(mn)$.

And in our example, the edit distance turns out to be 6:

The underlying dag

Every dynamic program has an underlying dag structure: think of each node as representing a subproblem, and each edge as a precedence constraint on the order in which the subproblems can be tackled. Having nodes $u_1, \ldots, u_k$ point to $v$ means "subproblem $v$ can only be solved once the answers to $u_1, \ldots, u_k$ are known."

In our present edit distance application, the nodes of the underlying dag correspond to subproblems, or equivalently, to positions $(i, j)$ in the table. Its edges are the precedence constraints, of the form $(i-1, j) \rightarrow (i, j)$, $(i, j-1) \rightarrow (i, j)$, and $(i-1, j-1) \rightarrow (i, j)$ (Figure 6.5).

In fact, we can take things a little further and put weights on the edges so that the edit distance is calculated as

$$E[k, l] = \min(E[k-1, l] + DC(x[k]), // \downarrow$$

$$E[k, l-1] + IC(y[l]), // \rightarrow$$

$$E[k-1, l-1] + SC(x[k], y[l])) // \downarrow$$
Towards a dynamic programming solution (5)

Figure 6.5

The underlying dag, and a path of length 6.

\[ E[k, l] = \min(E[k-1, l] + DC(x[k]), E[k, l-1] + IC(y[l]), E[k-1, l-1] + SC(x[k], y[l])) \]
Variations

**Approximate prefix:**

Is \( y \) approx. prefix of \( x \)? Decide based on

\[
max_{1 \leq k \leq m} E[k, n]
\]

**Approximate suffix:**

Initialize \( E[k, 0] = 0 \), use \( E[m, n] \) to determine if \( y \) is an approximate suffix of \( x \).

**Approximate substring:**

Initialize \( E[k, 0] = 0 \), use \( max_{1 \leq k \leq m} E[k, n] \) to decide if \( y \) is an approximate substring of \( x \).
More variations

Supporting transpositions:

Use a fourth term within \( \min \):

\[
E[k - 2, l - 2] + TC(x[k - 1]x[k], y[l - 1]y[l])
\]

where \( TC \) is a small value for transposed characters, and \( \infty \) otherwise.
Similarity Vs Edit-distance

**Edit-distance** cannot be interpreted on its own, and needs to take into account the lengths of strings involved.

**Similarity** can stand on its own.

\[ S[k, l] = \max(S[k-1, l] - DC(x[k]), S[k, l-1] - IC(y[l]), S[k-1, l-1] - SC(x[k], y[l])) \]

\[ S[0, l] = - \sum_{i=1}^{l} IC(y[i]) \]

\[ S[k, 0] = - \sum_{i=1}^{k} DC(x[i]) \]

- \( SC(r, r) \) should be negative, while \( IC \) and \( DC \) should be positive.
- Formulations in biology are usually based on similarity
Global alignment (DNA, proteins, ...)

- Similar to edit distance, but uses similarity scores

- Gaps are scored differently: a contiguous sequence of $n$ deletions does not get penalized as much as $n$ times a single deletion. (same applies to insertions.)

- Captures the idea that large deletions/insertions are much more likely in nature than many small ones. (Think of chromosomal crossover during meiotic cell division.)

- Obvious formulation to support such gap metrics will lead to more expensive algorithms: $S[k, l]$ depends on $S[k - d, l]$ and $S[k, l - i]$ for any $d < k$ and $i < l$. But a more careful formulation can get back to quadratic time

- Quadratic time still too slow for sequence alignment.
Local alignment

- Aimed at identifying local regions of similarity, specifically, the best matches between subsequences of $x$ and $y$

- $S[i, j]$ now represents the best alignment of some suffix of $x[1..i]$ and $y[1..j]$.

- A new term is introduced within $max$, namely, zero. This means that costs can never become negative.

- In other words, a subsequence does not incur costs because of mismatches preceding the subsequence.

- This change enables regions of similarity to stand out as positive scores.

- Initialize $F[i, 0] = F[0, j] = 0$
Improvements to ED Algorithm

Linear-space: $O(mn)$ is not so good for large $m, n$.

- Slow in terms of runtime
- (Possibly) unacceptable in terms of space usage
  - If we are only interested in ED, we can use linear space: retain only the last column computed.
  - But if want the actual edits, we need $O(mn)$ space with the algorithms discussed so far.

Linear-space algorithms developed to overcome this problem.

Better overall performance: $O(md)$ space and runtime if the maximum distance is limited to $d$.

In the interest of time, we won’t cover these extensions. They are fairly involved, but not necessarily hard.
LCS application: UNIX diff

Each line is considered a “character:”

- Number of lines far smaller than number of characters
- Difference at the level of lines is easy to convey to users
- Much higher degree of confidence when things line up. Leads to better results on programs.

**But does not work that well on document types where line breaks are not meaningful,** e.g., text files where each paragraph is a line.

Aligns lines that are preserved.

- The edits are then printed in the familiar “diff” format.
Software patches often distributed as “diffs.” Programs such as `patch` can apply these patches to source code or any other file.

Concurrent updates in version control systems are resolved using LCS.

- Let \( x \) be the version in the repository
- Suppose that user \( A \) checks it out, edits it to get version \( y \)
- Meanwhile, \( B \) also checks out \( x \), edits it to \( z \).
- If \( x \rightarrow y \) edits target a disjoint set of locations from those targeted by the \( x \rightarrow z \) edits, both edits can be committed; otherwise a conflict is reported.
Summary

- A general approach for optimization problems

Applicable in the presence of:

- Optimal substructure
- A natural ordering among subproblems
- Numerous subproblems (often, exponential), but only some (polynomial number) are distinct
Knapsack Problem (Recap)

- You have a choice of items you can pack in the sack
- Maximize value of sack, subject to a weight limit of $W$

<table>
<thead>
<tr>
<th>item</th>
<th>calories/lb</th>
<th>weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>bread</td>
<td>1100</td>
<td>5</td>
</tr>
<tr>
<td>butter</td>
<td>3300</td>
<td>1</td>
</tr>
<tr>
<td>tomato</td>
<td>80</td>
<td>1</td>
</tr>
<tr>
<td>cucumber</td>
<td>55</td>
<td>2</td>
</tr>
</tbody>
</table>

Fractional knapsack: Fractional quantities acceptable

0-1 knapsack: Take all of one item or none at all

Knapsack w/ repetition: Take any integral number of items.

No polynomial solution for the last two, but dynamic programming can solve them in \textit{pseudo-polynomial} time of $O(nW)$. 
Consider subproblems by reducing the weight

- Compute $K(W)$ in terms of $K(W')$ for $W' < W$

Which $W'$ values to consider?

- Since the $i$th item has a weight $w_i$, we should consider only $W - w_i$ for different $i$.

**Optimal substructure:** If $K(W)$ is the optimal solution and it includes item $i$, then $K(W) = K(W - w_i) + v_i$
Knapsack w/ repetition

\[ \text{KnapWithRep}(w, v, n, W) \]

\[
K[0] = 0 \\
\text{for } w = 1 \text{ to } W \text{ do} \\
K[w] = \max_{1 \leq i \leq n, w[i] \leq w}(K[w - w[i]] + v[i]) \\
\text{return } K[W]
\]

- Fills the array \( K \) from left-to-right
  - If you construct the dag explicitly, you will see that we are looking for the longest path!

- **Runtime:** Outer loop iterates \( W \) times, \( \max \) takes \( O(n) \) time, for a total of \( O(nW) \) time

- **Not polynomial:** input size logarithmic (not linear) in \( W \).
Previous algorithm does not work. We need to keep track of which items have been used up.

Key idea: Define 2-d array $K[u, j]$ which computes optimal value for weight $u$ achievable using items 1..$j$

- $K[u, j]$ can be computed from $K[\_, j - 1]$
  - Either item $j$ is not included in the optimal solution. Then $K[u, j] = K[u, j - 1]$
  - Or, $j$ is included, so $K[u, j] = v[j] + K[u - w[j], j - 1]$
- So, fill up the array $K$ as $j$ goes from 1 to $n$
- For each $j$, fill $K$ as $u$ goes from 1 to $W$
0-1 Knapsack Algorithm

\[ Knap01(w, v, n, W) \]

\[
K[u, 0] = K[0, j] = 0, \forall 1 \leq u \leq W, 1 \leq j \leq n
\]

for \( j = 1 \) to \( n \) do

\[
\text{for } u = 1 \text{ to } W \text{ do}
\]

\[
\text{if } w[j] > u \text{ then } K[u, j] = K[u, j - 1]
\]

\[
\text{else } K[u, j] = \max(K[u, j - 1],
K[u - w[j], j - 1] + v[j])
\]

return \( K[W, n] \)

Runtime: As compared to unbounded knapsack, we have a nested loop here, but the inner loop now executes in \( O(1) \) time. So runtime is still \( O(nW) \)
Chain Matrix Multiplication

(a) $A \times B \times C = A \times (B \times C)$

$A$ $50 \times 20$
$B$ $20 \times 1$
$C$ $1 \times 10$

(b) $(A \times (B \times C)) \times D$

$A$ $50 \times 20$
$B \times C$ $20 \times 10$
$D$ $10 \times 100$

(c) $A \times (B \times C)$

$A \times (B \times C)$ $50 \times 10$

(d) $(A \times (B \times C)) \times D$

$(A \times (B \times C)) \times D$ $50 \times 100$

<table>
<thead>
<tr>
<th>Parenthesization</th>
<th>Cost computation</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A \times ((B \times C) \times D)$</td>
<td>$20 \cdot 1 \cdot 10 + 20 \cdot 10 \cdot 100 + 50 \cdot 20 \cdot 100$</td>
<td>120,200</td>
</tr>
<tr>
<td>Greedy</td>
<td>$20 \cdot 1 \cdot 10 + 50 \cdot 20 \cdot 10 + 50 \cdot 10 \cdot 100$</td>
<td>60,200</td>
</tr>
<tr>
<td>$(A \times (B \times C)) \times D$</td>
<td>$50 \cdot 20 \cdot 1 + 1 \cdot 10 \cdot 100 + 50 \cdot 1 \cdot 100$</td>
<td>7,000</td>
</tr>
</tbody>
</table>
Chain MM: Formulating Optimal Solution

Consider outermost multiplication:

\[(M_1 \times \cdots \times M_j) \times (M_{j+1} \times \cdots \times M_n)\] — we could compute \(j\) using dynamic programming

Optimal substructure: Note that the optimal solution for

\[(M_1 \times \cdots \times M_j) \times (M_{j+1} \times \cdots \times M_n)\] must rely on optimal solutions to \(M_1 \times \cdots \times M_j\) and \(M_{j+1} \times \cdots \times M_n\) — or else we could improve the overall solution still

Cost function: This suggests a cost function \(C[k, l]\) to denote the optimal cost of \(M_k \times \cdots \times M_l\)
Figure 6.7 (a) \(((A \times B) \times C') \times D\); (b) \(A \times ((B \times C') \times D)\); (c) \((A \times (B \times C')) \times D\).

- Subproblems correspond to one of the subtrees
- Since order of multiplications can’t be changed, each subtree must correspond to a “substring” of multiplications, i.e., \(M_k \times \cdots \times M_l\)
Chain MM Algorithm

\textbf{chainMM}(m, n)

\[ C[i, i] = 0 \ \forall 1 \leq i \leq n \]

\textbf{for} \ s = 1 \textbf{ to } n - 1 \textbf{ do}

\hspace{1em} \textbf{for} \ k = 1 \textbf{ to } n - s \textbf{ do}

\hspace{2em} l = k + s

\hspace{2em} C[k, l] = \min_{k \leq i < l}(C[k, i] + C[i + 1, l] + m_{k-1} \times m_i \times m_l)

\textbf{return} \ C[1, n]

\textbf{Note:} \ m_i's \ give \ us \ the \ dimension \ of \ matrices, \ specifically, \ M_i \ is \ an \ m_{i-1} \times m_i \ matrix

\textbf{Complexity:} \ O(n^3)
Recursive formulation of Dynamic programming

- Recursive formulation can often simplify algorithm presentation, avoiding need for explicit scheduling
- Dependencies between subproblems can be left implicit an equation such as $K[w] = K[w - w[j]] + v[j]$
- A call to compute $K[w]$ will automatically result in a call to compute $K[w - w[j]]$ because of dependency
- Can avoid solving (some) unneeded subproblems

Memoization: Remember solutions to function calls so that repeat invocations can use previously returned solutions
Recursive 0-1 Knapsack Algorithm

**BestVal01**(u, j)

- if u = 0 or j = 0 return 0
- if w[j] > u return BestVal01(u, j−1)
- else return max(BestVal01(u, j−1), v[j] + BestVal01(u−w[j], j−1))

- Much simpler in structure than iterative version
- Unneeded entries are not computed, e.g. BestVal01(3, _) when all weights involved are even
- **Exercise:** Write a recursive version of ChainMM.

**Note:** m_i’s give us the dimension of matrices, specifically, M_i is an $m_{i−1} \times m_i$ matrix

**Complexity:** $O(n^3)$
Dyn. Prog. and Equation Solving

- The crux of a dynamic programming solution: set up equation to captures a problem’s optimal substructure. The equation implies dependencies on subproblem solutions.
- Dynamic programming algorithm: finds a schedule that respects these dependencies
- Typically, dependencies form a DAG: its topological sort yields the right schedule
- Cyclic dependencies: What if dependencies don’t form a DAG, but is a general graph.
- Key Idea: Use iterative techniques to solve (recursive) equations
Fixpoints

- A fixpoint is a solution to an equation:
- Substitute the solution on the rhs, it yields the lhs.

**Example 1:** \( y = y^2 - 12. \)
- A fixpoint is \( y = 4, \) another is \( y = -3. \)

\[
\left. \text{rhs} \right|_{y=4} = 4^2 - 12 = 4 = \left. \text{lhs} \right|_{y=4} \quad \text{— a fixpoint}
\]
A fixpoint is a solution to an equation:

**Example 2**: $7x = 2y - 4$, $y = x^2 + y/x + 0.5$.

- One fixpoint is $x = 2$, $y = 9$.

$$rhs_1|_{x=2,y=9} = 14 = lhs_1|_{x=2,y=9}$$

$$rhs_2|_{x=2,y=9} = 9 = lhs_2|_{x=2,y=9}$$

- The term “fixpoint” emphasizes an iterative strategy.

**Example techniques**: Gauss-Seidel method (linear system of equations), Newton’s method (finding roots), ...
Convergence

Convergence is a major concern in iterative methods

- *For real-values variables*, need to start close enough to the solution, or else the iterative procedure may not converge.
- *In discrete domains*, rely on *monotonicity* and *well-foundedness*.
  
  **Well-founded order:** An order that has no infinite ascending chain (i.e., sequence of elements $a_0 < a_1 < a_2 < \cdots$ where there is no maximum)

  **Monotonicity:** Successive iterations produce larger values with respect to the order, i.e., $\text{rhs}|_{\text{sol}_i} \geq \text{sol}_i$

  **Result:** Start with an initial guess $S^0$, note $S^i = \text{rhs}|_{S^{i-1}}$.
  
  - Due to monotonicity, $S^i \geq S^{i-1}$, and
  - by well-foundedness, the chain $S^0, S^1, \ldots$ can’t go on forever.
  - Hence iteration must converge, i.e., $\exists k \forall i > k \ S^i = S^k$
Role of Iterative Solutions

- **Fixpoint iteration resembles an inductive construction**
  - $S^0$ is the base case, $S^i$ construction from $S^{i-1}$ is the induction step.

- Drawback of *explicit fixpoint iteration*: hard to analyze the number of iterations, and hence the runtime complexity

- So, algorithms tend to rely on inductive, bottom-up constructions with enough detail to reason about runtime.

- Fixpoint iteration thus serves two main purposes:
  - When it is possible to bound its complexity in advance, e.g., non-recursive definitions
  - As an intermediate step that can be manually analyzed to uncover inductive structure explicitly.
Shortest Path Problems

Graphs with cycles: Natural example where the optimal substructure equations are recursive.

Single source: \[ d_v = \min_{u \mid (u,v) \in E} \left( d_u + l_{uv} \right) \]

All pairs: \[ d_{uv} = \min_{w \mid (w,v) \in E} \left( d_{uw} + l_{wv} \right) \]

or, alternatively, \[ d_{uv} = \min_{w \in V} \left( d_{uw} + d_{wv} \right) \]

Our study of shortest path algorithms is based on fixpoint formulation

- Shows how different shortest path algorithms can be derived from this perspective
- Highlights the similarities between these algorithms, making them easier to understand/remember
**Single-source shortest paths**

For the source vertex $s$, $d_s = 0$. For $v \neq s$, we have the following equation that captures the optimal substructure of the problem. We use the convention $l_{uu} = 0$ for all $u$, as it simplifies the equation:

$$d_v = \min_{u \mid (u,v) \in E} (d_u + l_{uv})$$

Expressing edge lengths as a matrix, this equation becomes:

$$
\begin{bmatrix}
  d_1 \\
  d_2 \\
  \vdots \\
  d_j \\
  \vdots \\
  d_n
\end{bmatrix} = 
\begin{bmatrix}
  l_{11} & l_{21} & \cdots & l_{1n} \\
  l_{12} & l_{22} & \cdots & l_{1n} \\
  \vdots & \vdots & \ddots & \vdots \\
  l_{1j} & l_{2j} & \cdots & l_{1n} \\
  \vdots & \vdots & \ddots & \vdots \\
  l_{1n} & l_{2n} & \cdots & l_{nn}
\end{bmatrix}
\begin{bmatrix}
  d_1 \\
  d_2 \\
  \vdots \\
  d_j \\
  \vdots \\
  d_n
\end{bmatrix}
$$

Matches the form of linear simultaneous equations, except that point-wise multiplication and addition become the integer “+” and $\min$ operations respectively.
Single-source shortest paths

SSP, written as a recursive matrix equation is:

\[ D = LD \]

Now, solve this equation iteratively:

\[
\begin{align*}
D^0 &= Z \\
D^1 &= LZ \\
D^2 &= LD^1 = L(LZ) = L^2Z
\end{align*}
\]

Or, more generally, \( D^i = L^iZ \)

- \( L \) is the generalized adjacency matrix, with entries being edge weights (aka edge lengths) rather than booleans.

- Side note: In this domain, multiplicative identity \( I \) is a matrix with zeroes on the main diagonal, and \( \infty \) in all other places.

- So, \( L = I + L \), and hence \( L^* = \lim_{r \to \infty} L^r \)
Single-source shortest paths

- Recall the connection between paths and the entries in \( L^i \).
- Thus, \( D^i \) represents the shortest path using \( i \) or fewer edges!
- Unless there are cycles with negative cost in the graph, all shortest paths must have a length less than \( n \), so:
  - \( D^n \) contains all of the shortest paths from the source vertex \( s \)
  - \( d^n_i \) is the shortest path length from \( s \) to the vertex \( i \).

Computing \( L \times L \) takes \( O(n^3) \), so overall SSP cost is \( O(n^4) \).
SSP: Improving Efficiency of Matrix Formulation

- Compute the product from right: \((L \times (L \times \cdots (L \times Z) \cdots))\)
  - Each multiplication involves \(n \times n\) and \(1 \times n\) matrix, so takes \(O(n^2)\) instead of \(O(n^3)\) time.
  - Overall time reduced to \(O(n^3)\).

- To compute \(L \times d_j\), enough to consider neighbors of \(j\), and not all \(n\) vertices
  \[d^i_j = \min_{k \mid (k, j) \in E} (d^{i-1}_k + l_{kj})\]

- Computes each matrix multiplication in \(O(|E|)\) time, so we have an overall \(O(|E||V|)\) algorithm.

- *We have stumbled onto the Bellman-Ford algorithm!*
Further Optimization on Iteration

\[ d_j^i = \min_{k \mid (k,j) \in E} (d_k^{i-1} + l_{kj}) \]

- **Optimization 1**: If none of the \( d_k \)'s on the rhs changed in the previous iteration, then \( d_j^i \) will be the same as \( d_j^{i-1} \), so we can skip recomputing it in this iteration.

- Can be an useful improvement in practice, but asymptotic complexity unchanged from \( O(|V||E|) \)
Optimizing Iteration

\[ d_j^i = \min_{k \mid (k,j) \in E} (d_{k}^{i-1} + l_{kj}) \]

**Optimization 2:** Wait to update \( d_j \) on account of \( d_k \) on the rhs until \( d_k \)'s cost stabilizes

- Avoids repeated propagation of min cost from \( k \) to \( j \) — instead propagation takes place just once per edge, i.e., \( O(|E|) \) times
- If all weights are non-negative, we can determine when costs have stabilized for a vertex \( k \)
  - There must be at least \( r \) vertices whose shortest path from the source \( s \) uses \( r \) or fewer edges.
  - In other words, if \( d_k^i \) has the \( r \)th lowest value, then \( d_k^i \) has stabilized if \( r \leq i \)

Voila! We have Dijkstra’s Algorithm!
All pairs Shortest Path (l)

\[ d_{uv}^i = \min_{w \mid (w, v) \in E} (d_{uw}^{i-1} + l_{wv}) \]

- Note that \( d_{uv} \) depends on \( d_{uw} \), but not on any \( d_{xy} \), where \( x \neq u \).
- So, solutions for \( d_{xy} \) don’t affect \( d_{uv} \).
- i.e., we can solve a separate SSP, each with one of the vertices as source
- i.e., we run Dijkstra’s \(|V|\) times, overall complexity \( O(|E||V| \log |V|) \)
All pairs Shortest Path (II)

\[ d_{uv}^i = \min_{w \in E} (d_{uw}^{i-1} + d_{wv}^{i-1}) \]

Matrix formulation:

\[ D = D \times D \]

with \( D^0 = L \).

Iterative formulation of the above equation yields

\[ D^i = L^{2i} \]

We need only consider paths of length \( \leq n \), so stop at \( i = \log n \).

Thus, overall complexity is \( O(n^3 \log n) \), as each step requires \( O(n^3) \) multiplication.

*We have just uncovered a variant of Floyd-Warshall algorithm!*

- Typically used with matrix-multiplication based formulation.

*Matches ASP I complexity for dense graphs* (\(|E| = \Theta(|V|^2))
Further Improving ASP II

Each step has $O(n^3)$ complexity as it considers all $(u, w, v)$ combinations.

*Note:* Blind fixpoint iteration “breaks” recursion by limiting path length.

- Converts $d_{uv}$ into $d_{uv}^i$ where $i$ is the path length
- Worked well for SSP & ASP I, not so well for ASP II

*Can we break cycles by limiting something else,* say, vertices on the path?

*Floyd-Warshall:* Define $d_{uv}^k$ as the shortest path from $u$ to $v$ that only uses intermediate vertices 1 to $k$.

$$d_{uv}^k = \min(d_{uv}^{k-1}, d_{uk}^{k-1} + d_{kv}^{k-1})$$

*Complexity:* Need $n$ iterations to consider $k = 1, \ldots, n$ but each iteration considers only $n^2$ pairs, so overall runtime becomes $O(n^3)$
Summary

- A versatile, robust technique to solve optimization problems

- **Key step:** Identify *optimal substructure* in the form of an equation for optimal cost

- If equations are non-recursive, then either
  - identify underlying DAG, compute costs in topological order, or,
  - write down a memoized recursive procedure

- For recursive equations, “break” recursion by introducing additional parameters.
  - A fixpoint iteration can help expose such parameters.

- Remember the choices made while computing the optimal cost, use these to construct optimal solution.