

Alignment

Sept 16, 2015

ANNOUNCEMENTS

ALIGNMENT – THINK BLAST

Q
D

ANCQE
ANC**G**E

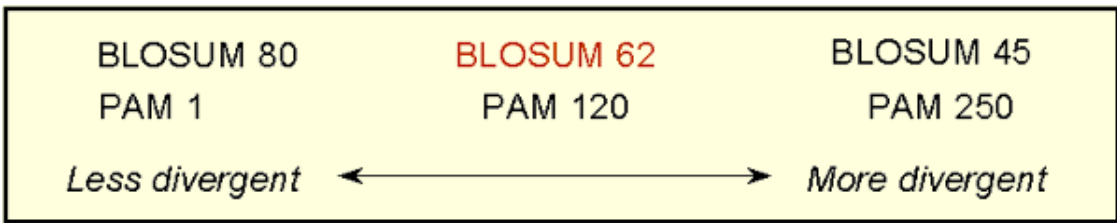
versus

ANCQE
ANC**H**E

BLOSUM MATRIX

| | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---|
| Ala | 4 | | | | | | | | | | | | | | | | | | | |
| Arg | -1 | 5 | | | | | | | | | | | | | | | | | | |
| Asn | -2 | 0 | 6 | | | | | | | | | | | | | | | | | |
| Asp | -2 | -2 | 1 | 6 | | | | | | | | | | | | | | | | |
| Cys | 0 | -3 | -3 | -3 | 9 | | | | | | | | | | | | | | | |
| Gln | -1 | 1 | 0 | 0 | -3 | 5 | | | | | | | | | | | | | | |
| Glu | -1 | 0 | 0 | 2 | -4 | 2 | 5 | | | | | | | | | | | | | |
| Gly | 0 | -2 | 0 | -1 | -3 | -2 | -2 | 6 | | | | | | | | | | | | |
| His | -2 | 0 | 1 | -1 | -3 | 0 | 0 | -2 | 8 | | | | | | | | | | | |
| Ile | -1 | -3 | -3 | -3 | -1 | -3 | -3 | -4 | -3 | 4 | | | | | | | | | | |
| Leu | -1 | -2 | -3 | -4 | -1 | -2 | -3 | -4 | -3 | 2 | 4 | | | | | | | | | |
| Lys | -1 | 2 | 0 | -1 | -3 | 1 | 1 | -2 | -1 | -3 | -2 | 5 | | | | | | | | |
| Met | -1 | -1 | -2 | -3 | -1 | 0 | -2 | -3 | -2 | 1 | 2 | -1 | 5 | | | | | | | |
| Phe | -2 | -3 | -3 | -3 | -2 | -3 | -3 | -3 | -1 | 0 | 0 | -3 | 0 | 6 | | | | | | |
| Pro | -1 | -2 | -2 | -1 | -3 | -1 | -1 | -2 | -2 | -3 | -3 | -1 | -2 | -4 | 7 | | | | | |
| Ser | 1 | -1 | 1 | 0 | -1 | 0 | 0 | 0 | -1 | -2 | -2 | 0 | -1 | -2 | -1 | 4 | | | | |
| Thr | 0 | -1 | 0 | -1 | -1 | -1 | -1 | -2 | -2 | -1 | -1 | -1 | -1 | -2 | -1 | 1 | 5 | | | |
| Trp | -3 | -3 | -4 | -4 | -2 | -2 | -3 | -2 | -2 | -3 | -2 | -3 | -1 | 1 | -4 | -3 | -2 | 11 | | |
| Tyr | -2 | -2 | -2 | -3 | -2 | -1 | -2 | -3 | 2 | -1 | -1 | -2 | -1 | 3 | -3 | -2 | -2 | 2 | 7 | |
| Val | 0 | -3 | -3 | -3 | -1 | -2 | -2 | -3 | -3 | 3 | 1 | -2 | 1 | -1 | -2 | -2 | 0 | -3 | -1 | 4 |
| Ala | Arg | Asn | Asp | Cys | Gln | Glu | Gly | His | Ile | Leu | Lys | Met | Phe | Pro | Ser | Thr | Trp | Tyr | Val | |

BLOSUM MATRIX



Alignment Algorithms

Sept 16, 2015

ALGORITHMS

Global Alignment : Needleman – Wunsch

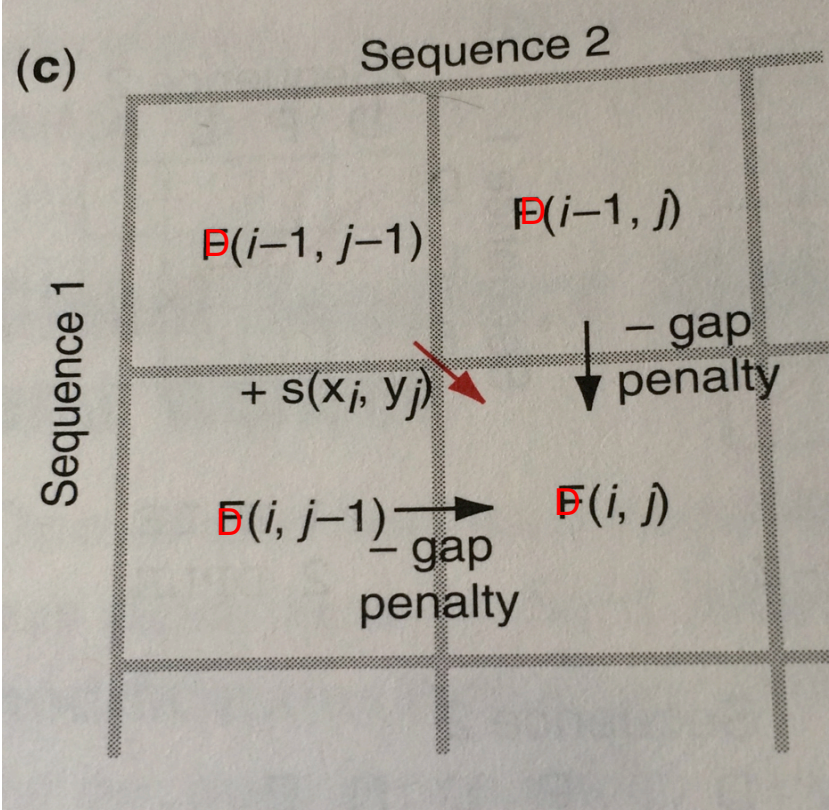
ALGORITHMS

Global Alignment Step 1: set up scoring matrix

| | | | | |
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ALGORITHMS

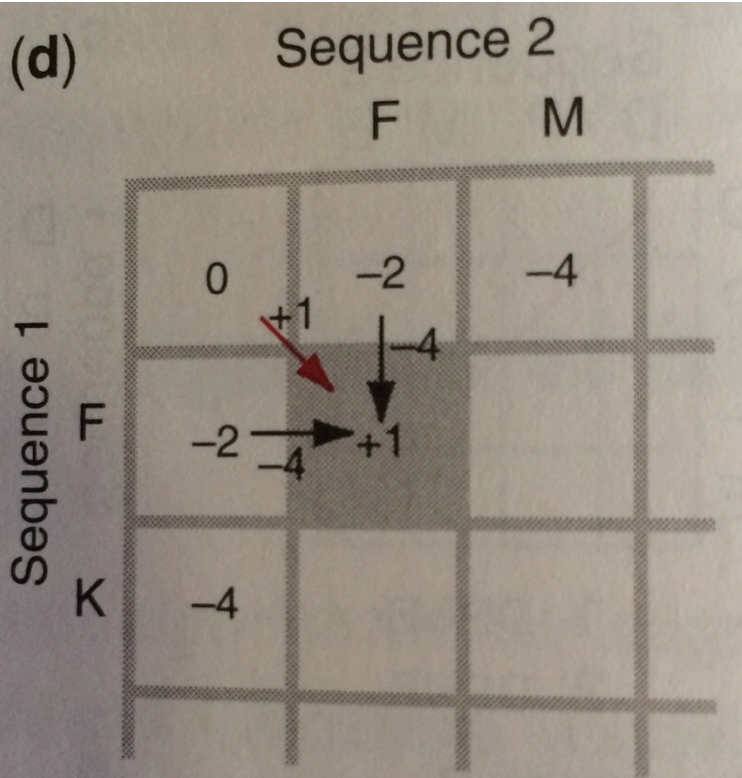
Global Alignment
Step 2: score matrix



$$D(i, j) = \max \begin{cases} D(i-1, j-1) + s(x_i, y_j) \\ D(i-1, j) + g \\ D(i, j-1) + g \end{cases}$$

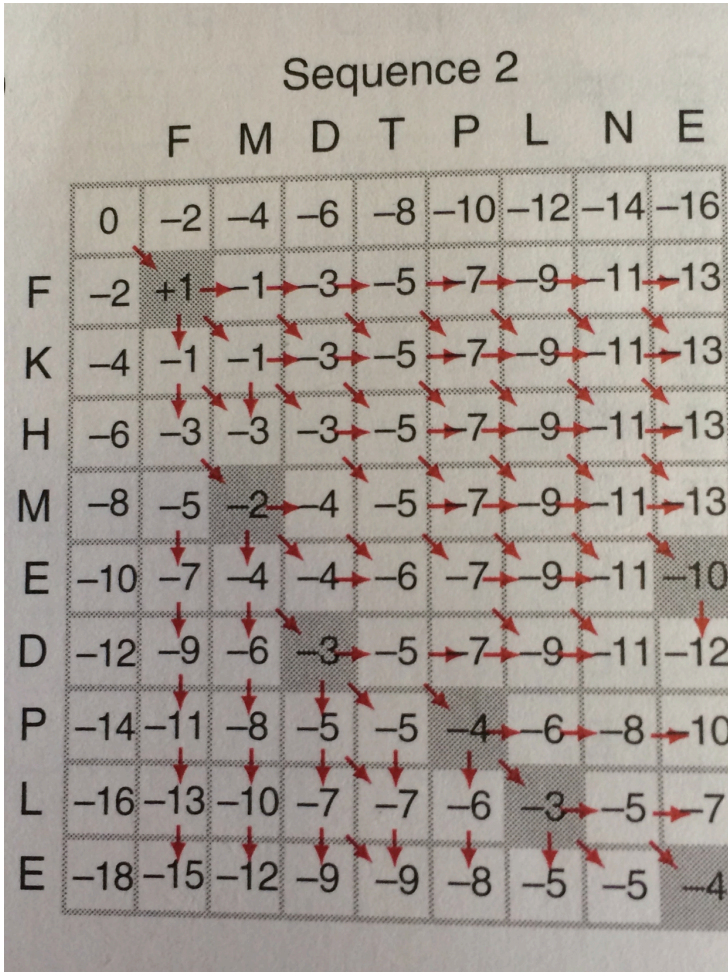
ALGORITHMS

Global Alignment Step 2: score matrix



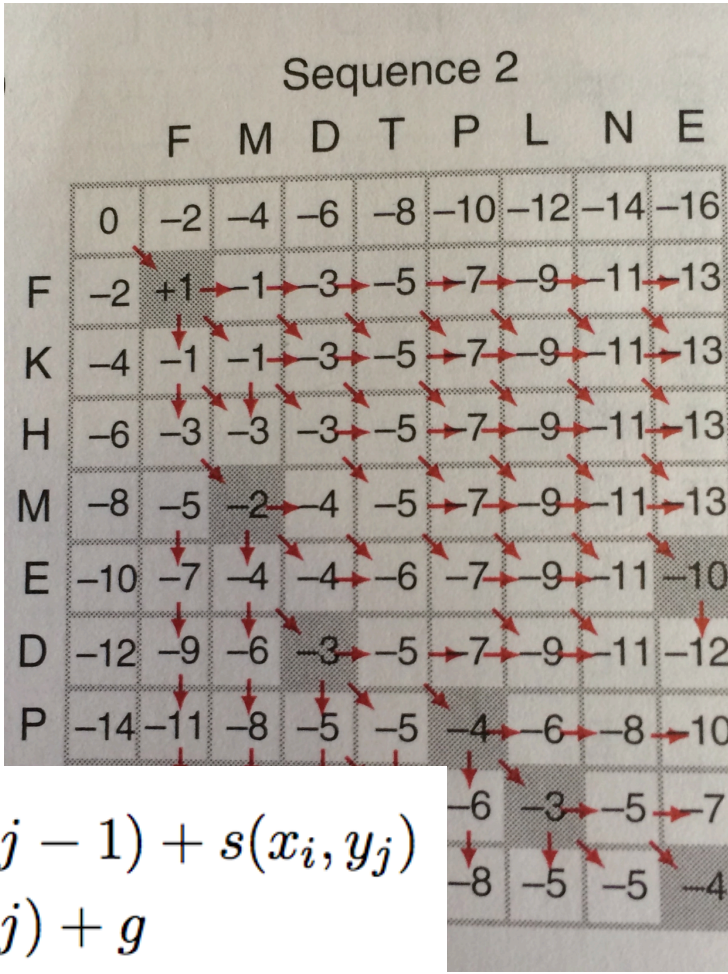
ALGORITHMS

Global Alignment
Step 2: score matrix



ALGORITHMS

Global Alignment
Step 2: score matrix



$$D(i, j) = \max \begin{cases} D(i - 1, j - 1) + s(x_i, y_j) \\ D(i - 1, j) + g \\ D(i, j - 1) + g \end{cases}$$

ALGORITHMS

Global Alignment

Step 3:

ID optimal alignment

ALGORITHMS

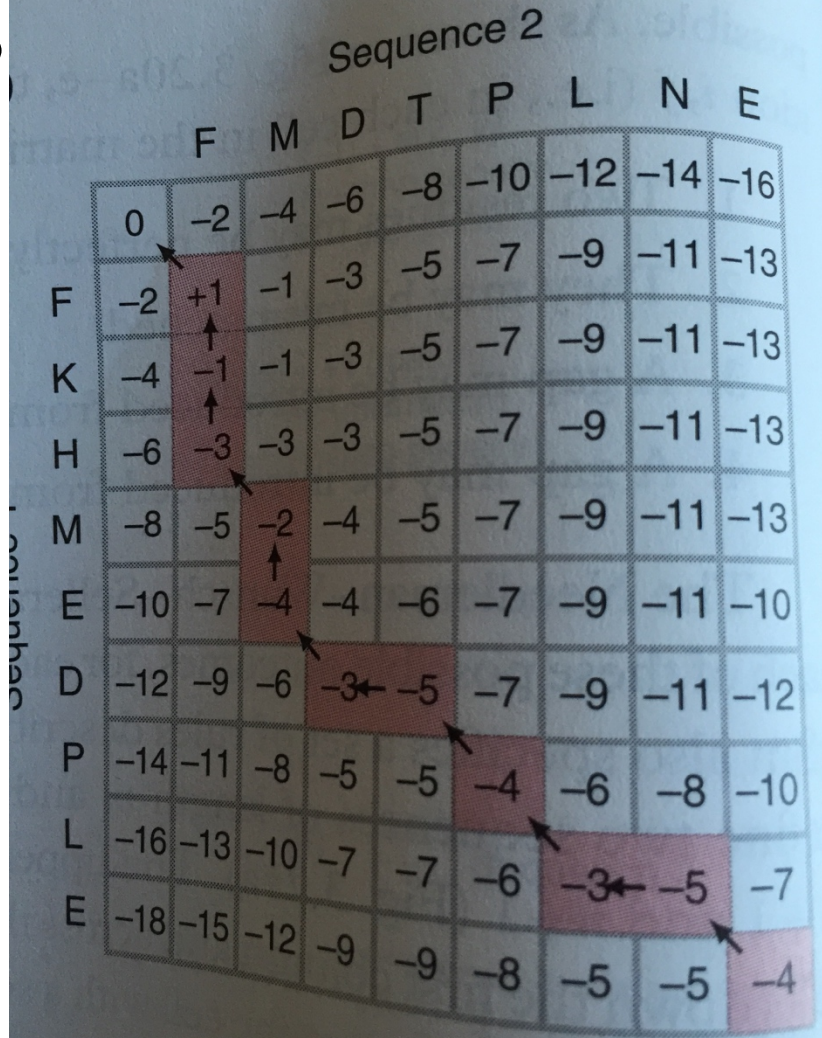
Global Alignment
Step 3:
ID optimal alignment

Sequence 2

| | F | M | D | T | P | L | N | E | |
|---|-----|-----|-----|----|-----|-----|-----|-----|-----|
| 0 | -2 | -4 | -6 | -8 | -10 | -12 | -14 | -16 | |
| F | -2 | +1 | -1 | -3 | -5 | -7 | -9 | -11 | -13 |
| K | -4 | -1 | -1 | -3 | -5 | -7 | -9 | -11 | -13 |
| H | -6 | -3 | -3 | -3 | -5 | -7 | -9 | -11 | -13 |
| M | -8 | -5 | -2 | -4 | -5 | -7 | -9 | -11 | -13 |
| E | -10 | -7 | -4 | -4 | -6 | -7 | -9 | -11 | -10 |
| D | -12 | -9 | -6 | -3 | -5 | -7 | -9 | -11 | -12 |
| P | -14 | -11 | -8 | -5 | -5 | -4 | -6 | -8 | -10 |
| L | -16 | -13 | -10 | -7 | -7 | -6 | -3 | -5 | -7 |
| E | -18 | -15 | -12 | -9 | -9 | -8 | -5 | -5 | -4 |

ALGORITHMS

Global Alignment
Step 3:
ID optimal alignment



Advanced Search

Sept 16, 2015

ADVANCED SEARCH

PSI-BLAST

ADVANCED SEARCH

PSI-BLAST

```
66  FTVDENGQMSATAKGRVRLFNNDVCDMIGSFTD TEDPAKFKMKYWGVA SF LQKGNDDH 125
63  FSVDEKGHMSATAKGRVRLLSNWEVCADMVGTFTD TEDPAKFKMKYWGVA SF LQKGNDDH 122
34  FSVDEKGHMSATAKGRVRLLSNWEVCADMVGTFTD TEDPAKFKMKYWGVA SF LQKGNDDH 93
2   MSATAKGRVRLLNNDVCDMIGSFTD TEDPAKFKMKYWGVA SF LQKGNDDH 53
65  FKIEDNGKTTATAKGRVRLDKLELCANMVGTFT IE TNDPAKFKMKYHGALAILERGLDDH 124
44  FSVDESGKVTATAHGRVILNNDWEMCANMFGTFEDTPDPAKFKMRYWGAA SF LQKGNDDH 103
44  FSVDSGKVTATAQGRVILNNDWEMCANMFGTFEDTPDPAKFKMRYWGAA SF LQKGNDDH 100
63  FTIHEDGAMTATAKGRVILNNDWEMCADMMATFETTPDPAKFKMRYWGAA SF LQKGNDDH 121
60  FKVEEDGTMTATAIGRVILNNDWEMCANMFGTFEDTEDPAKFKMKYWGAA SF LQKGYDDH 118
81  FKVQEDGTMTATATGRVILNNDWEMCANMFGTFEDTEEPARFKMKYWGAA SF LQKGYDDH 141
1   MVGTFD TEDPAKFKMKYWGVA SF LQKGNDDH 32
38  FSVDSGKMTATAQGRVILNNDWEMCANMFGTFEDTPDPAKFKMRYWGAA SF LQKGNDDH 97
65  YTVEEDGTMTASSKGRVKLFGFVVICADMAAQYTDPTTPAKMYMTYQGLAS SF LSSGGDNY 12
```

↑ ↑ ↑ ↑ ↑

R,I,K C D,E,T K,R,T N,L,Y,G

ADVANCED SEARCH

PSI-BLAST

