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Algorithms in Genome Research

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Exercises

Number 6, Discussion: 2025-December-12

1. Given a list of peaks from a Tandem Mass Spectrum (MS/MS) for peptide de-novo sequencing, one important obstacle for recovering the peptide sequence is to assign peaks to the main ion types b and y (prefix and suffix strings of the peptide sequence, respectively).

   If we know that only b-ions are present in the spectrum, then recovering the sequence becomes simple. Describe an algorithm to do so: Input are the parent mass W and an ordered list of prefix masses $w_1, \ldots, w_k$. (Some peaks may be missing, though.)

2. We modify the above problem such that there are "noise peaks" (of unknown origin) in the mass spectrum. Describe an algorithm that finds a peptide sequence maximizing the number of explained peaks. The algorithm should run in $O(k|\Sigma|)$ time where k is the number of peaks and Σ is the underlying alphabet of amino acids. Hint: Use dynamic programming.

3. Word puzzling:

   - How many different words can be built by using all the letters of the string $S =$ `GLÜHWEIN` exactly once? Compute the actual value.
   - How many different words can be built by using all the letters of the string $S =$ `TEELICHT` exactly once? Note that all words need to have the same length and must use the letters the specified number of times: For `ABA`, there are three such words, `AAB`, `ABA`, `BAA`.
   - Try and find a general formula for the number of different words wordnum(S) that can be created from the letters of a string S. Hint: For $S =$ `GLÜHWEIN`, the formula depends only on the length of S, but not for $S =$ `TEELICHT` - what else does it depend on?

4. Suppose that we do not know the order of characters in a string: For example, the strings `AACCC`, `ACACC`, ..., `CCCAA` are indistinguishable to us. We call such "strings without order" *compomers* (denoted $\mathtt{A}_2\mathtt{C}_3$ for our example). The *length* of a compomer is the length of the corresponding string (5 in our example).

   - Let $\Sigma = \{\mathtt{A}, \mathtt{C}, \mathtt{G}, \mathtt{T}\}$ be our alphabet, then there exist 4 compomers of length 1 ($\mathtt{A}_1, \mathtt{C}_1, \mathtt{G}_1, \mathtt{T}_1$) and 10 compomers of length 2 ($\mathtt{A}_2, \mathtt{A}_1\mathtt{C}_1, \mathtt{A}_1\mathtt{G}_1, \mathtt{A}_1\mathtt{T}_1, \mathtt{C}_2, \mathtt{C}_1\mathtt{G}_1, \mathtt{C}_1\mathtt{T}_1, \mathtt{G}_2, \mathtt{G}_1\mathtt{T}_1, \mathtt{T}_2$). How many compomers exist of lengths 3 and 4?
   - Derive a general formula for the number of compomers of length n over an arbitrary alphabet Σ of size σ.