

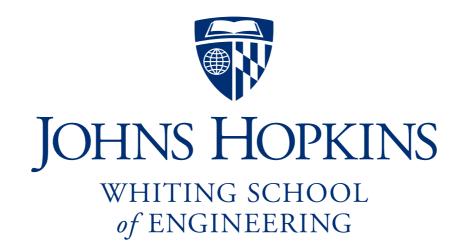
Sequence Learning

Comparing Sequences

Korbinian Riedhammer

Dynamic programming and edit distance

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Department of Computer Science

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Beyond approximate matching: sequence similarity

In many settings, Hamming and edit distance are too simple. Biologically-relevant distances require algorithms. We will expand our tool set accordingly.

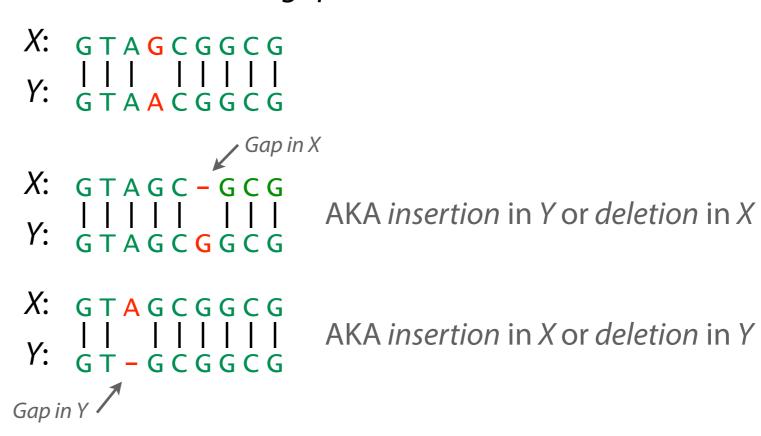
```
Score = 248 bits (129), Expect = 1e-63
Identities = 213/263 (80%), Gaps = 34/263 (12%)
Strand = Plus / Plus
Query: 161 atatcaccacgtcaaaggtgactccaactcca---ccactccattttgttcagataatgc 217
Sbjct: 481 atatcaccacgtcaaaggtgactccaact-tattgatagtgttttatgttcagataatgc 539
Query: 218 ccgatgatcatgtcatgcagctccaccgattgtgagaacgacagcgacttccgtcccagc 277
               Sbjct: 540 ccgatgactttgtcatgcagctccaccgattttg-g-----ttccgtcccagc 586
Query: 278 c-gtgcc--aggtgctgcctcagattcaggttatgccgctcaattcgctgcgtatatcgc 334
Sbjct: 587 caatgacgta-gtgctgcctcagattcaggttatgccgctcaattcgctgggtatatcgc 645
Query: 335 ttgctgattacgtgcagctttcccttcaggcggga-----ccagccatccgtc 382
Query: 383 ctccatatc-accacgtcaaagg 404
                                 Example BLAST alignment
          Sbjct: 706 atccatatcaaccacgtcaaagg 728
```



Approximate string matching

A *mismatch* is a single-character substitution:

An *edit* is a single-character substitution or *gap* (*insertion* or *deletion*):





Alignment

Above is an *alignment*: a way of lining up the characters of x and y

Could include mismatches, gaps or both

Vertical lines are drawn where opposite characters match



Hamming and edit distance

Finding Hamming distance between 2 strings is easy:

Edit distance is harder:



If strings x and y are same length, what can we say about **editDistance**(x, y) relative to **hammingDistance**(x, y)?

editDistance $(x, y) \le \text{hammingDistance}(x, y)$

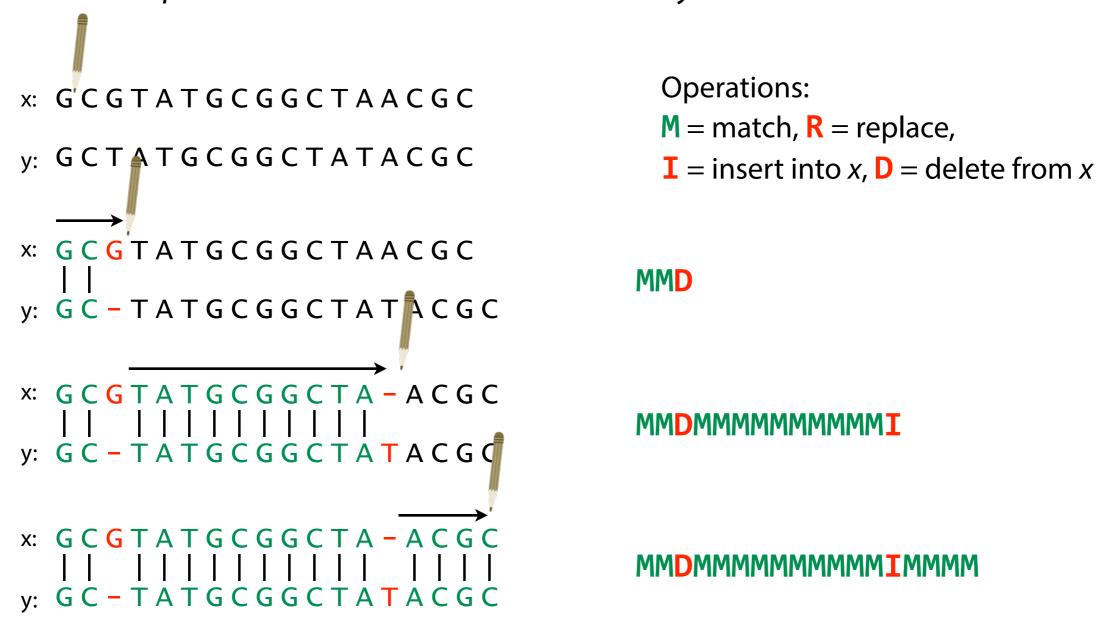
If strings x and y are different lengths, what can we say about editDistance(x, y)?

editDistance
$$(x, y) \ge ||x| - |y||$$

Python example: http://bit.ly/CG DP EditDist



Can think of edits as being introduced by an *optimal editor* working left-to-right. *Edit transcript* describes how editor turns *x* into *y*.





Alignments:

Edit transcripts with respect to *x*:

MMDMMMMMMMMM I MMMM

Distance = 2

MMDMMMMRMMMMMIMMMM

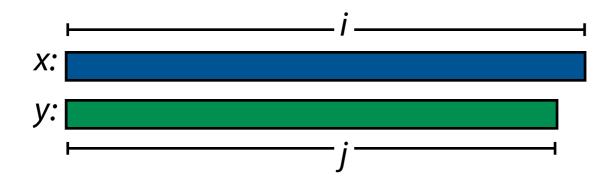
Distance = 3

DDDDMMMMMMIIII

Distance = 8



D[i, j]: edit distance between length-i prefix of x and length-j prefix of y



Think in terms of edit transcript. Optimal transcript for D[i, j] can be built by extending a shorter one by 1 operation. Only 3 options:

Append D to transcript for D[i-1, j]

Append I to transcript for D[i, j-1]

Append M or R to transcript for D[i-1, j-1]

D[i, j] is minimum of the three, and D[|x|, |y|] is the overall edit distance



Let D[0, j] = j, and let D[i, 0] = i

Otherwise, let
$$D[i,j] = \min \left\{ \begin{array}{l} D[i-1,j]+1 \\ D[i,j-1]+1 \end{array} \right.$$
 $\bigwedge^{\mathsf{N}} \mathsf{or} \, \mathsf{R}$ $D[i-1,j-1]+\delta(x[i-1],y[j-1])$

 $\delta(a,b)$ is 0 if a=b,1 otherwise



```
Let D[0,j] = j, and let D[i,0] = i  \text{Otherwise, let } D[i,j] = \min \left\{ \begin{array}{l} D[i-1,j] + 1 \\ D[i,j-1] + 1 \\ D[i-1,j-1] + \delta(x[i-1],y[j-1]) \end{array} \right.
```

```
A simple recursive algorithm:

prefixes of x and y currently under consideration
```

 $\delta(a,b)$ is 0 if a=b, 1 otherwise

Python example: http://bit.ly/CG DP EditDist



```
def edDistRecursive(x, y):
    if len(x) == 0: return len(y)
    if len(y) == 0: return len(x)
    delt = 1 if x[-1] != y[-1] else 0
    diag = edDistRecursive(x[:-1], y[:-1]) + delt
    vert = edDistRecursive(x[:-1], y) + 1
    horz = edDistRecursive(x, y[:-1]) + 1
    return min(diag, vert, horz)
```

```
>>> import datetime as d
>>> st = d.datetime.now(); \
... edDistRecursive("Shakespeare", "shake spear"); \
... print (d.datetime.now()-st).total_seconds()
3
31.498284
```

Simple, but takes >30 seconds for a small problem



Subproblems (D[i, j]s) can be reused instead of being recalculated:

```
def edDistRecursive(x, y):
                        if len(x) == 0: return len(y)
                        if len(y) == 0: return len(x)
                        delt = 1 if x[-1] != y[-1] else 0
                        diag = edDistRecursive(x[:-1], y[:-1]) + delt
                        vert = edDistRecursive(x[:-1], y) + 1
                        horz = edDistRecursive(x, y[:-1]) + 1
                        return min(diag, vert, horz)
                                              def edDistRecursiveMemo(x, y, memo=None):
                                                  if memo is None: memo = {}
                                                  if len(x) == 0: return len(y)
Reusing
                             Return
                                                  if len(y) == 0: return len(x)
solutions to
                                                  if (len(x), len(y)) in memo:
                             memoized
                                                      return memo[(len(x), len(y))]
subproblems is
                             answer, if
                                                  delt = 1 if x[-1] != y[-1] else 0
                             avaialable
                                                  diag = edDistRecursiveMemo(x[:-1], y[:-1], memo) + delt
memoization:
                                                  vert = edDistRecursiveMemo(x[:-1], y, memo) + 1
                                                  horz = edDistRecursiveMemo(x, y[:-1], memo) + 1
                                                  ans = min(diag, vert, horz)
                        Memoize D[i, j] \longrightarrow memo[(len(x), len(y))] = ans
                                                  return ans
```

Python example: http://bit.ly/CG_DP_EditDist



```
def edDistRecursiveMemo(x, y, memo=None):
    if memo is None: memo = {}
    if len(x) == 0: return len(y)
    if len(y) == 0: return len(x)
    if (len(x), len(y)) in memo:
        return memo[(len(x), len(y))]
    delt = 1 if x[-1] != y[-1] else 0
    diag = edDistRecursiveMemo(x[:-1], y[:-1], memo) + delt
    vert = edDistRecursiveMemo(x[:-1], y, memo) + 1
    horz = edDistRecursiveMemo(x, y[:-1], memo) + 1
    ans = min(diag, vert, horz)
    memo[(len(x), len(y))] = ans
    return ans
```

```
>>> import datetime as d
>>> st = d.datetime.now(); \
... edDistRecursiveMemo("Shakespeare", "shake spear"); \
... print (d.datetime.now()-st).total_seconds()
3
0.000593
```



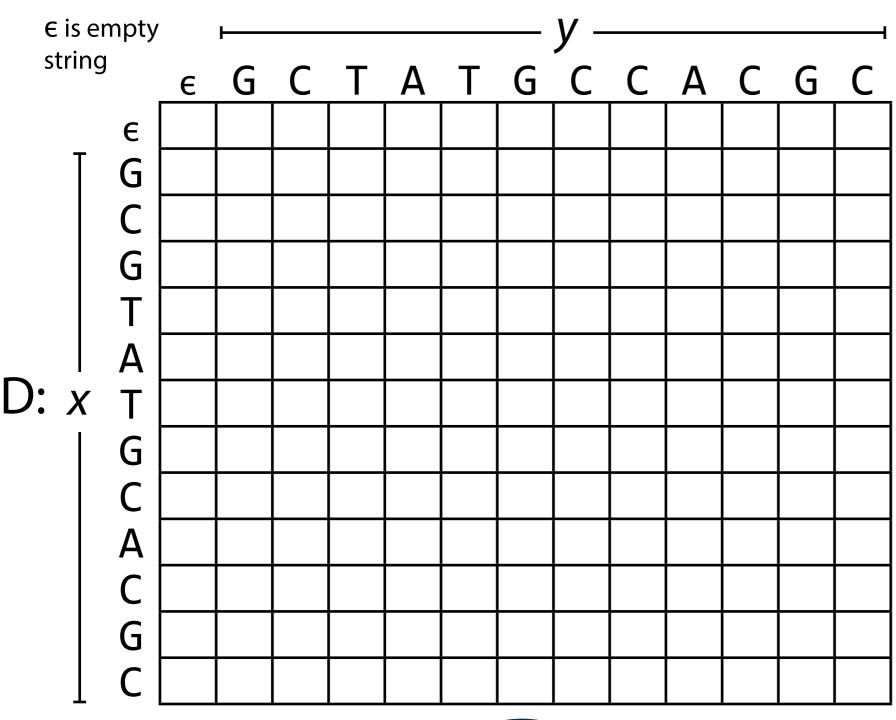


edDistRecursiveMemo is a top-down dynamic programming approach

Alternative is *bottom-up*. Here, bottom-up recursion is pretty intuitive and interpretable, so this is how edit distance algorithm is usually explained.

Fills in a table (matrix) of D(i, j)s:



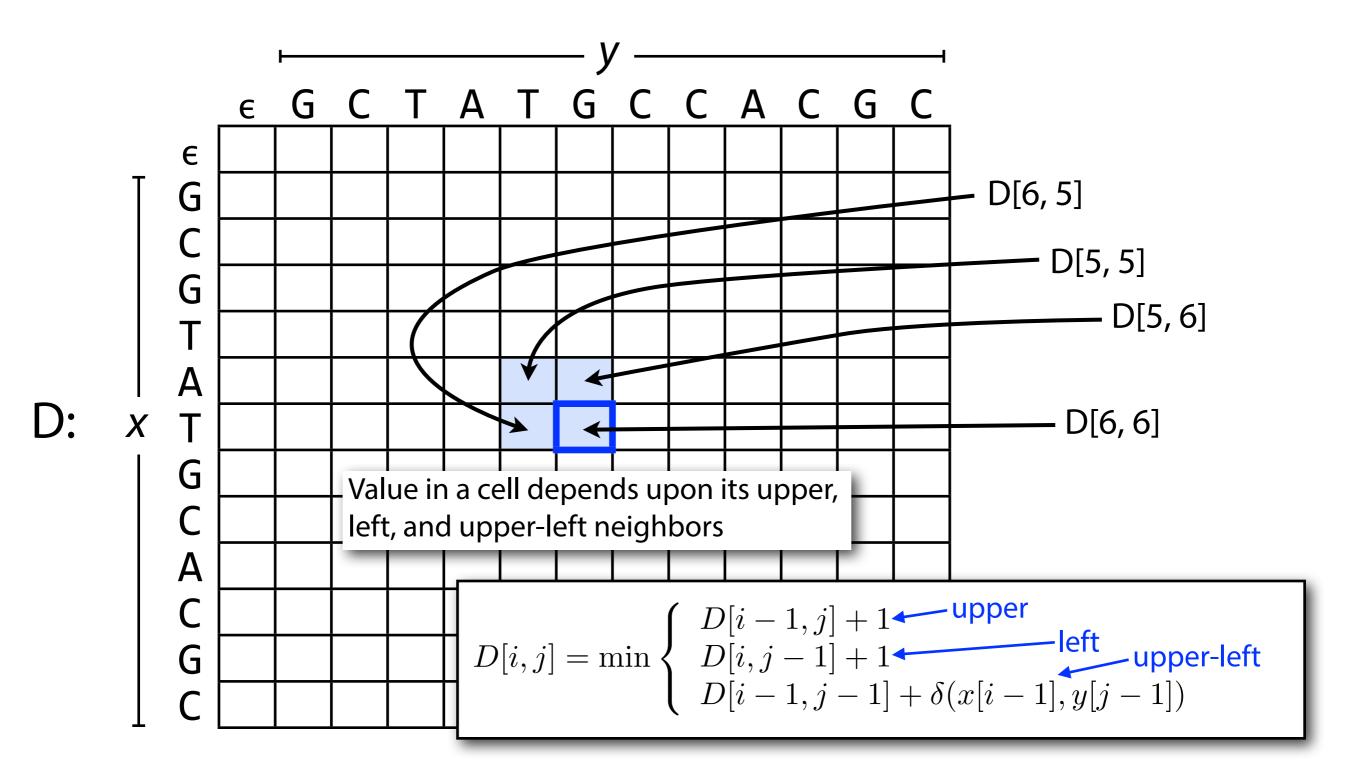


Let
$$n = |x|, m = |y|$$

D: $(n+1) \times (m+1)$ matrix

D[i, j] = edit distance b/tlength-i prefix of x and length-j prefix of y







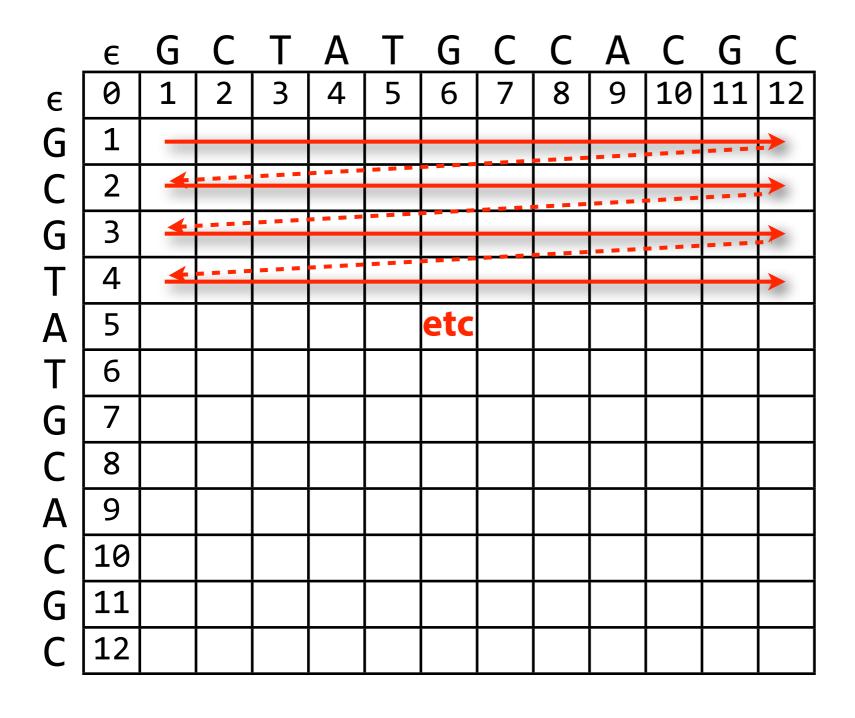
```
First few lines
Of edDistDp:

D = numpy.zeros((len(x)+1, len(y)+1), dtype=int)
D[0, 1:] = range(1, len(y)+1)
D[1:, 0] = range(1, len(x)+1)
```

	€	G	C	<u>T</u>	<u>A</u>	<u>T</u>	G	C	<u>C</u>	Α	C	G	<u>C</u>
ϵ	0	1	2	3	4	5	6	7	8	9	10	11	12
G	1												
C	2												
G	3												
Τ	4												
Α	5												
Τ	6												
G	7												
C	8												
Α	9												
C	10												
G	11												
C	12												

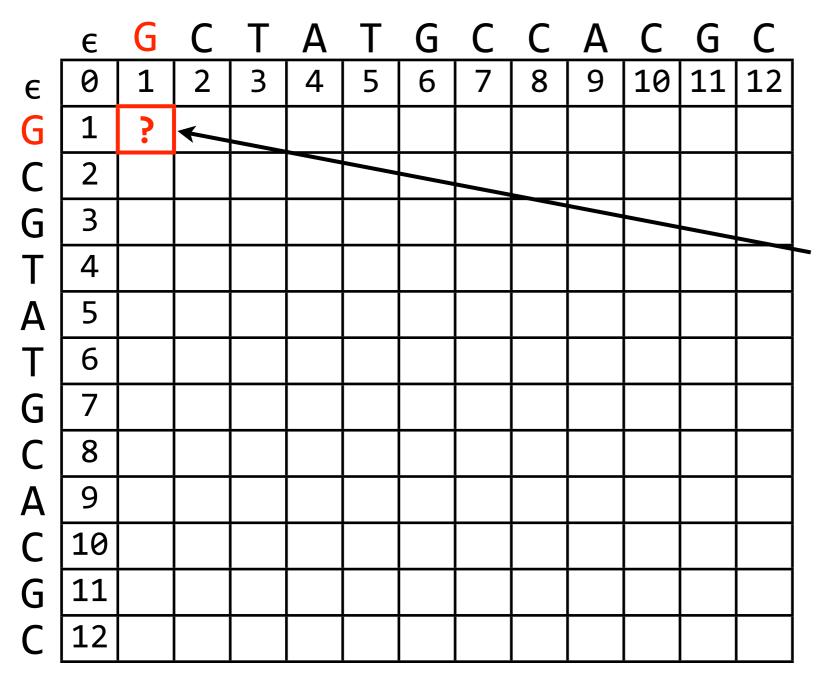
Initialize D[0, j] to j, D[i, 0] to i





Fill remaining cells from top row to bottom and from left to right





Fill remaining cells from top row to bottom and from left to right

What goes here in i=1,j=1?

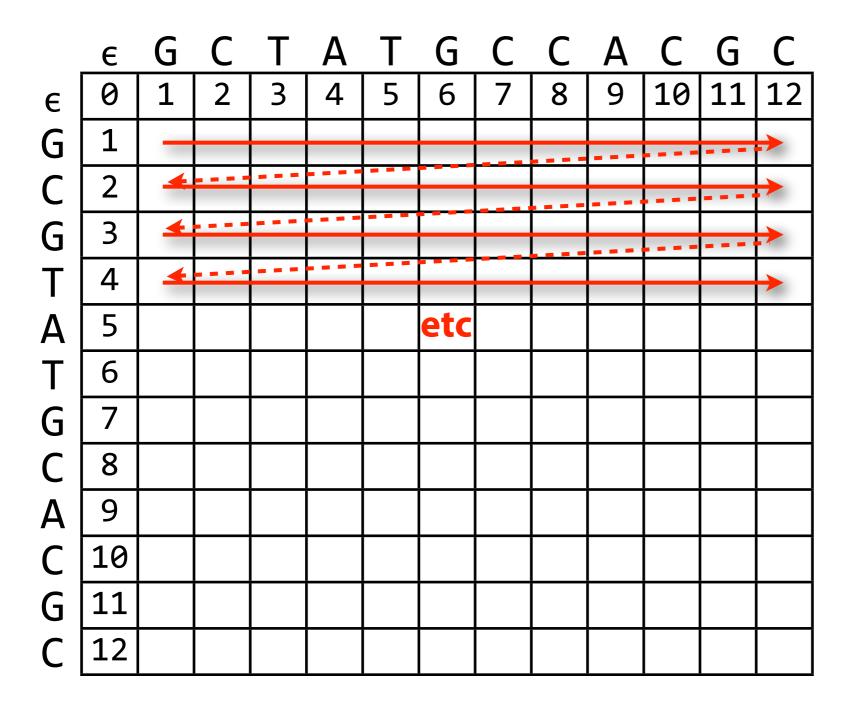


	ε	G	C	Τ	Α	Τ	G	C	C	Α	C	G	C
ϵ	0	1	2	M	4	5	6	7	8	9	10	11	12
G	1	0	1	2	3	4	5	6	7	8	9	10	11
C	2	1	0	1	2	3	4	5	6	7	8	9	10
G	3	2	1	1	2	3	3	4	5	6	7	8	9
Т	4	3	2	1	2	2	3	4	5	6	7	8	9
Α	5	4	3	2	1	2	3	4	5	5	6	7	8
Т	6	5	4	3	2	1	2	3	4	5	6	7	8
G	7	6	5	4	3	2	1	2	3	4	5	6	7
C	8	7	6	5	4	3	2	1	2	3	4	5	6
Α	9	8	7	6	5	4	3	2	2	2	3	4	5
C	10	9	8	7	6	5	4	3	2	3	2	3	4
G	11	10	9	8	7	6	5	4	3	3	3	2	3
C	12	11	10	9	8	7	6	5	4	4	3	3	2

Fill remaining cells from top row to bottom and from left to right

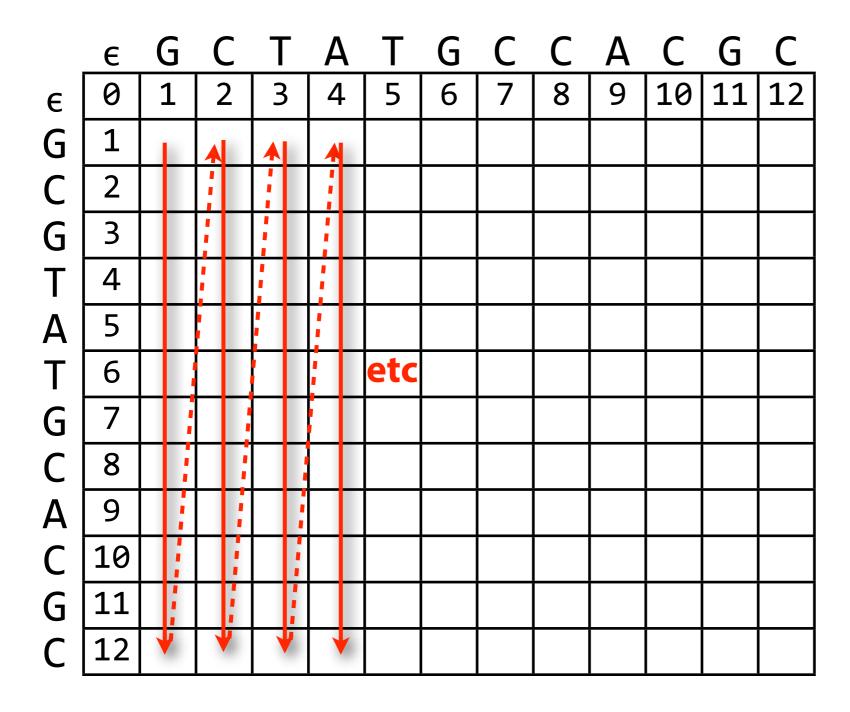
Edit distance for x, y





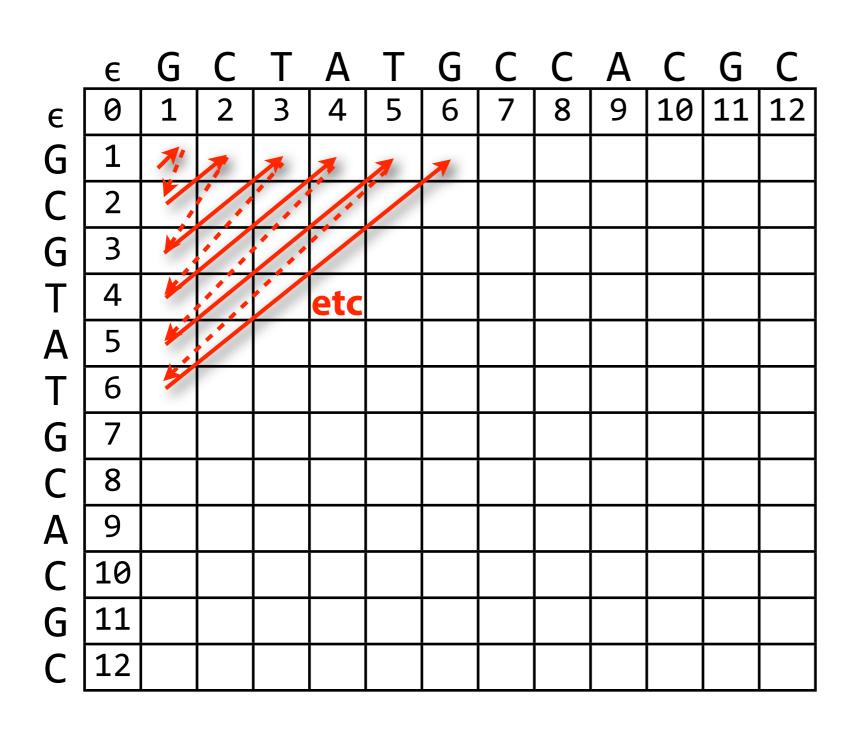
Could we have filled the cells in a different order?





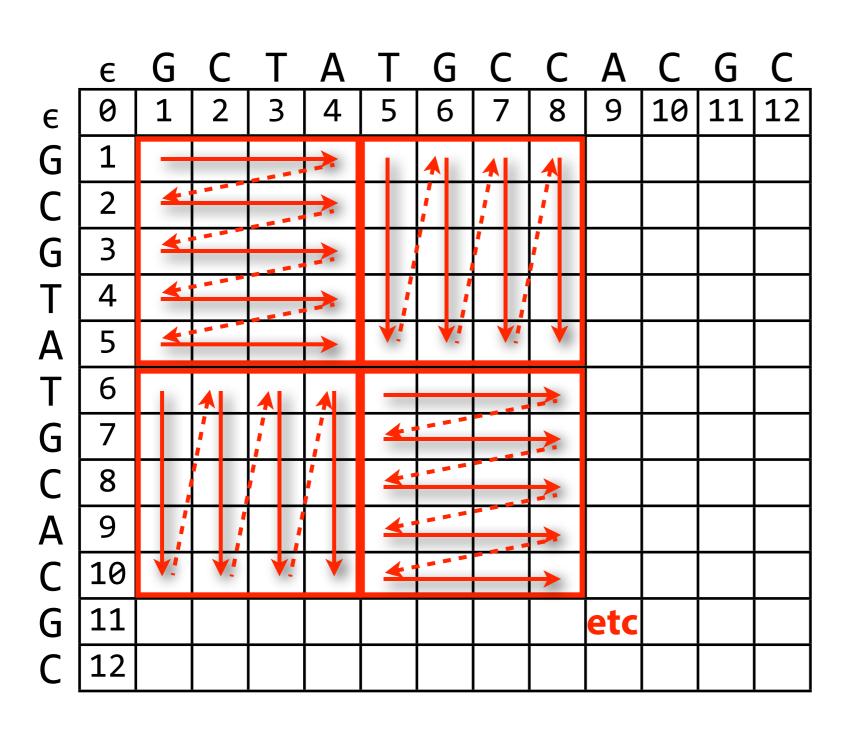
Yes: e.g. invert the loops





Or by anti-diagonal





Or blocked



Full backtrace path corresponds to an optimal alignment / edit transcript:

Start at end; at each step, ask: which predecessor gave the minimum?

	€	G	C	<u>T</u>	Α	T	G	<u>C</u>	<u>C</u>	Α	C	G	<u>C</u>	
ϵ	0	1	2	3	4	5	6	7	8	9	10	11	12	
G	1	0	1	2	3	4	5	6	7	8	9	10	11	
C	2	1	0	1	2	3	4	5	6	7	8	9	10	
G	3	2	1	1	2	3	3	4	5	6	7	8	9	
Т	4	3	2	1	2	2	3	4	5	6	7	8	9	
Α	5	4	3	2	1	2	3	4	5	5	6	7	8	
Т	6	5	4	3	2	1	2	3	4	5	6	7	8	
G	7	6	5	4	3	2	1	2	3	4	5	6	7	
C	8	7	6	5	4	3	2	1	2	3	4	5	6	
Α	9	8	7	6	5	4	3	2	2	2	3	4	5	
C	10	9	8	7	6	5	4	3	2	3	2<	3	4	A: From here
G	11	10	9	8	7	6	5	4	3	3	3	2	7	——— Q: How did I get here?
C	12	11	10	9	8	7	6	5	4	4	3	3	2	
														JOHNS HOPKINS WHITING SCHOOL of ENGINEERING

Full backtrace path corresponds to an optimal alignment / edit transcript:

Start at end; at each step, ask: which predecessor gave the minimum?

	ϵ	G	C	Τ	Α	Τ	G	C	C	Α	C	G	C	
ϵ	0	1	2	3	4	5	6	7	8	9	10	11	12	
G	1	0	1	2	3	4	5	6	7	8	9	10	11	
C	2	1	0	1	2	3	4	5	6	7	8	9	10	
G	3	2	1	1	2	3	3	4	5	6	7	8	9	
T	4	3	2	1	2	2	3	4	5	6	7	8	9	
Α	5	4	3	2	1	2	3	4	5	5	6	7	8	
T	6	5	4	3	2	1	2	3	4	5	6	7	8	
G	7	6	5	4	3	2	1	2	M	4	5	6	7	
C	8	7	6	5	4	M	2	1	2	3	4	5	6	
Α	9	8	7	6	5	4	3	2	2	2 1	(3	4	5	A: From here
C	10	9	8	7	6	5	4	3	2	3	2	3	4	——— Q: How did I get here?
G	11	10	9	8	7	6	5	4	3	3	3	2	3	
C	12	11	10	9	8	7	6	5	4	4	3	3	2	
'														JOHNS HOPKINS WHITING SCHOOL GENCINEERING

Full backtrace path corresponds to an optimal alignment / edit transcript:

Start at end; at each step, ask: which predecessor gave the minimum?

	€	G	C	Т	Α	Т	G	C	C	Α	C	G	C	
ϵ	0	1	2	3	4	5	6	7	8	9	10	11	12	
G	1	0	1	2	3	4	5	6	7	8	9	10	11	
C	2	1	0	1	2	3	4	5	6	7	8	9	10	
G	3	2	1	1	2	3	3	4	5	6	7	8	9	
Т	4	3	2	1	2	2	3	4	5	6	7	8	9	
Α	5	4	3	2	1	2	3	4	5	5	6	7	8	
Т	6	5	4	3	2	1	2	3	4	5	6	7	8	A: From here
G	7	6	5	4	3	2	1	2	(1)	4	5	6	7	—— Q: How did I get here?
C	8	7	6	5	4	3	2	1	/2	3	4	5	6	
A	9	8	7	6	5	4	3	2	2	2	3	4	5	
C	10	9	8	7	6	5	4	3	2	3	4	3	4	
G	11	10	9	8	7	6	5	4	3	3	3	7	3	
C	12	11	10	9	8	7	6	5	4	4	3	3	2	
						•				•	•		•	IOHNS HOP

Full backtrace path corresponds to an optimal alignment / edit transcript:

Start at end; at each step, ask: which predecessor gave the minimum?

	E	G	C	Т	Α	Т	G	C	C	Α	C	G	<u>C</u>
€	0	1	2	3	4	5	6	7	8	9	10	11	12
G	1	2	1	2	3	4	5	6	7	8	9	10	11
C	2	1	9	1	2	3	4	5	6	7	8	9	10
G	3	2	1	1	2	3	3	4	5	6	7	8	9
T	4	3	2	×	2	2	3	4	5	6	7	8	9
Α	5	4	3	2	×	2	3	4	5	5	6	7	8
T	6	5	4	3	2	×	2	3	4	5	6	7	8
G	7	6	5	4	3	2	H	4	3	4	5	6	7
C	8	7	6	5	4	3	2	1	C	3	4	5	6
Α	9	8	7	6	5	4	3	2	2	SA	3	4	5
C	10	9	8	7	6	5	4	3	2	3	24	3	4
G	11	10	9	8	7	6	5	4	3	3	3	2	3
C	12	11	10	9	8	7	6	5	4	4	3	3	2

Alignment:

Edit transcript:

MMDMMMMIMMMMM



Edit distance: summary

Matrix-filling dynamic programming algorithm is O(mn) time and space

FillIng matrix is O(mn) space and time, and yields edit distance

Backtrace is O(m + n) time, yields optimal alignment / edit transcript



Levenshtein

Basic edit distance

- Works for different-length sequences
- Uniform cost for substitution/ insertion/deletion

```
def edit(x, y):
    D = np.zeros((len(x) + 1, len(y) + 1), dtype=int)
    # for the empty word, costs match the length of
    # the other string
    D[0, 1:] = range(1, len(y) + 1)
    D[1:, 0] = range(1, len(x) + 1)
    for i in range(1, len(x) + 1):
        for j in range(1, len(y) + 1):
            delta = 1 if x[i-1] != y[j-1] else 0
            D[i, j] = min(
                D[i-1, j] + 1,
                D[i, j-1] + 1,
                D[i-1, j-1] + delta
    return D[len(x), len(y)]
```

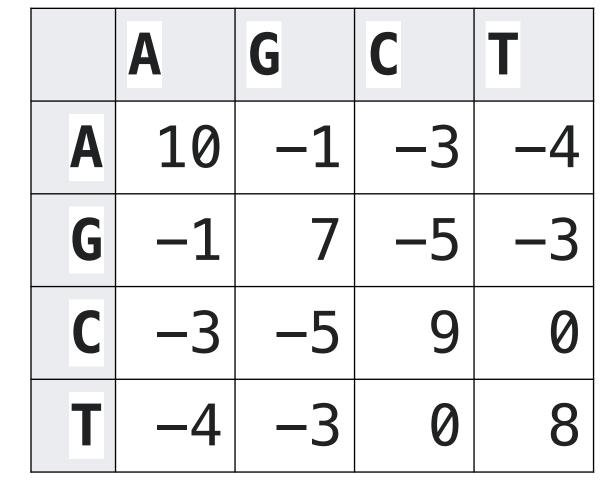
Levenshtein

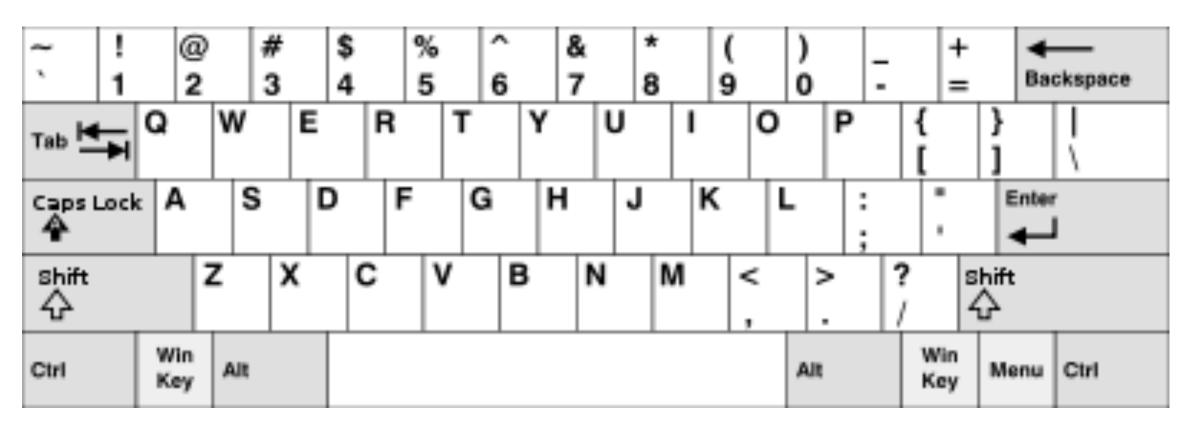
Custom Cost

```
def edit(x, y, cost={'m': 0, 's': 1, 'i': 1, 'd': 1}):
    D = np_z eros((len(x) + 1, len(y) + 1), dtype=int)
    # for the empty word, costs match the length of the
    # other string
   D[0, 1:] = range(1, len(y) + 1)
   D[1:, 0] = range(1, len(x) + 1)
    for i in range(1, len(x) + 1):
        for j in range(1, len(y) + 1):
            delta = cost['m'] if x[i-1] == y[j-1] else cost['s']
            D[1, ]] = min(
                D[i-1, j] + cost['d'],
                D[i, j-1] + cost['i'],
                D[i-1, j-1] + delta
    return D[len(x), len(y)]
```

Needleman-Wunsch Algorithm

- Biology: not all edits "cost the same", gaps typically treated separately
- Gap penalty (eg. -1)
- Similarity (match reward, mismatch penalty)
- DP finds maximum similarity



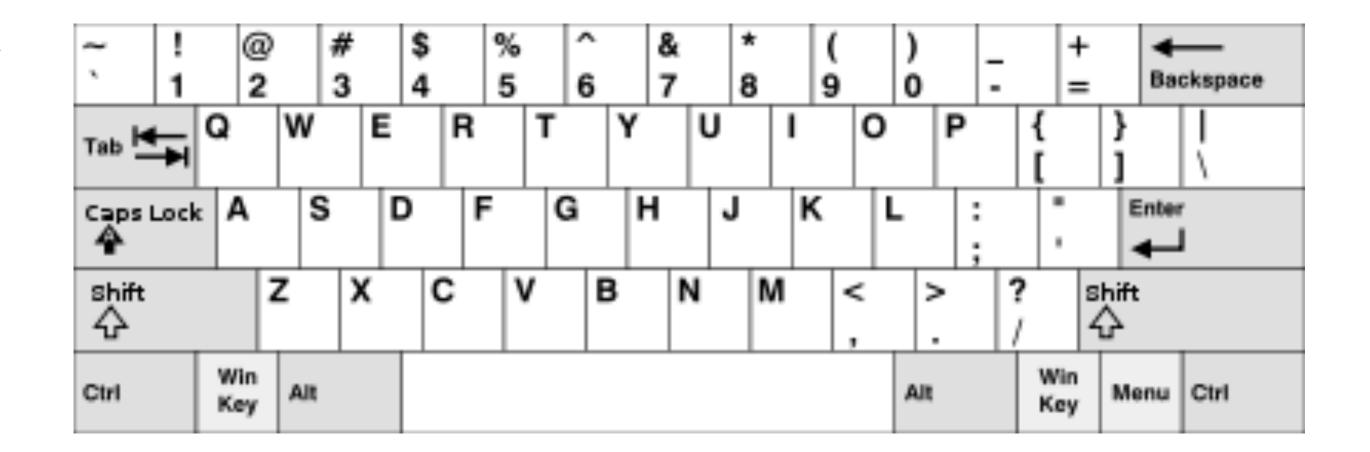


Needleman-Wunsch Algorithm

```
def nw(x, y, d, sim):
    D = np.zeros((len(x) + 1, len(y) + 1), dtype=int)
    # for the empty word, costs match the length of the other string
    D[0, 1:] = range(1, len(y) + 1); D[0, 1:] *= d
    D[1:, 0] = range(1, len(x) + 1); D[1:, 0] *= d
    for i in range(1, len(x)):
        for j in range(1, len(y)):
            cs = D[i-1, j-1] + sim(x[i], y[j])
            cd = D[i-1, j] + d
            ci = D[i, j-1] + d
            D[i,j] = max(cs, cd, ci)
    print(D)
    return D[len(x)][len(y)]
```

Keyboard-aware Substitutions?

- Compute cost of substitution by proximity of keys
- Map keys to grid, compute euclidean distance
- What about g <> h etc.?

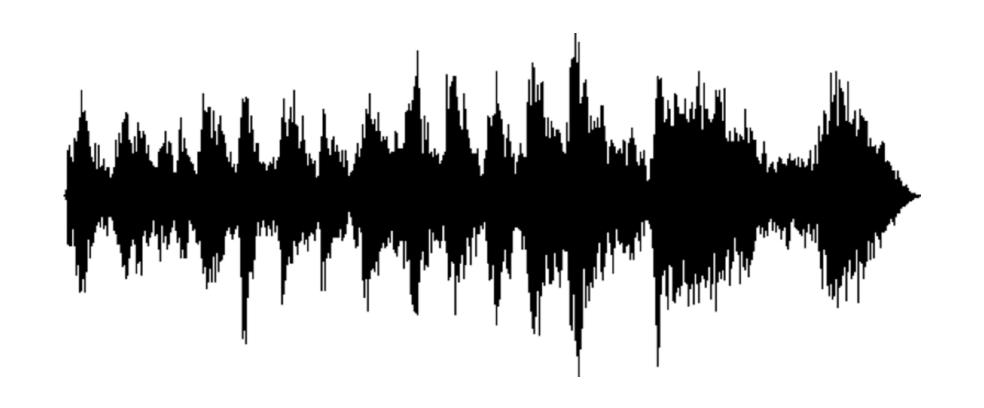


https://commons.wikimedia.org/wiki/File:KB_United_States.svg#/media/File:KB_United_States.svg

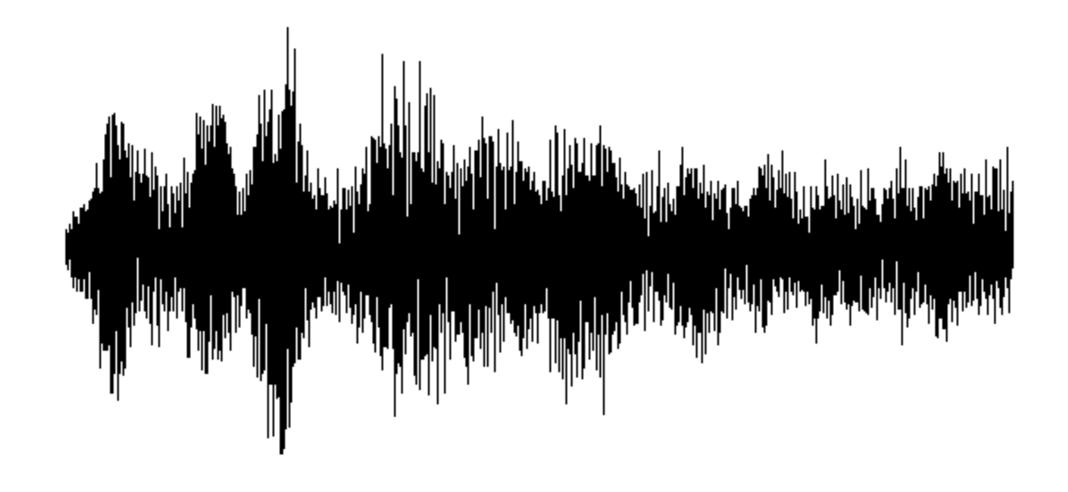
Outlook: <u>Damerau-Levenshtein</u> with adjacent transpositions

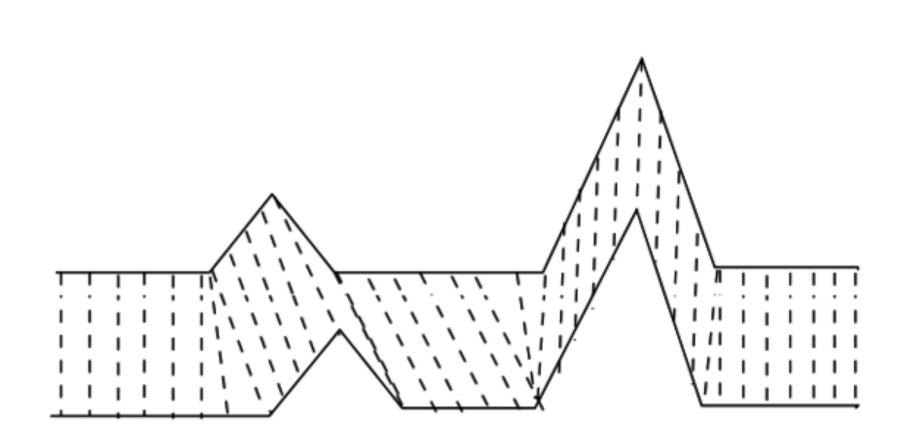
Comparing Sequences

... of non-discrete signals?

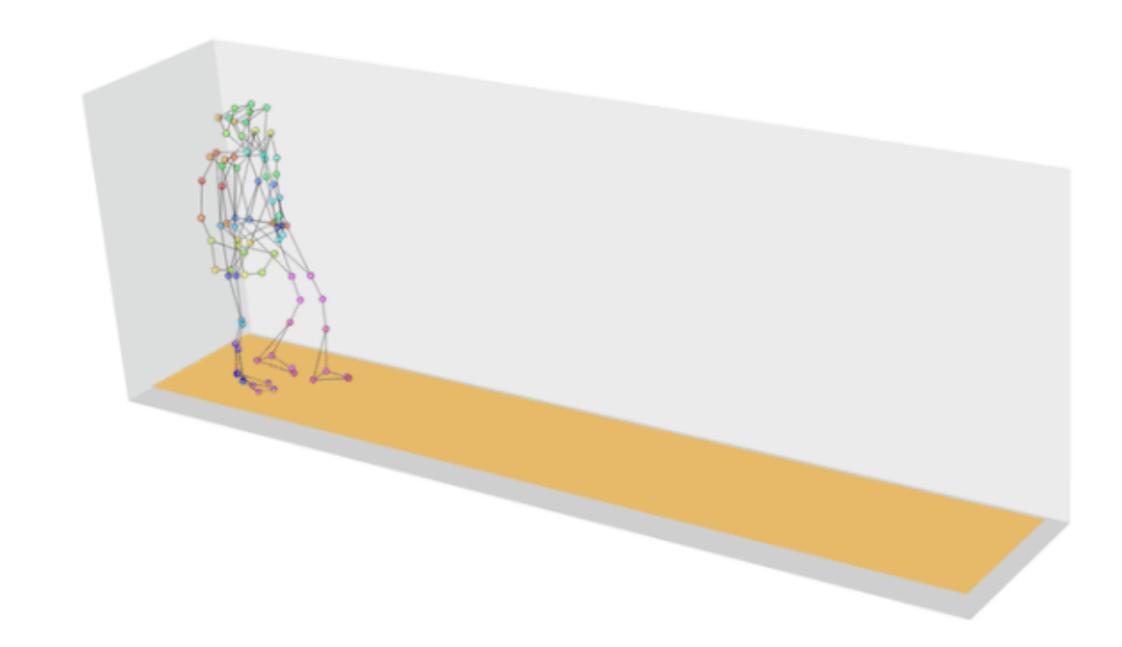


VS.





https://en.wikipedia.org/wiki/File:Dynamic_time_warping.png



- Sequences assumed to be similar, no notion of insert
 - -> first row/col is *inf*!
- Observations are continuous (not drawn from vocab)
 - There is always a cost
 - No explicit modeling of insertion/deletion/substitution

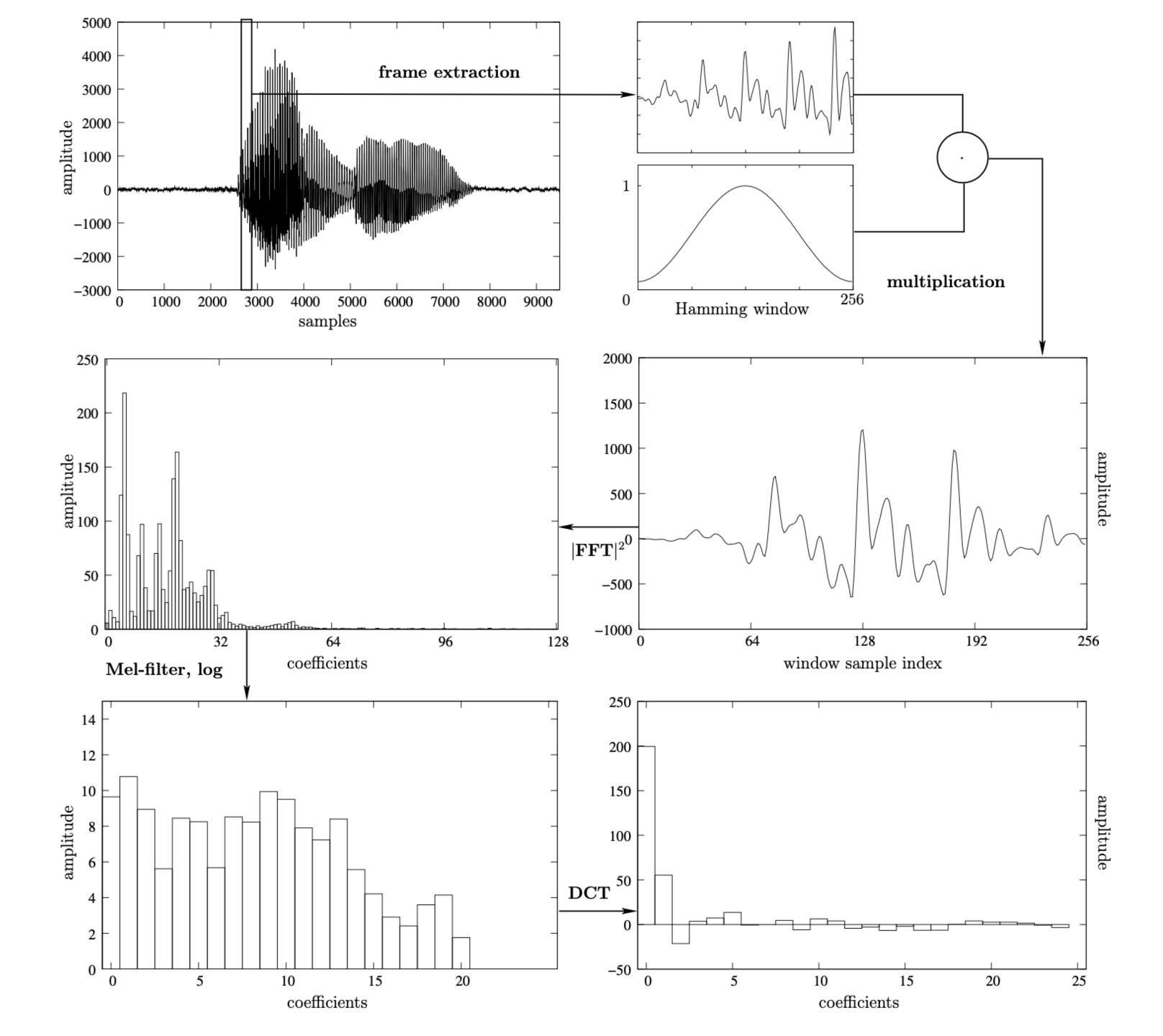
```
def dtw(x: list, y: list, d) -> float:
    D = np.full((len(x) + 1, len(y) + 1), np.inf, dtype=float)
    D[0, 0] = 0

for i in range(1, len(x)):
    for j in range(1, len(y)):
        cost = d(x[i], y[j])
        D[i, j] = cost + min(D[i-1, j],
        D[i, j-1],
        D[i-1, j-1])
return D[len(x)][len(y)]
```

On audio data

- Raw sample data is way to numerous
- Compute spectral (cepstral) features, eg. MFCC
- Use euclidean distance on feature vectors

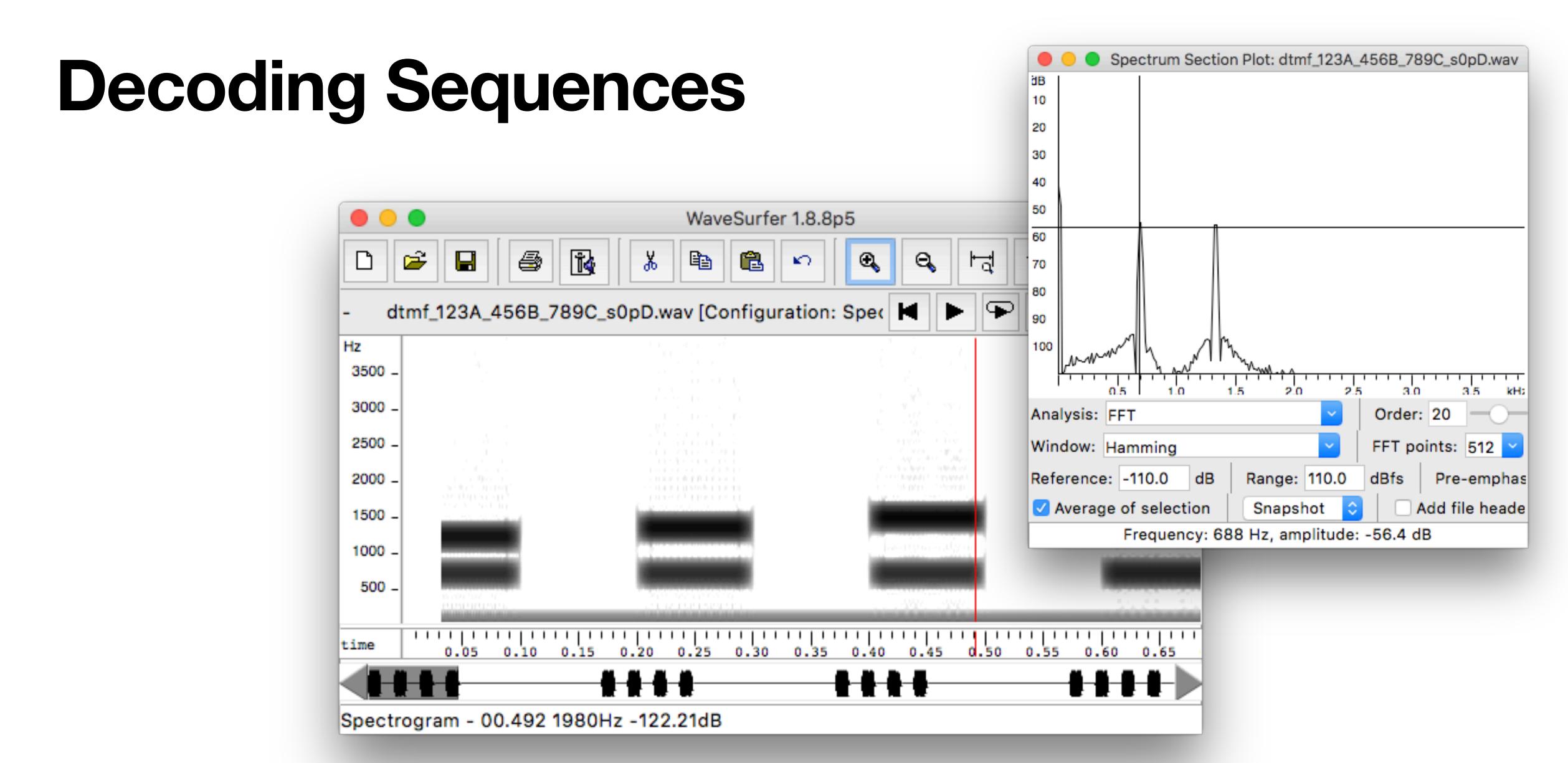
MFCC pipeline



Multi-class Sequence Classification

Eg. Isolated word recognition

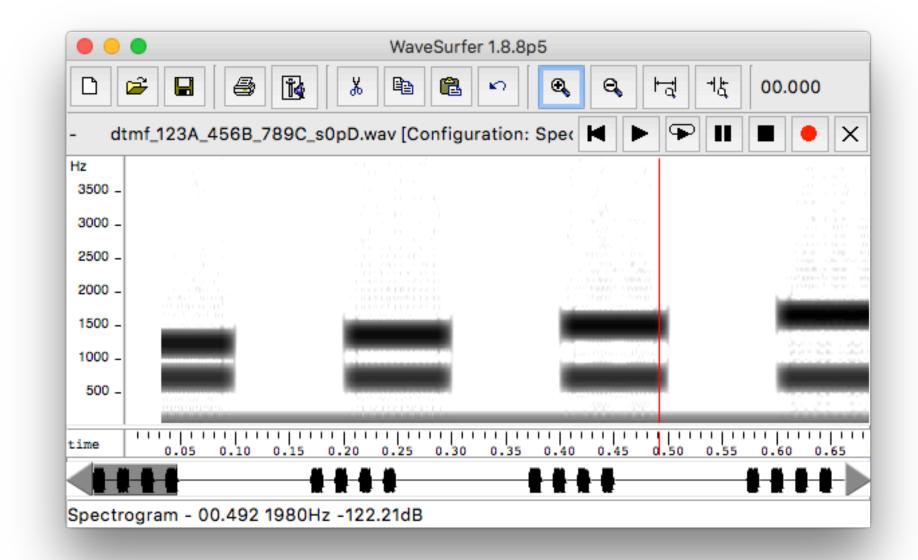
- Have (at least) one reference sequence per class (word)
- Compute DTW distance for test sequence to each reference
- Chose class with minimum distance
- How to speed up...?

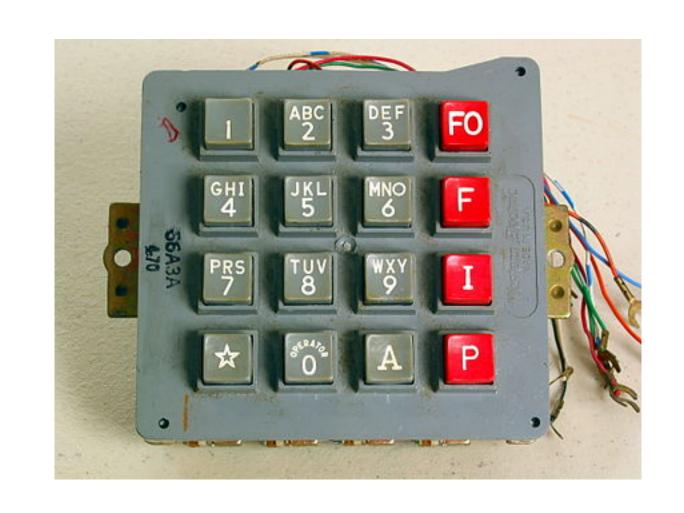


Dual-tone multi-frequency signaling (DTMF)

Decoding States

- Observation: pause 1 pause 2 pause ...
- If we ignore noise etc.: 12+1 classes
 - model each class, eg. with a reference vector
 - apply a sliding window, map each window to class
 - output: - 1 1 1 - 2 2 2 2 - 3 3 ...
 - collapse (uniq)
 - output: 123





Assignment 1

Due April 8

- Edit distances (Hamming, Levenshtein, Needleman-Wunsch)
- Auto-Complete (using basic word stats)
- Isolated Word Recognition using DTW (on digits)
- DTMF sequence decoding using DP on states
- Submit via Teams to Files > Assignment Submissions

https://github.com/seqlrn/assignments/tree/master/1-dynamic-programming