

# MstatX User Manual

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# Contents

1	Introduction . . . . .	1
2	Installation . . . . .	1
3	User side . . . . .	3
3.1	Getting started . . . . .	3
3.2	Options . . . . .	3
3.3	Available statistics . . . . .	3
	Trident . . . . .	3
4	Programmer side . . . . .	5
4.1	The Statistics virtual class . . . . .	5

# 1 Introduction

MstatX provides a simple and easy-to-extend solution for multiple alignment scores calculation.

A multiple alignment can be produced in many ways, including the use of an application like CLUSTALW [5] or MUSCLE [1], but also manually. Once obtained, automatic methods gives a global score for the alignment. But we often need to calculate the conservation on one or many columns. Or we want to calculate a global score with another method or statistic.

When we searched the web for such a tool, we found nothing. Many scores exist to evaluate a multiple alignment, but no simple command-line tool can do it easily. That is why we created MstatX.

In MstatX, things are simple. A multiple alignment is simply defined by an alphabet of symbols and a list of words made with this alphabet. The calculation of a given score is completely independent from the other scores. The output is a simple text file with the score of each column of the multiple alignment (or the global score only if asked).

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 statistics, you can refer to [6] and [3]. Some of the statistics use scoring matrices. We choose to use matrices in the AAindex format [4] from the AAindex website<sup>1</sup>. Although it has not been updated since 2008, this website provide a useful list of amino acids scoring matrices in a simple format. The user can use his own scoring matrix by the flag `-sp` and `-sc`.

#### Trident

The trident statistic module is based on the work of William S.J. Valdar [6]. 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:

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

---

<sup>1</sup><http://www.genome.jp/aaindex/>

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 alignement 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 [2]:

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

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

## 4 Programmer side

### 4.1 The Statistics virtual class



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