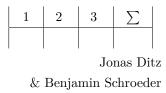
Bioinformatics I

WS 15/16

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Blatt 7

(Abgabe am 19. October 2015)

Exercise 1 - Smith Waterman today

The 30 years old Smith-Waterman (SW) algorithm is one of the fundamental algorithms in bioinformatics. This algorithm allows in a biological sense for example the detection of Domains in a protein or a Protein in a larger sequence. But the dynamic programmed algorithm has to face the problem of complexity of $O(n \times m)$. This complexity is getting a problem when starting to compare large sequences or even whole genomes. The classical example for todays usage of the Smith Waterman algorithm is the BLAST algorithm. [Li, H., Homer, N.]

Exercise 2 - DP Algorithm for finding motifs

```
\begin{array}{l} \underline{\text{for}} \ i = 0 \ \underline{\text{to}} \ \underline{\text{length}}(X) \\ \underline{\text{if}} \ X[i] == Y[0] \\ \text{Score} = 0 \qquad \underline{\text{for}} \ j = 0 \ \underline{\text{to}} \ \underline{\text{length}}(Y) \\ \underline{\text{if}} \ (X[i+j] == Y[j]) \ \text{Score} \ += 1 \\ \text{if} \ (\text{Score} > T) \qquad \text{print}(\text{motif found at position i}) \qquad i \ += \text{length}(Y) \end{array}
```

Exercise 3 - Programming assignment: Needleman-Wunsch alignment

One task was to handle command line options. We wrote a new class to have a modular and easy way to provide this functionality. The java package args4j has everything we need. So we used that package to write our own option handler class. The code can be found in CommandLineParser.java. We did the same with gap penalties. A gap penalty class gives one the advantage of modular gap handling. If a gap penalties are needed, just reuse this class.

A new member function of our NeedlemanWunsch class takes care of file writing. If a user wants the resulting alignment in a FastA file, this function takes care of it.

References

[Li, H., Homer, N.] Li, H., Homer, N. (2010). A survey of sequence alignment algorithms for next-generation sequencing. Briefings in Bioinformatics, 11(5), 473-483. http://doi.org/10.1093/bib/bbq015