wScatFit

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4-6-2002

Abstract

This pages provide a brief introduction to handle the computer program **wScatFit®**, which has been developed by the author. This program has been designed *ad hoc* for estimating the McGhee and von Hippel Equation.

1 Introduction

wScatFit® is a computer program which carries out the estimation of the equation for the non-cooperative interacting ligand-lattice case by several statistical procedures.

From a theoterical point of view, this equation is derived in McGhee and von Hippel (1974). However, in practice the parameters of this equation have to be estimated from experimental data. Since different probabilitstic models on the noisy experimental data can be considered, different statistical procedures must be used. Some explanations about the statistical procedures which are implemented in **wScatFit®** appear in Talavera *et al* (2002).

Roughly speaking, the problem consists of fitting the nonlinear equation

$$\frac{\nu}{L} \; = \; K\,(1 \; - \; n\,\nu)\,\left[\frac{1 \; - \; n\,\nu}{1 \; - \; (n-1)\,\nu}\right]^{n-1} \tag{1}$$

from data given by

$$\{(\nu_i, L_i) \; : \; i = 1, \ldots, M\} \; ,$$

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where the unknown parameters, denoted by n and K, are assumed to be positive real numbers. It is usually assumed that n is subjected to $n \leq n_{max}$, where n_{max} is a given (known) positive integer.

However the data set $\{(\nu_i, L_i) \ : \ i = 1, \ldots, M\}$ are not directly observed in the laboratory. In the laboratory the observed (experimental) data are given by $\{([E]_b(i), [E]_f(i)) : i = 1, \ldots, M\}$ and $[DNA]_0$, where

- $[E]_b(i)$ is the concentration of bound ligands in the experiment i,
- $[E]_f(i)$ is the concentration of free ligands in the experiment i,
- $[DNA]_0$ is the concentration of macromolecules.

Once the experimental data are obtained, it follows that

$$\nu_i \stackrel{def}{=} \frac{[E]_b(i)}{[DNA]_0} \qquad \text{and} \qquad L_i \stackrel{def}{=} [E]_f(i)\,.$$

More details about the McGhee and von Hippel Equation can be obtained in McGhee and von Hippel (1974). The datafile for **wScatFit®**will contain data given by $\{([E]_b(i), [E]_f(i)) : i = 1, \ldots, M\}$ and $[DNA]_0$.

2 Getting started

wScatFit® is a program under MS-Windows. This makes very easy to handle the program in the windows environment. It is important to note that the experimental data have to be previously stored in an ASCII file (MSDOS Text file) with extension ***.DAT** following a fixed syntaxis by using any word processor (WordPad, Notepad, ...).

If we run **wScatFit®**, we firstly indicate the name of the data file (*.DAT) and we then execute the program by clicking in the **Execute** menu. After some seconds, the program will thus indicate the end of calculations. In this point, **wScatFit®** has already created another ASCII file with extension *.OUT, where the estimated parameters and other results are stored. In order to display or to print this output file any ASCII word processor can be considered.

In the next section the syntaxis for the data file to be followed by the user is outlined. Note that the output file (i.e. the file containing numerical results) is made automatically by **wScatFit®**.

$[DNA]_0$	
M	
$[E]_b(1)$	$[E]_f(1)$
$[E]_b(2)$	$[E]_f(2)$
$\vdots$	$\vdots$
$[E]_b(M)$	$[E]_f(M)$

Table 1: Data file syntaxis.

2.1 Data file syntaxis

The user for making any data file has to follow the following conditions:

1. $[DNA]_0$ appears in the first line of the data file.
2. The number of experimental data M is included in the second line.
3. Each pair of data is included in a line.

An example of the structure of a input file can be seen in Table 1.

3 References to wScatFit®

Finally, the author would like to note that this computer program has been firstly used in the paper by Talavera *et al* (2002). As the details about this program appears in this article, this program could be referenced through including a cite for the article by Talavera *et al* (2002).

References

[1] McGhee, J. and von Hippel, P. (1974). Theoretical aspects of DNA–protein interactions: co–operative and non-co-operative binding of large ligands to a one-dimensional homogeneous lattice. *Journal of Molecular Biology* **86**, 469–489.

[2] Talavera, E.M., Guerrero, P., Ocana, F. and Alvarez-Pez, J.M. (2002). Photophysical and Direct Determination of Binding Constants of Ethidium Bromide complexed to E. coli DNA. *Applied Spectroscopy* **56**(3),