Biomedica informatics: Lecture 14

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1 Lecture 14: Longest Common Subsequence

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Longest common subsequence (LCS) problem

Dynamic Programming Approach

LCS : Longest Common Subsequence

Let $X, Y \in Seq$ be the sequences to compare, and X_i, Y_j be the subsequences of their first i, j characters, respectively.

The integer function

$$LCS : Seq \times Seq \rightarrow Nat$$

gives the integer length of longest common subsequence of any two (sub)sequences, as follows:

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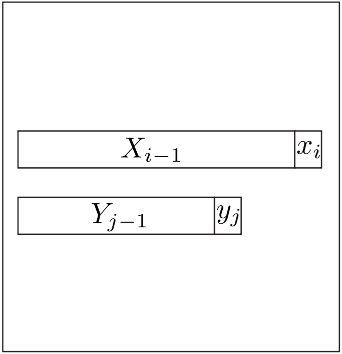
$$LCS(X_i, Y_j) = \begin{cases} 0 & \text{if } i = 0 \text{ or } j = 0 \\ LCS(X_{i-1}, Y_{j-1}) + 1 & \text{if } x_i = y_j \\ \max(LCS(X_i, Y_{j-1}), LCS(X_{i-1}, Y_j)) & \text{if } x_i \neq y_j \end{cases}$$

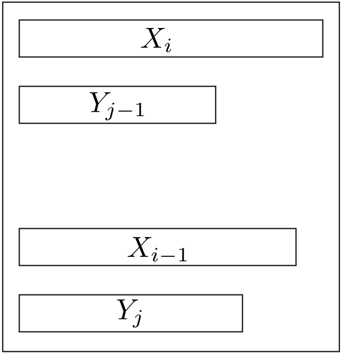
Longest common subsequence

LCS function defined

$x_i = y_j$

$LCS(X_i, Y_j) = LCS(X_{i-1}, Y_{j-1}) + 1$





$x_i \neq y_j$

$LCS(X_i, Y_j) = \max(LCS(X_i, Y_{j-1}), LCS(X_{i-1}, Y_j))$

Recursive implementation

just write down in Python the recursive equations above

```python
def cls(X,Y):
    i,j = len(X),len(Y)
    if i == 0 or j == 0: return 0
    elif X[i-1] == Y[j-1]: return cls(X[:i-1],Y[:j-1])+1
    else: return max(cls(X[:i],Y[:j-1]),cls(X[:i-1],Y[:j]))
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```
print cls("BASKETBALL","BASEBALL") ≡ 8
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OK !

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print cls("ABRACADABRA","SUPERCALIFRAGILISTICESPIRALIDOSO")
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print cls("BASKETBALL","BASEBALL") ≡ 8
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OK !

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print cls("ABRACADABRA","SUPERCALIFRAGILISTICESPIRALIDOSO")
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VERY long execution time ... WHY ?

... because of recursion nonlinearity

the execution time is exponential with the sequence lengths

a recursion is said linear if the definition right-hand side contains at most one recursive function call

- nonlinear recursion: $\binom{n}{k} = \binom{n-1}{k} + \binom{n-1}{k-1}$ complexity: $O(2^n)$

```
def binomial(n,k):
    if k == 0 or n == k: return 1
    else: return binomial(n-1,k) + binomial(n-1,k-1)
```

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```
def binomial(n,k):
    if k == 0 or n == k: return 1
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```

- linear recursion: $\binom{n}{k} = \binom{n-1}{k-1} \times \frac{n}{k}$ complexity: $O(n)$

```
def binomial(n,k):
    if k == 0 or n == k: return 1
    else: return binomial(n-1,k-1) * n / k
```

Memoization technique

In computing, "memoization" is an optimization technique used primarily to speed up computer programs by having function calls avoid repeating the calculation of results for previously-processed input

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- This technique of saving values that have already been calculated is frequently used
- Memoization is a means of lowering a function’s time cost in exchange for space cost; that is, memoized functions become optimized for speed in exchange for a higher use of computer memory space.
- An efficient LCS procedure requires: saving the solutions to one level of subproblem in a table so that the solutions are available to the next level of subproblems.

Length of the Longest Common Subsequence

computing the function *LCS* : *Seq* × *Seq* → *Nat* with memoization

```python
def LCS(X, Y):
    m,n = len(X),len(Y)
    # An (m+1) times (n+1) matrix
    C = [[0] * (n+1) for i in range(m+1)]
    for i in range(1, m+1):
        for j in range(1, n+1):
            if X[i-1] == Y[j-1]:
                C[i][j] = C[i-1][j-1] + 1
            else:
                C[i][j] = max(C[i][j-1], C[i-1][j])
    return C
```

Usage example — LCSfunction

```
>>> X = "AATCC"
>>> Y = "ACACG"
>>> m = len(X)
>>> n = len(Y)
>>> C = LCS(X, Y)
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>>> C = LCS(X, Y)
```

```
>>> print C
[[0, 0, 0, 0, 0, 0],
 [0, 1, 1, 1, 1, 1],
 [0, 1, 1, 2, 2, 2],
 [0, 1, 1, 2, 2, 2],
 [0, 1, 2, 2, 3, 3],
 [0, 1, 2, 2, 3, 3]]
```

Usage example — LCSfunction

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>>> C = LCS(X, Y)
```

```
>>> print C
[[0, 0, 0, 0, 0, 0, 0, 0, 0, 0],
 [0, 1, 1, 1, 1, 1, 1, 1, 1, 1],
 [0, 1, 2, 2, 2, 2, 2, 2, 2, 2],
 [0, 1, 2, 2, 2, 3, 3, 3, 3, 3],
 [0, 1, 2, 2, 2, 3, 4, 4, 4, 4],
 [0, 1, 2, 3, 3, 3, 4, 4, 5, 5],
 [0, 1, 2, 3, 4, 4, 4, 4, 5, 6],
 [0, 1, 2, 3, 4, 4, 4, 4, 5, 6],
 [0, 1, 2, 3, 4, 5, 5, 5, 5, 6],
 [0, 1, 2, 3, 4, 5, 6, 6, 6, 6],
 [0, 1, 2, 3, 4, 5, 6, 7, 7, 7],
 [0, 1, 2, 3, 4, 5, 6, 7, 8, 8]]
```

Reading out an LCS

Backtracking on the table from the lower-right corner

```python
def backTrack(C, X, Y, i, j):
    if i == 0 or j == 0:
        return ""
    elif X[i-1] == Y[j-1]:
        return backTrack(C, X, Y, i-1, j-1) + X[i-1]
    else:
        if C[i][j-1] > C[i-1][j]:
            return backTrack(C, X, Y, i, j-1)
        else:
            return backTrack(C, X, Y, i-1, j)
```

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>>> X = "AATCC"
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>>> m = len(X)
>>> n = len(Y)
>>> C = LCS(X, Y)
```

```
>>> print "Some LCS: '%s'" % backTrack(C, X, Y, m, n)
Some LCS: 'AAC'
```

Usage example — backTrack function

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>>> X = "ATGGCCTGGAC"
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```
>>> X = "ATGGCCTGGAC"
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>>> m = len(X)
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>>> C = LCS(X, Y)
```

```
>>> print "Some LCS: '%s'" % backTrack(C, X, Y, m, n)
Some LCS: 'ATCCGGAC'
```

Reading out all LCSs

```
def backTrackAll(C, X, Y, i, j):
    if i == 0 or j == 0:
        return set([""])
    elif X[i-1] == Y[j-1]:
        return set([Z + X[i-1]
                   for Z in backTrackAll(C, X, Y, i-1, j-1)])
    else:
        R = set()
        if C[i][j-1] >= C[i-1][j]:
            R.update(backTrackAll(C, X, Y, i, j-1))
        if C[i-1][j] >= C[i][j-1]:
            R.update(backTrackAll(C, X, Y, i-1, j))
        return R
```

Usage example — backTrackAll function

```
>>> X = "AATCC"
>>> Y = "ACACG"
>>> m = len(X)
>>> n = len(Y)
>>> C = LCS(X, Y)
```

Usage example — backTrackAll function

```
>>> X = "AATCC"
>>> Y = "ACACG"
>>> m = len(X)
>>> n = len(Y)
>>> C = LCS(X, Y)
```

```
>>> print "All LCSs: %s" % backTrackAll(C, X, Y, m, n)
All LCSs: set(['ACC', 'AAC'])
```

Usage example — backTrackAll function

```
>>> X = "ATGGCCTGGAC"
>>> Y = "ATCCGGACC"
>>> m = len(X)
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>>> C = LCS(X, Y)
```

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```

```
>>> print "All LCSs: %s" % backTrackAll(C, X, Y, m, n)
All LCSs: set(['ATCCGGAC'])
```

BLAST (Basic Local Alignment Search Tool)

BLAST program

Comparison of nucleotide or protein sequences

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How to do Batch BLAST jobs

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- Most likely these are isolated as amplified products from a library of some sort
- There is no need to manually cut and paste a 100 sequences in to the BLAST web pages
- Using the BLAST web pages it is possible to input "batches" of sequences into one form and retrieve the results
- There are two methods to do batch BLAST jobs
- The first is through the web interface and the second is using the standalone BLAST binaries and downloaded NCBI databases

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BLAST

Example

- BLAST paper
- QuickStart: Example-Driven Web-Based BLAST Tutorial

FASTA (FAST Alignement)

FASTA

Example

FASTA stands for FAST-ALL, reflecting the fact that it can be used for a fast protein comparison or a fast nucleotide comparison

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- Increasing the ktup decreases the number of background hits
- Not every word hit is investigated but instead initially looks for segment's containing several nearby hits

FASTA Web services

Both REST and SOAP web service interfaces are exposed

REST Sample clients are provided for a number of programming languages.

SOAP RPC/encoded SOAP service