Nonlinear Parameter-estimation

Name

gfit – interactive parameter-estimation using gnuplot

Synopsis

`gfit [model] [data_file]`

This program prepares a model definition for loading in the gnuplot program. The user must then run a series of interactive commands to obtain parameter estimates.

Purpose

This program is a simple script that runs "gnuplot[1]", a general purpose interactive plotting and curve fitting utility. It is used to obtain estimates for some of the input parameters required for other programs in this package. Many other programs can be used to generate these estimates. For those wishing to use an alternate programs, the model equations and sample results shown below may be helpful.

Unlike the other programs in this package, gfit does not support batch operation. The hardware requirements for gfit are more demanding than for the other programs in the ocean production package.

Description

The gfit script creates a file containing the model definition and starts the gnuplot program. The user must issue interactive commands to plot a data file and fit the model. The most commonly used commands are:

help invokes a comprehensive help system for gnuplot;

show displays current values of variables (*show variables*) and lists user-defined functions (*show functions*);

plot displays a graph of functions and data;

replot repeats the last *plot* command (functions will be evaluated using the current parameter values);

fit performs nonlinear least-squares regression; and

load reads and executes a file containing gnuplot commands; and

quit ends the session.

[1] available without charge in versions that run on a wide range of systems. A new version (3.6) is now (summer 1996) undergoing beta testing. Current information is available through the internet at URL `http://www.cs.dartmouth.edu/gnuplot`. Note that not all executables include the parameter-estimation module (fit) used here.

z m	$B(z)$ mg Chl m^{-3}	z m	$B(z)$ mg Chl m^{-3}
0	0.6	60	0.48
10	0.7	70	0.52
20	1.0	80	0.50
30	1.6	90	0.40
40	1.3	100	0.60
50	0.6	–	–

Table 1. Example profile data file (`etc\profile.dat`). The file is formatted in two columns: depth, z; and the corresponding chlorophyll biomass, $B(z)$.

Gnuplot supports command-line history editing using the cursor keys. It is not necessary to retype an entire command to repeat an operation with minor changes. Most gnuplot commands can be abbreviated.

Examples

The first example shows the use of gfit to estimate the profile parameters z_m, B_0, h, and σ for the shifted-Gaussian model. The data set used for the example is shown in Table 1.

A Gaussian profile was used by Lewis *et al.* (1983) to describe the vertical distribution of chlorophyll biomass in the ocean. Later, Platt *et al.* (1988) introduced the shifted-Gaussian model, that is a Gaussian superimposed on a constant background, to provide a more versatile profile (Figure 1 of Platt *et al.* 1994). It allows one to match the surface values without compromising the structure of the rest of the profile. This is the standardised profile that has been adopted by subsequent authors (Morel & Berthon 1989, Sathyendranath & Platt 1989, Sathyendranath *et al.* 1989, André 1992, Gordon 1992). It has been found that a shifted Gaussian provides a suitable description of the vertical distribution of chlorophyll at a wide range of locations in the ocean. The shifted-Gaussian model for biomass depth profiles is expressed (in one of many mathematically-equivalent formulations) by the model equation:

$$B(z) = B_0 + \frac{h}{\sigma\sqrt{2\pi}} e^{-\frac{(z-z_m)^2}{2\sigma^2}},$$

where $B(z)$ is chlorophyll biomass as a function of depth, z (positive downwards). B_0 represents the "background" concentration on which a Gaussian curve whose peak is centered at depth z_m is superimposed. In some cases, a degenerate form of the model (with $B_0 \equiv 0$ or $h \equiv 0$) may be appropriate.

In practice, the change of variables $h = \exp(a)$, $\sigma = \exp(b)$, and $B_0 = \exp(c)$ is introduced so that the numerical algorithm will not attempt to evaluate the function using meaningless (negative) values for the parameters.

The first step is to prepare the files and load the definitions. This will also produce a plot of the data and of the model function with all the parameter values set to zero. An edited transcript of a typical session follows:

```
C:\OP\DATA> gfit sgauss profile.dat
gnuplot> load 'sgauss'

        User-Defined Functions:
        ef(z) = (z-zm)*(z-zm)/(2*exp(2*b))
        f(z) = exp(c) + exp( a - ef(z) - b - 0.9184 )

model variables are a=log(h), b=log(sigma), c=log(B_0), and zm
```

The next step is to examine the plot to obtain starting estimates. The value for the depth of the chlorophyll maximum, z_m, is seen to be approximately 30 m. The value for the background concentration, B_0, is seen to be approximately 0.4 mg Chl m^{-3}. The remaining two parameters are less easy to estimate by inspection, so we will start with arbitrary values. Note that some versions of gnuplot require that floating point numbers be entered with explicit decimal points (*e.g.*, 'zm=30.0', *not* 'zm=30'). A semi-colon can be used to separate multiple assignments on a line (this makes it easier to restore earlier parameter values from the command-line history if required). Some versions of gnuplot may display variables with many non-significant digits. The following commands set starting values, display the updated plot of the model and data together, and list current values of the variables[2]:

```
gnuplot> a=log(1); b=log(1); c=log(0.4); zm=30.0
gnuplot> replot
gnuplot> sho var

        Variables:
        pi = 3.14159265358979
        FIT_INDEX = 0
        zm = 30.0000000000000
        b = 0
        c = -0.916290731874155
        a = 0
```

The resulting plot (Figure 1) confirms the choices for B_0 and z_m, but suggests that both h and σ must be increased.

By continuing to experiment with different settings for the remaining two variables, a more reasonable starting fit is obtained (note that it is not necessary to retype the entire line to make each change; simply recall the previous line and edit the value to be changed):

[2] Note that the *show* command in the version of gnuplot used to generate these examples displays variables to fourteen decimal places. When reporting these values, the number of decimal places should be reduced commensurate with the uncertainties in the estimates.

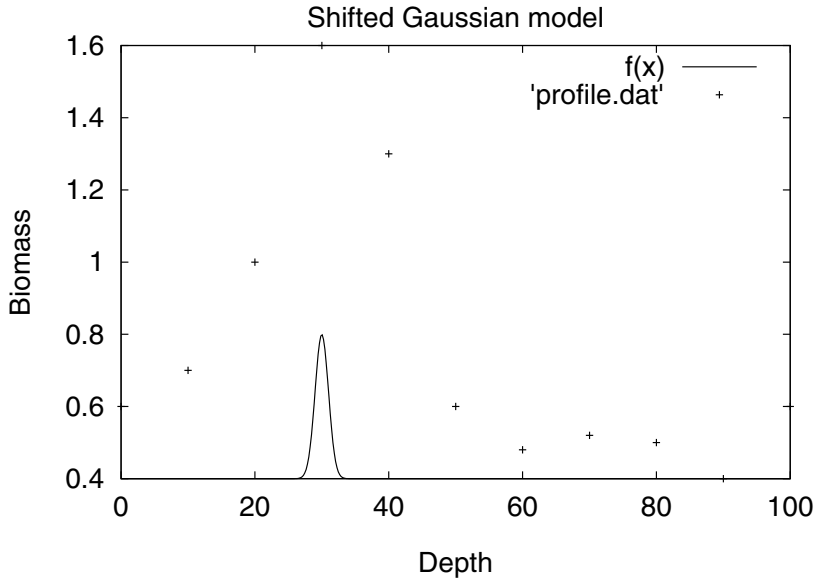

Figure 1. Preliminary plot for parameter-estimation of profile parameters using the shifted-Gaussian model. Crosses represent data points; the smooth curve represents the model.

```
gnuplot> a=log(2);b=log(1);c=log(0.4);zm=30.0
gnuplot> replot
gnuplot> a=log(2);b=log(10);c=log(0.4);zm=30.0
gnuplot> replot
gnuplot> a=log(10);b=log(10);c=log(0.4);zm=30.0
gnuplot> replot
gnuplot> a=log(30);b=log(10);c=log(0.4);zm=30.0
gnuplot> replot
gnuplot> sho var

        Variables:
        pi = 3.14159265358979
        FIT_INDEX = 0
        zm = 30.0000000000000
        b = 2.30258509299405
        c = -0.916290731874155
        a = 3.40119738166216
```

Having obtained reasonable starting values, we first refine the estimates for $a = \log(h)$ and $b = \log(\sigma)$:

```
gnuplot> fit f(x) 'profile.dat' via a,b
...
gnuplot> sho var
```

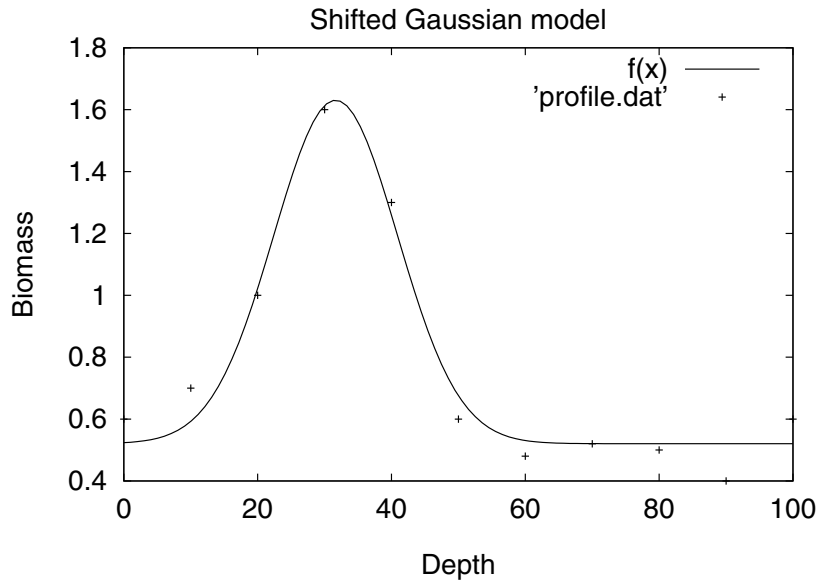

Figure 2. Plot showing the final parameter estimates for shifted-Gaussian model.

```
Variables:
pi = 3.14159265358979
FIT_INDEX = 0
zm = 30.0000000000000
b = 2.44663029314006
c = -0.916290731874155
a = 3.50415149941879
```

Finally, a fit is obtained using all four parameters (note that, by defining the variables h, σ, and B_0 as functions of the parameters used in fitting, the program provides estimates for the original parameterization) and the result plotted (Figure 2):

```
gnuplot> fit f(x) 'profile.dat' via a,b,c,zm
...
gnuplot> h=exp(a);sigma=exp(b);B_0=exp(c)
gnuplot> sho var

Variables:
pi = 3.14159265358979
FIT_INDEX = 0
zm = 31.6535747998782
b = 2.22460670745325
c = -0.652869482620909
a = 3.24750564253516
h = 25.7260897550485
sigma = 9.24984419365467
B_0 = 0.520549922667341
```

I W m^{-2}	$P^B(I)$ mg C (mg Chl)$^{-1}$ h^{-1}	I W m^{-2}	$P^B(I)$ mg C (mg Chl)$^{-1}$ h^{-1}
536.8	2.80	30.9	0.68
408.5	2.51	27.6	0.58
356.3	2.31	19.0	0.46
313.5	2.55	15.7	0.38
161.5	2.43	13.8	0.32
133.0	2.14	12.2	0.21
111.2	2.10	11.1	0.16
98.8	1.95	9.9	0.14
89.3	1.71	6.6	0.10
79.3	1.47	5.6	0.07
53.2	1.36	4.9	0.05
42.8	1.06	2.2	0.02
38.0	0.98	1.9	0.01
34.2	0.88	–	–

Table 2. Example data file (`etc\p-i.dat`). The file is formatted in two columns: light intensity, I; and the resulting production normalized to biomass, P^B.

```
gnuplot> replot
```

Once acceptable estimates have been obtained using the numerical procedure, the number of significant figures in the estimates must be reduced commensurate with the uncertainties.

A second example is the photosynthesis – irradiance model defined by the following equation (Platt *et al.* 1980):

$$P^B = P/B = P_m^B(1 - \exp(-\alpha^B I/P_m^B)),$$

where P is the instantaneous rate of primary production per unit volume of water, B is the photosynthetically active biomass, I the irradiance, and the parameters are α^B and P_m^B.

The data file used for the example is shown in Table 2.

The first step is to prepare the files and load the definitions. This will also produce a plot of the data and of the model function with all the parameter values set to zero. An edited transcript of the session follows:

```
C:\OP\DATA> gfit p-i p-i.dat
gnuplot> load 'p-i'

        User-Defined Functions:
        f(I) = exp(p)*(1-exp(-I*exp(q)/exp(p)))

model variables are q=log(alphaB) and p=log(PmB)
```

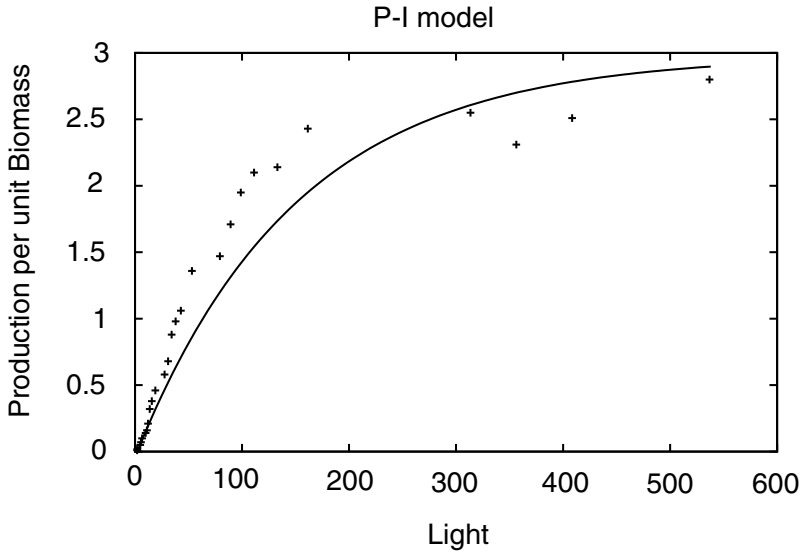

Figure 3. Preliminary plot for parameter-estimation using photosynthesis–irradiance model.

The next step is to examine the plot to obtain starting estimates. The value for the maximum, P_m^B, is seen to be approximately 3. The slope at the origin, α^B , is seen to be approximately 0.02. These estimates can easily be improved by trial and error:

```
gnuplot> p=log(3);q=log(.02)
gnuplot> replot
```

The trial plot (Figure 3) confirms the choices $\alpha^B = 0.2$ and $P_m^B = 3$ as reasonable starting estimates.

Having obtained reasonable starting values, a fit is obtained and the result plotted (Figure 4):

```
gnuplot> fit f(x) 'p-i.dat' via p,q
...
Final set of parameters     68.3% confidence interval (one at a time)
=======================================================

p               = 0.96895          q   0.0244208
q               = -3.4726          q   0.0447196

correlation matrix of the fit parameters:

               p      q
p               1.000 -0.445
q              -0.445  1.000
gnuplot> alphaB=exp(q);PmB=exp(p)
```

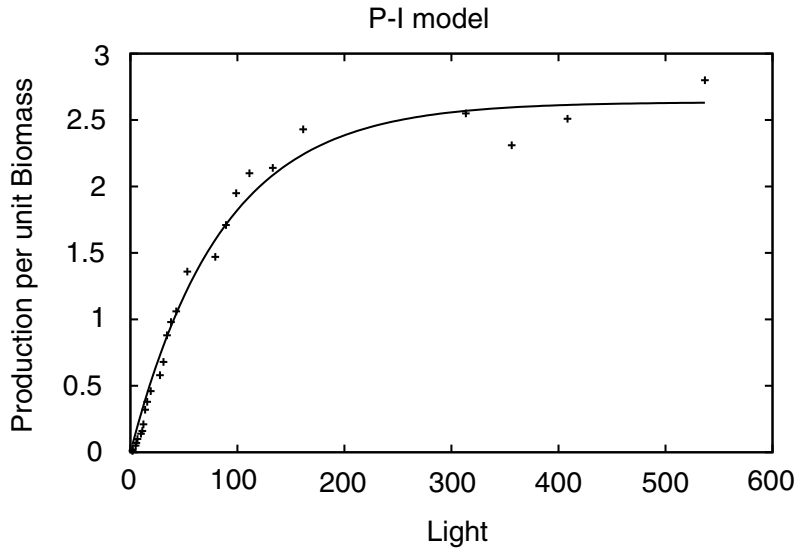

Figure 4. Plot showing the curve produced by the final parameter estimates, $\alpha^B = 0.031$ and $P_m^B = 2.6$, for the photosynthesis–irradiance model.

```
gnuplot> sho var

        Variables:
        pi = 3.14159265358979
        FIT_INDEX = 0
        p = 0.968949538557486
        q = -3.47259930892269
        alphaB = 0.0310362529142556
        PmB = 2.6351748553479
```

Again, the number of significant figures should be adjusted reflect the uncertainties when reporting these estimates.

Input

The input data file for gnuplot consists of one or more data records with no header. Each record has two fields. Any line in the file that begins with the # character is treated as a comment.

Output

A record of the nonlinear parameter-estimation is placed in the file "`fit.log`". This file will continue to grow over time. The gnuplot source distribution includes drivers capable of generating plots in a wide variety of file formats. Including all these formats would result in a very large executable program, so most compiled versions support a subset of the available drivers.

Special cases

In some cases it is not appropriate to use the full, shifted-Gaussian model. Examples include the case where $B_0 = 0$ or $h = 0$. In the case $B_0 = 0$, the appropriate model is "`gauss`", which is almost identical to "`sgauss`", but omits the background term. The case $h = 0$ corresponds to the model "`constant`".

```
gnuplot> f(x)=B_0
gnuplot> fit f(x) 'profile.dat' via B_0
```

Files

In addition to the binary executable program, one input data file and a file defining the model are required. A log file containing a record of the processing is created. The files are:

1) the gnuplot program (executable) file (`gnuplot.exe`);
2) input data (ASCII text, `.dat` extension);
3) a log of the job (ASCII text, `fit.log`); and
4) model (ASCII text, no extension).

The log file will continue to grow in size for each new calculation, and should be truncated or removed periodically.

Requirements

The numerical calculations are not demanding. An effort has been made to ensure that the results will remain consistent across a range of hardware platforms. It is assumed that double precision variables conform to the IEEE floating point arithmetic standard. This is the most efficient data type for floating point computations on modern microprocessors with hardware floating point support.

To run the program under MS-DOS, approximately 512k of free, low-DOS memory is required.

Bugs

There are many different versions of gnuplot available on the internet. Most of these suffer to some extent from bugs associated with the compilers used to build them. The nonlinear parameter-estimation module has been improved over time, but not all versions incorporate all of the available improvements.

It is difficult to protect against all possible combinations of input parameters that generate run-time errors due to floating point underflow or overflow. In general, care taken in the choice of a parameterization and in choosing initial parameter estimates will reduce the likelihood of such errors.

Limits

The maximum number of input records is a function of available memory and the compiler used to compile the gnuplot program.

Diagnostics

It is not unusual for the fit command to fail, either due to a floating point error or a "singular matrix". These errors often occur when the fitting procedure generates trial parameter values that produce numerical underflow or overflow. A number of factors may contribute to these errors:

1) initial parameter estimates were not sufficiently close to the solution;
2) a mistake was made entering the model equations;
3) the data do not fit the model well;
4) poorly-scaled data; or
5) inappropriate parameterization of the model.

References

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Notation

α^B	initial slope of $P^B - I$ curve, defined as $\partial P^B/\partial I\|_{I\to 0}$, mg C (mg Chl)$^{-1}$ h^{-1} (W m^{-2})$^{-1}$.
B	biomass, as concentration of chlorophyll *a*, mg Chl m^{-3}.
$B(z)$	chlorophyll concentration as a function of depth, mg Chl m^{-3}.
B_0	background concentration in the shifted-Gaussian model, mg Chl m^{-3}.
h	parameter for the amplitude of the chlorophyll maximum in the shifted-Gaussian model, mg Chl m^{-2}.
I	irradiance, W m^{-2}.
P^B	primary production rate normalized to biomass, $P^B \equiv P/B$, mg C (mg Chl)$^{-1}$ h^{-1}.
P_m^B	assimilation number, specific production at saturating light, in the absence of photoinhibition, $P_m^B = P^B\|_{I\to\infty}$, mg C (mg Chl)$^{-1}$ h^{-1}.
σ	scale parameter for the width of the peak in the shifted-Gaussian model, m.
z	depth (origin at surface, positive downwards), m.
z_m	"depth" (in rare cases, the value of z_m may be negative) of chlorophyll maximum, in the shifted-Gaussian model, m.