

MstatX User Manual

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1 Introduction

MstatX aims to provide a simple and easy-to-extend solution for multiple alignment statistics calculation. A multiple alignment is simply defined by an alphabet of symbols and a list of words made with this alphabet. The definition of statistics calculation is completely independant and can be seen as a module or a plug-in.

The default usage of MstatX is for multiple alignment of protein sequences, so, it uses amino acids substitution matrix to calculate statistics. But it is possible to use it for any alphabet with any scoring scheme defined by the user.

MstatX has two side: the end-user side and the programmer side. If you wants to calculate statistics already available in MstatX, then read the section 3. If you want to add a new statistics module in MstatX, then read the section 4 to have some examples of already coded statistics modules.

2 Installation

If you read this, then you have downloaded MstatX from my github repository. When you are at the root of MstatX, just open a terminal and:

```
make
```

This will compile MstatX with `g++`. So you need it in order to compile.

MstatX uses only one environment variable: `SCORE_MAT_PATH`. This variable gives the path to the substitution matrices directory. You can set this variable in your `.bashrc` file or you can also use the `-sd` option to specify the substitution matrices directory to MstatX.

3 User side

This section is dedicated to the usage of MstatX. If you want to add a statistics module in MstatX, read section 4.

3.1 Getting started

The basic use of MstatX is like the following:

```
mstatx -ma example.mali
```

This command will calculate the trident statistic of each columns in the multiple sequences alignment given in file `example.mali`. The trident statistic scores are written in file `example.stat`. Line 1 of file `example.stat` corresponds to column 1 in file `example.mali`, etc. This definition allows the calculation of multiple scores for a given column.

The trident statistic is defined in section 3.3.

3.2 Options

3.3 Available statistics

Statistics proposed in MstatX comes from many articles. For a review of these scores, you can refer to [3] and [2]

Trident

The trident statistic module is based on the work of William S.J. Valdar [3]. It is composed of three parts, each measures a different aspect of column conservation.

The first part, noted $t(x)$, measures the entropy of a column x by the Shannon formula:

$$t(x) = \frac{1}{\log(\min(N, K))} \sum_{a=1}^K p_a \log(p_a) \quad (1)$$

In this formule, N is the number of sequences in the multiple alignment, K is the size of the alphabet, and p_a is the probability of symbol a in the column x . The redundancy between the sequences in the multiple alignment is measured in p_a by this formula:

$$p_a = \sum_{i \in \{i | s(i)=a\}} w_i \quad (2)$$

In this formula, w_i is the weight of sequence i and it is added to the probability p_a only if the symbol of sequence i and column x is a . The weight is calculated by the formula from Henikoff & Henikoff [1]:

$$w_i = \frac{1}{L} \sum_{x=1}^L \frac{1}{K_x n_{x_i}} \quad (3)$$

In this formula, L is the length of the alignment,

4 Programmer side

4.1 The Statistics virtual class

Bibliography

- [1] Steven Henikoff and Jorja G. Henikoff. Position-based sequence weights. *Journal of Molecular Biology*, 243(4):574 – 578, 1994.
- [2] Fredrik Johansson and Hiroyuki Toh. A comparative study of conservation and variation scores. *BMC bioinformatics*, 11:388, 2010.
- [3] W.S.J Valdar. Scoring residue conservation. *Proteins: Structure, Function, and Bioinformatics*, 48(2):227–241, 2002.

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