

# BGFit



---

## INESC-ID

### USER AND TECHNICAL DOCUMENTATION

Supplementary material to reference to paper

---

*Authors:*

André VERÍSSIMO  
Susana Vinga

*Contacts:*

svinga@kdbio.inesc-id.pt

April 24, 2013

## Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
1.1	Source Code . . . . .	3
1.2	Availability . . . . .	3
<b>2</b>	<b>Architecture</b>	<b>3</b>
<b>3</b>	<b>Data organization</b>	<b>4</b>
<b>4</b>	<b>Tutorials on how to perform tasks in BGFIt</b>	<b>6</b>
4.1	Layout Description . . . . .	6
4.2	Create a New Team . . . . .	6
4.3	Adding an existing User to a Team . . . . .	7
4.4	Sign Up with a New User . . . . .	8
4.5	Login . . . . .	8
4.6	Insert new data measurements . . . . .	10
4.7	Estimate Parameters . . . . .	13
4.8	Multiple Estimation . . . . .	15
4.8.1	Aggregation . . . . .	16
4.8.2	Batch estimation . . . . .	17
4.9	Generate a new Model . . . . .	19
4.9.1	Create a new Model . . . . .	19
4.9.2	Add models parameters (if added later on the details page)	21
4.9.3	Generate source files . . . . .	21
4.9.4	Download source files . . . . .	22
4.10	Manual Regression . . . . .	24
<b>5</b>	<b>Modeling Extensions</b>	<b>27</b>
5.1	Overview . . . . .	27
5.2	Download . . . . .	27
5.3	Technical Overview . . . . .	27
5.4	Models . . . . .	27
5.5	Requirements . . . . .	28
5.5.1	Requirements for Octave-based models . . . . .	28
5.5.2	Requirements for Matlab-based models . . . . .	29
5.5.3	Requirements for SBTOOLBOX2-based models . . . . .	29
5.6	Structure . . . . .	29
5.7	Create a new model blackbox . . . . .	29
5.7.1	Octave / Matlab model . . . . .	29
5.7.2	Compile for octave . . . . .	30
5.7.3	Compile for matlab . . . . .	30
5.7.4	Compile for SBTOOLBOX2 model . . . . .	30
5.8	Test the model . . . . .	30
5.9	Deploy . . . . .	31
5.9.1	Octave . . . . .	31

5.9.2	Matlab or SBTOOLBOX2 . . . . .	31
<b>6</b>	<b>Questions and Sugestions</b>	<b>32</b>

**List of Figures**

1	Application's Architecture . . . . .	4
2	Data structure . . . . .	5
3	Layout of application . . . . .	6

## 1 Introduction

Existing tools to model bacterial growth curves do not offer enough automated methods adequate for large datasets neither present a standard nor a flexible approach. BGFIt provides a unified tool that offers a rich set of dynamic models for automatically estimate model parameters along with efficiently manage experimental time-series data in an structured way.

BGFIt was designed with a flexible architecture that focus on extensibility and leverages free software with existing tools and methods. BGFIt positions itself as a platform to compare and evaluate different data modeling techniques and extract relevant information from data.

The application is described in the context of bacterial growth data fitting, but it is also applicable to other types of two-dimensional data, e.g., from cancer growth experiments to macroeconomic data.

### 1.1 Source Code

- BGFIt source code
- Model extension source code

*All results are stored by the application and are downloadable by the user.*

### 1.2 Availability

BGFIt is currently available online at <http://oracle.inesc-id.pt> with all available functionality and several dynamic models that are further described at section 5.4.

The application is available for a guest user, that can browse and access detail on public data. However, to introduce and manage data or models it is required to register a user with a valid email.

## 2 Architecture

BGFIt is developed using open-source frameworks and free libraries allowing for a high dregree of flexibility and creating a modular system. Ruby on Rails, MySQL, Octave, MathJax and Google Chart Tools are some examples.

The application is designed using a model-view-controller architecture effectively separating data-management and dynamic modeling that is performed using extensions that are decoupled from the web-application.

The modeling extensions only require the implementation of the necessary interface and for it to be deployed on a location that is accessible by BGFIt. This approach allows for every component of BGFIt to be deployed online, encouraging collaboration and the reutilization of these tools. Nevertheless, it can also be used in a local installation.

The default modeling extension pack that describes different bacterial growth models (such as Baranyi, Gompertz, Logistics, etc. . . ) is implemented in Octave/Matlab. These modeling extensions are also released with BGFIt and are described in their documentation, as well as a template model from which all the implemented models derive. This provides a starting point for users to create their own models.

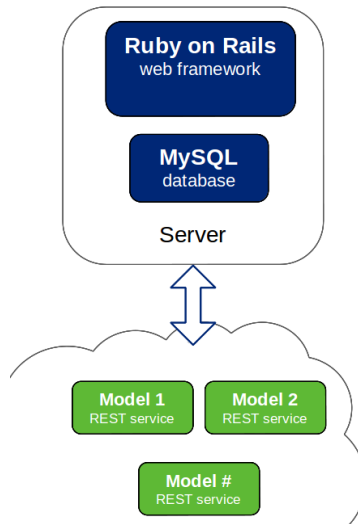


Figure 1: Application's Architecture

### 3 Data organization

Data management is divided in three layers: project (top-level folder) → experiment (folder) → measurement (actual data)

- Project: Top-level folder where permissions and other properties are set;
- Experiment: Folder to organize and aggregate data by typology;
- Measurement: Actual data, e.g. replicates.

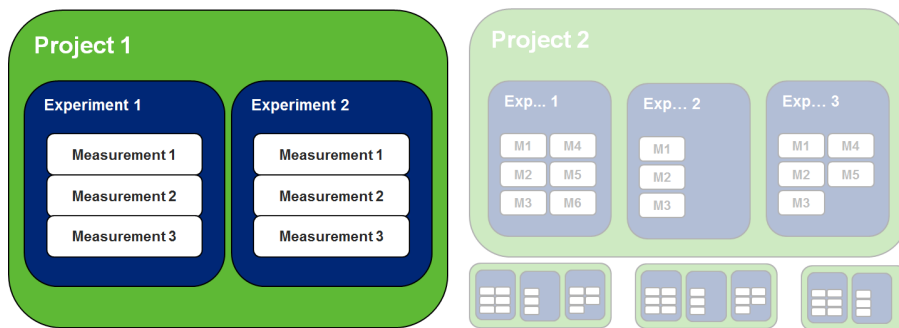


Figure 2: Data structure

## 4 Tutorials on how to perform tasks in BGFit

### 4.1 Layout Description

The application's layout is organized in three different areas (as shown in the image below):

1. Primary menu: Main navigation and contextual actions are available here;
2. User/Team management: Manage its account and the teams where he collaborates;
3. Content

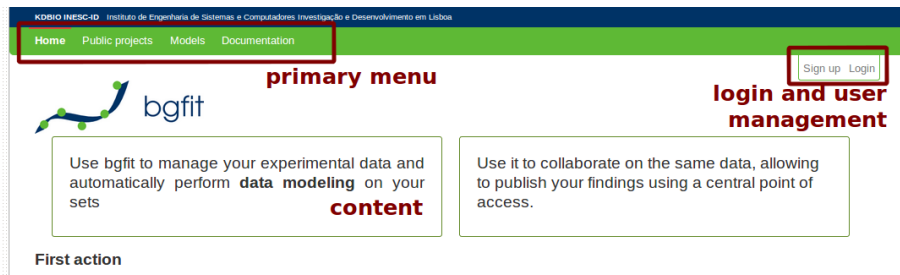
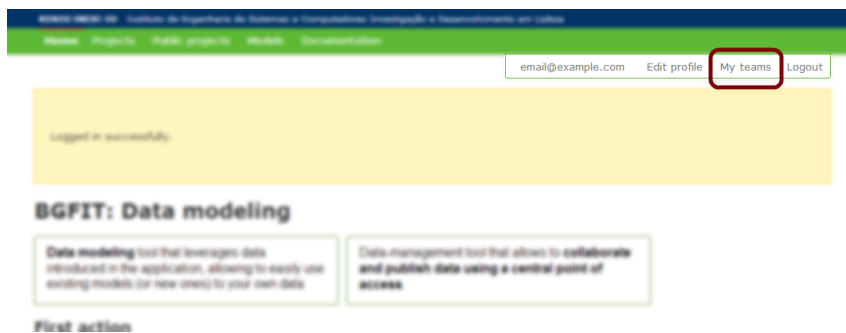


Figure 3: Layout of application

### 4.2 Create a New Team

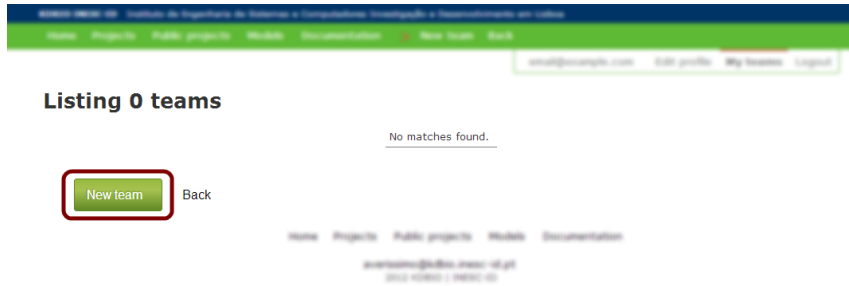
BGFit allows for teams to collaborate on the project at hand, being able to work and share on the same data.

1. To create a new team a user needs to login to the application and click on the “My teams” link on to top right corner

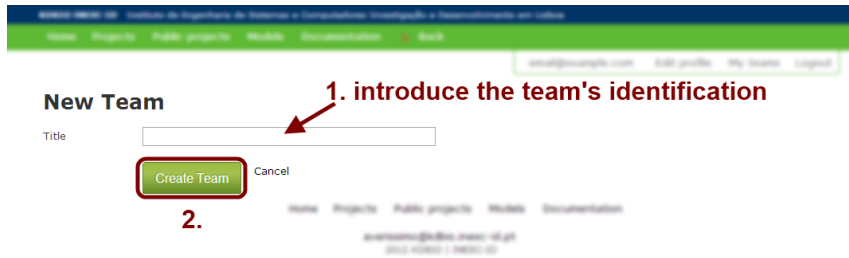


2. Click on “New team”

### 4.3 Adding an existing User to a Team's User and Technical Documentation

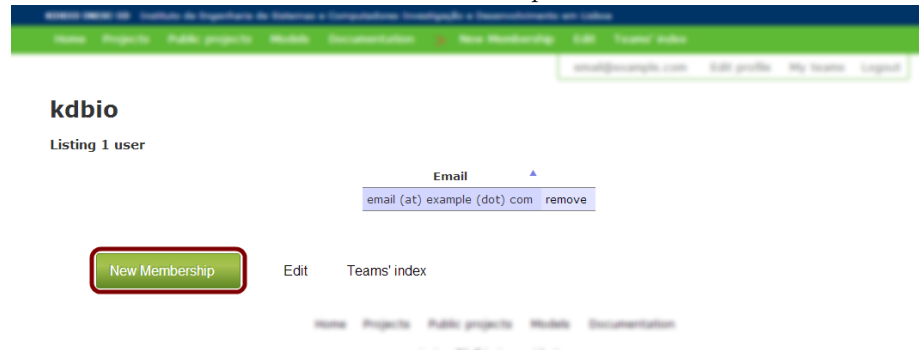


3. Select a name for the team



### 4.3 Adding an existing User to a Team

Goto the desired team and add a membership





## 4.4 Sign Up with a New User

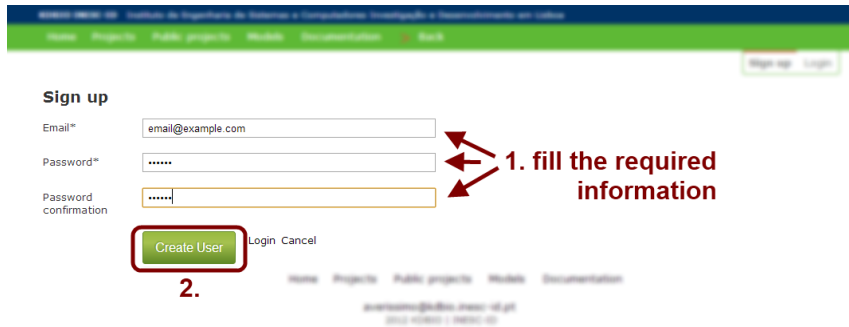
Any user can register a new user in BGFIT, having to provide an email address and a password.

This process is available using the “User/Team management” menu on the top right corner.

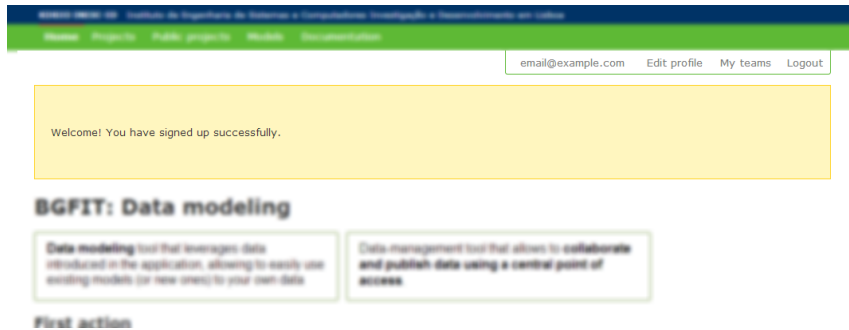
1. Click on the “Sign up” link on the top right corner



2. Introduce the required information



3. Success message

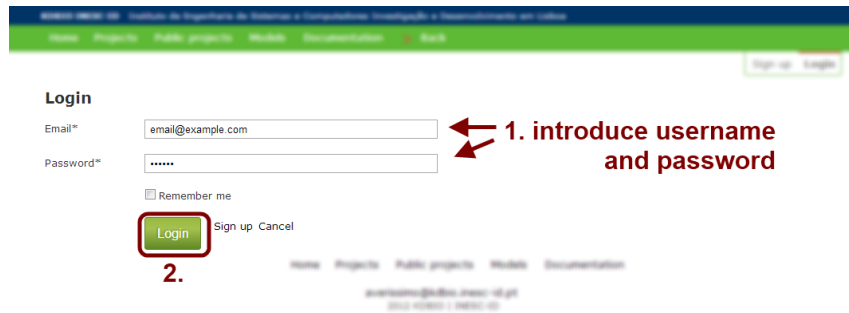


## 4.5 Login

1. Click on the “Login” link on the top right corner



## 2. Introduce the login information



## 4.6 Insert new data measurements

1. Start by creating a new project



2. Fill information about the project

Check the “published?” checkbox if the project should be public

### New Project

Title\*  1. fill information

identifier used for this project

Description  1. fill information

text describing the scope of this project

Published?  
if checked then the data is visible to the world, otherwise, only owner and associated teams can view it.

2. create project

3. Insert data

This can be accomplished in one of two ways:

- (a) Create a measurement directly using the default experiment folder
- (b) First create an experiment folder and then introduce measurements inside the folder

## 4.6 Insert new data measurement BGFIIt's User and Technical Documentation

### My project

#### Description

the description of my project

#### Domain

Owner: afsverissimo (at) gmail (dot) com  
Project is not yet public

Associate team

tip: give write or read permissions to a team.

Listing 0 experiments

New measurement

New Experiment

introduce new data directly to a 'default' experiment

organize your data by creating an experiment folder

tip: an experiment aggregates different measurements. You can use different experiments to aggregate identical conditions or if you wish to logically separate your results, otherwise just use the default experiment.

New Experiment

Edit Associate team Projects' index

### 4. Filling data

**My project**

Experiment: Default

Title: replicate 1

2007 January 2

Original data

0	0
1	1
2	4
3	9
4	16
5	25
6	36

data should be copied as tab delimited columns:  
X Y Z note

Create Measurement Cancel

identifier's title

data separated by tabs  
(can be copied from excel)

### 5. A view of the data showing the plot

## 4.6 Insert new data measurement BGFI's User and Technical Documentation

Home Projects Public projects Models Documentation **New measurement** Associate dynamic model Edit Goto project

afsvrissimo@gmail.com Edit profile My teams Logout

### Default (experiment)

Using My project scope  
the description of my project

**Experiment Description**  
(not defined)

Displaying 1 measurement

Project	Experiment	Title	Date
My project	Default	replicate 1	goto download .csv

[New measurement](#) [Associate dynamic model](#) [Edit](#) [Goto project](#)

**Proxy Models (0)**  
No matches found.

**Measurements chart**

Download chart as .svg

## 4.7 Estimate Parameters

1. Associate a model to measurement / experiment

An user must first navigate to a measurement or experiment and click on “Associate model”

### Default (experiment)

Using My project scope

the description of my project

Experiment Description

(not defined)

Displaying 1 measurement

Project	Experiment	Title	Date
My project	Default	replicate 1	goto download .csv

Proxy Models (0)

No matches found.

2. Choose from existing models

### New proxy dyna model

Title

used to differentiate models in case of using different set of ranges or manual tuning

- Gompertz  
 Baranyi  
 Logistics  
 Richards  
 LENP type 1b (ode)

No death phase

removes any sequential values in the end that show a declining pattern

← 1. choose a model and fill information

3. Calculate the parameters for the model

Select a range for each of the parameters to better narrow the value each parameter can take. Or leave the default values that are taken from the model definition.

## Baranyi

### Description

(not defined)

### Options

Does not include death phase  
 =====  
 Estimation is performed on log scale (base e)  
 =====

### Listing 7 parameters

Title	Estimated parameter	Description	Bottom range for estimation	Top range for estimation
h0		dimensionless parameter quantifying the initial physiological state of the population. From that, the lag time lambda can be calculated as h0/mu.	<input type="text" value="-5.0"/>	<input type="text" value="5.0"/>
m		curvature parameter to characterize the transition from the exponential phase	<input type="text" value="0.0"/>	<input type="text" value="5.0"/>
Optimal Cost		fitting cost (not used in the solver and estimator)	(n/a)	(n/a)
v		curvature parameter to characterize the transition to the exponential phase	<input type="text" value="0.0"/>	<input type="text" value="10.0"/>
y0		initial population density	<input type="text" value="-5.0"/>	<input type="text" value="5.0"/>
ymax		asymptotic for the population density	<input type="text" value="0.0"/>	<input type="text" value="10.0"/>
μ max.		maximum specific growth rate	<input type="text" value="0.0"/>	<input type="text" value="3.0"/>

1. fill range for each parameter



RMSE R<sup>2</sup> Bias Accuracy

Calculate parameters

2. Calculate parameters

[Edit this proxy model](#) [Goto experiment](#) [Goto model](#) [.csv](#)

## 4. Results

After successfully calculating the parameters the user is presented with the results: parameters values, statistical measures and a visual plot of the fitting.

If the estimated parameters reaches the internal range, displayed as a highlighted shadow in red, a new range should be tested and a recalculation should be performed.

### Baranyi

Laura S. pneumoniae | ITQB model's description for 18-1-2011 (2) measurement:

(not defined)

**Description**

(not defined)

**Options**

Does not include death phase  
 \*\*\*\*\*  
 Estimation is performed on log scale (base e)  
 \*\*\*\*\*

**Listing 7 parameters**

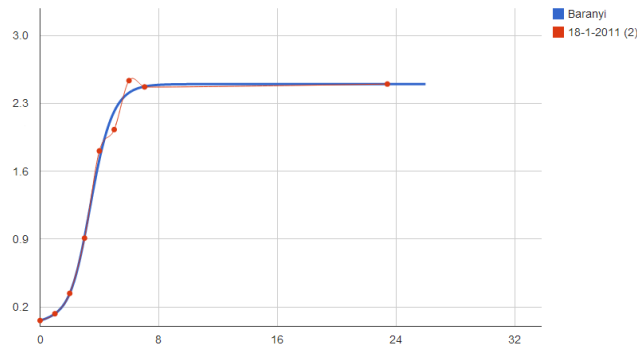
Title ▲	Estimated parameter	Description	Bottom range for estimation	Top range for estimation
h0	3.455956	dimensionless parameter quantifying the initial physiological state of the population. From that, the lag time lambda can be calculated as h0/mu.	-5.0	5.0
m	0.675574	curvature parameter to characterize the transition from the exponential phase	0.0	5.0
Optimal Cost	0.01313001196375	fitting cost (not used in the solver and estimator)	(n/a)	(n/a)
v	1.946531	curvature parameter to characterize the transition to the exponential phase	0.0	10.0
y0	-2.813356	inital population density	-5.0	5.0
ymax	0.0	asymptotic for the population density	0.0	10.0
μ max.	1.812065	maximum specific growth rate	0.0	3.0

RMSE	R <sup>2</sup>	Bias	Accuracy
0.08071	0.99347	1.00011	0.99989

Recalculate parameters

[Edit this proxy model](#)   [Goto measurement](#)   [Goto model](#)   .csv

**Baranyi's Curve**



## 4.8 Multiple Estimation

There are two methods to perform multiple parameter estimation, one using different measurements to estimate parameters and the other to perform the parameter estimation on several measurements in parallel.

1. Aggregation: Perform parameter estimation on several measurements under an experiment;
2. Batch estimation: Performs parallel estimation to multiple measurements.



### 4.8.1 Aggregation

The process to perform parameter estimation using as input all experiment's measurements is identical to the process described above.

The difference lays in the context where the model association is performed. To aggregate the measurement the "Associate model" should be done in the experiment's detail page.

The proxy models will be editable and shown identically as above.

**30 mM Glc (experiment)** **1. select one experiment with several measurements**

Using Laura S. pneumoniae | ITQB scope

**Experiment Description**

Summary growt\_muc\_Laura1 tratado laura  
02/02/2012

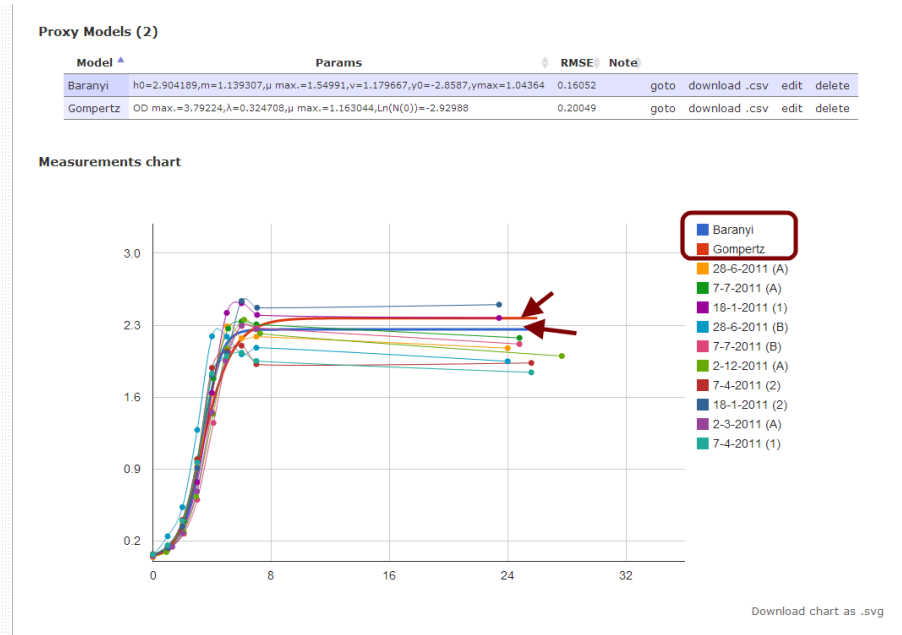
Displaying all 10 measurements

Project	Experiment	Title	Date	
Laura S. pneumoniae   ITQB	30 mM Glc	28-6-2011 (A)	2011-06-28	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	28-6-2011 (B)	2011-06-28	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	7-7-2011 (A)	2011-07-07	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	7-7-2011 (B)	2011-07-07	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	7-4-2011 (1)	2011-04-07	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	7-4-2011 (2)	2011-04-07	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	18-1-2011 (1)	2011-01-18	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	18-1-2011 (2)	2011-01-18	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	2-3-2011 (A)	2011-03-02	goto download .csv
Laura S. pneumoniae   ITQB	30 mM Glc	2-12-2011 (A)	2011-12-02	goto download .csv

**2. associate model**

New measurement Associate model Edit Goto project

Proxy Models (2)



### 4.8.2 Batch estimation

Batch estimation allows to perform multiple estimation in parallel, testing different parameter's range for datasets in different projects / experiments.

This is suited to perform simultaneous parameter estimation to a large dataset (using a fixed parameter range) or to recalculate results using the last known good parameter range.

1. Navigate to a model's detail page
2. Click on "Estimate in batch"

$\mu$	$\mu \text{ max.}$	maximum specific growth rate	0.0	3.0	false	false	<a href="#">edit</a>	<a href="#">delete</a>
$\alpha$	Optimal Cost	fitting cost (not used in the solver and estimator)			true	false	<a href="#">edit</a>	<a href="#">delete</a>
$v$	$v$	curvature parameter to characterize the transition to the exponential phase	0.0	10.0	false	false	<a href="#">edit</a>	<a href="#">delete</a>
$y_0$	$y_0$	initial population density	-5.0	5.0	false	false	<a href="#">edit</a>	<a href="#">delete</a>
$y_{\text{max}}$	$y_{\text{max}}$	asymptotic for the population density	0.0	10.0	false	false	<a href="#">edit</a>	<a href="#">delete</a>

[Estimate in batch](#)
[Statistical data](#)
[Edit](#)
[New parameter](#)
[Generate source](#)
[Models' index](#)
[Back](#)

Home Projects Public projects Models Documentation

avensmo@kibio.inesc-id.pt  
2013 KDEIO | INESC-ID

3. Select the parameter range

Either the last known parameter range used for the parameter estimation (for each measurement), or a fixed range.

### Baranyi

**Description**

Baranyi J., Roberts T.A. and McClure P.J. (1993a). A non-autonomous differential equation to model bacterial growth. Food Microbiol. 10, 43-59.

**Parameters**

What type of parameters should be used for estimation?

Last parameters used with each proxy model

Same parameters for all (defined at the table)

These are the default parameters defined at the model level, and they will override the estimates that are executed.

Title *	Bottom	Top
h0	-5.0	5.0
m	0.0	5.0

**Projects**

**Example**

**Experiment 1**

Title	Rmse		
Replicate 1	0.051051	show below	goto

click on one of the links above to see a chart

**Experiment 2**

Title	Rmse		
Replicate 1	0.000000	show below	goto
Replicate 2	1.303977	show below	goto

click on one of the links above to see a chart

**Experiment 3**

Title	Rmse		
-------	------	--	--

4. Click on “Estimate parameters” to start

As this operation uses a background process to perform all the parameter estimation, a note is added to the proxy model. When the results are calculated the note is removed and the parameter values are shown.

click on one of the links above to see a chart

[Show model details](#) [Statistical data](#) [Back](#) [Estimate parameters](#)

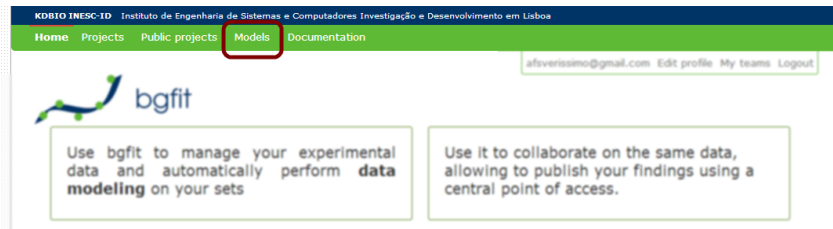
## 4.9 Generate a new Model

There are two existing methods to create a new model to use in the application.

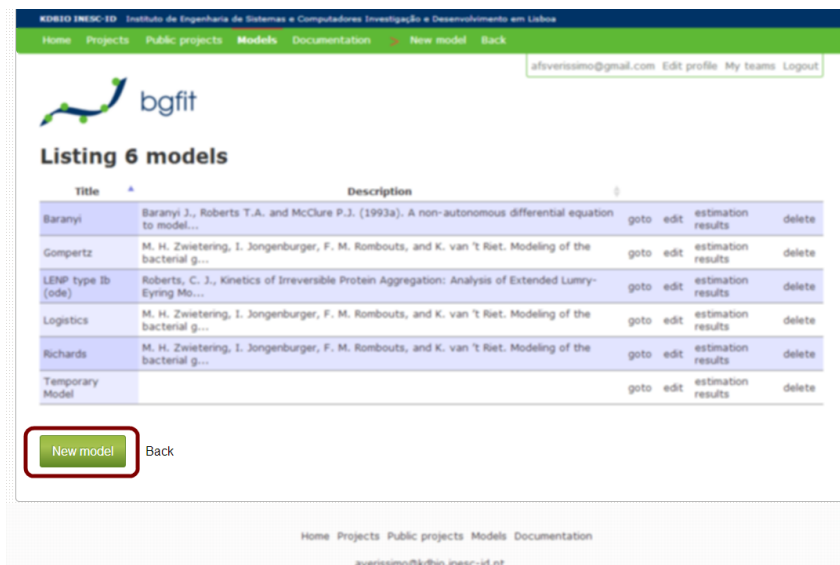
1. The first is described in 5.7;
2. The second can be done through the BGFIt application itself, generating the necessary source files.

### 4.9.1 Create a new Model

1. Navigate to the model index by clicking on the Models menu



2. Click on New model button



3. Introduce the necessary information The user needs to introduce the necessary information to define the model. A model can be defined by:
  - (a) An already published model that has a simulation and estimation interface (i.e. two urls that indicate these interfaces)
  - (b) The equation that defines it.

*note:* for both cases it is necessary to define the parameters (either on the creation page or later in the models page)

Add parameters and the necessary parameters and other options. To add a parameter the user needs to click on + add new parameter and define the parameters detail.

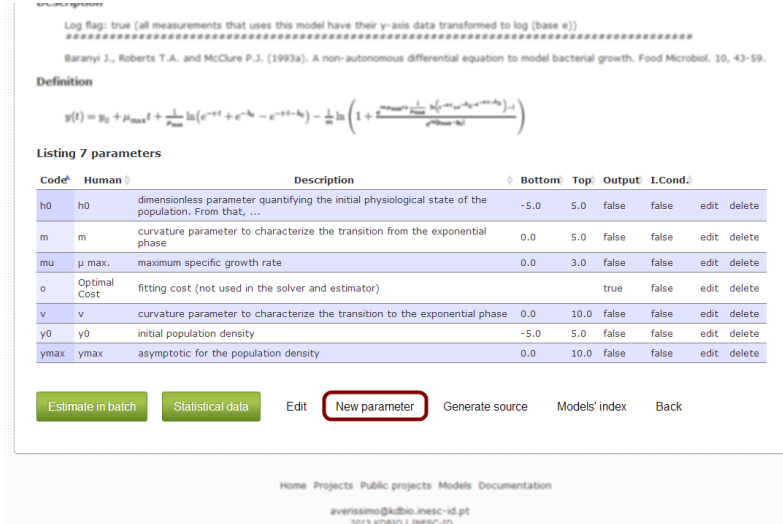
More information on this on section 2.2.

*note:* the code defines the parameter as described in the equation, it should start with an letter and cannot contain spaces or special characters (think of a matlab variable).

### 4.9.2 Add models parameters (if added later on the details page)

Click on the New parameter button and add the models necessary parameters

(a) Click on New parameter



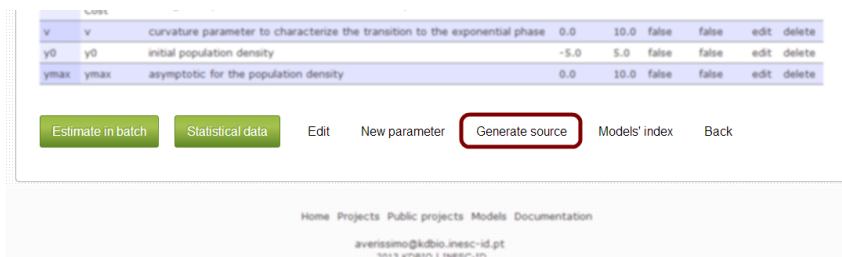
(b) Introduce the necessary information:

- Code: the variable name that will uniquely identify the parameter;
- Human: the human friendly symbol or name for the parameter;
- Output only: If true this parameter will not be passed to the model, but will be determined as a result of a model call;
- Initial condition: If true this will be used as an initial condition for differential models.

### 4.9.3 Generate source files

The equation can be latter defined or corrected.

4. Click on “Generate source” on the model’s detail page



## 5. Select the equation

- Algebraic;
- Differential.

## 6. Describe the equation

Introduce the right hand side of the equation. Such as  $f(t) = a + b^2 \exp(t)$  with parameters  $a$  and  $b$ :

$$a + b * t^2 + \exp(t)$$

example for differential equation that has parameter  $a$  (as initial condition) and  $b$ :

$$2 * b * t + x$$

## 7. Save the model

Click on “Update model”

Parameters

Code	Human	Description	Initial Condition
h0	h <sub>0</sub>		false
mu	μ max.		false

Algebraic  
 Differential

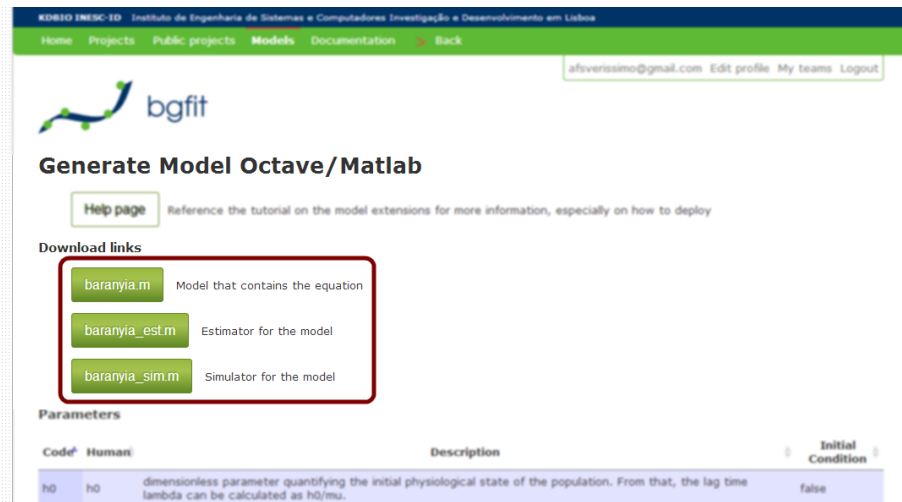
Equation\*

describe the equation using the parameters' code that is listed above as f(t)=x  
 example for parameters a and b: a+bt^2 + exp(t)  
 example for differential equation that has parameter a as initial condition: 2bt + x

Update Model [Back](#)

## 4.9.4 Download source files

The generated files are then accessible as links in the page (model, estimator and simulator functions)



KDRI10 INESC-ID Instituto de Engenharia de Sistemas e Computadores Investigação e Desenvolvimento em Lisboa

Home Projects Public projects **Models** Documentation Back

afiverissimo@gmail.com Edit profile My teams Logout

 **Generate Model Octave/Matlab**

[Help page](#) Reference the tutorial on the model extensions for more information, especially on how to deploy

**Download links**

- [baranyia.m](#) Model that contains the equation
- [baranyia\\_est.m](#) Estimator for the model
- [baranyia\\_sim.m](#) Simulator for the model

**Parameters**

Code	Human	Description	Initial Condition
h0	h0	dimensionless parameter quantifying the initial physiological state of the population. From that, the lag time lambda can be calculated as h0/mu.	false



## 4.10 Manual Regression

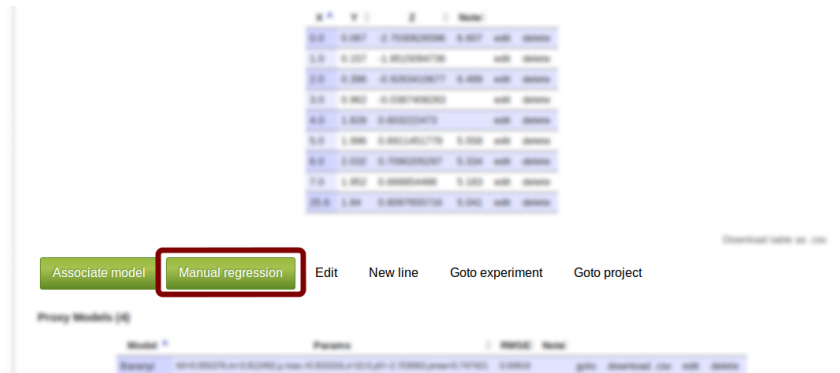
A manual regression allows to calculate a linear regression on the data using a subset of points from the measurement. This calculation is performed on a logarithm scale.

1. Navigate to the Measurement's detail page

To start the user should navigate to the measurement's detail page from an existing project.

2. Click on "Manual regression"

To perform a manual linear regression on measurement data the user should navigate to a measurement's detail page



3. Select points

The user should select two or more points from the data table.

To select points the user should use the mouse and click on the points that will be used in the linear regression.

In order to select multiple points the user should click on two (or more) different entries on the table by either:

- (a) Press the "shift" key to select sequential points;
- (b) Press the "ctrl" key to select specific points.

Laura S. pneumoniae | ITQB model and part of 30 mM Glc experiment

**Data Visualization**

To determine the linear regression for the data you need to select multiple lines in the table below. This can be performed by clicking on multiple lines pressing "Shift" or "Ctrl" keys.

Time	Ln( OD600 )	Regression
0.000	-2.813	
1.000	-2.120	
2.000	-1.238	
3.000	-0.261	
4.000	0.495	
5.000	0.884	
6.000	0.922	
7.050	0.875	
23.420	0.863	

click →

click while pressing shift →

click while pressing ctrl →

$\mu_{max}$  = (select multiple lines in the table)

Save regression

---

Laura S. pneumoniae | ITQB model and part of 30 mM Glc experiment

**Data Visualization**

To determine the linear regression for the data you need to select multiple lines in the table below. This can be performed by clicking on multiple lines pressing "Shift" or "Ctrl" keys.

Time	Ln( OD600 )	Regression
0.000	-2.813	-2.608
1.000	-2.120	-1.944
2.000	-1.238	-1.279
3.000	-0.261	-0.614
4.000	0.495	0.050
5.000	0.884	0.715
6.000	0.922	1.379
7.050	0.875	2.077
23.420	0.863	12.957

$\mu_{max}$  = 0.6646357195115865

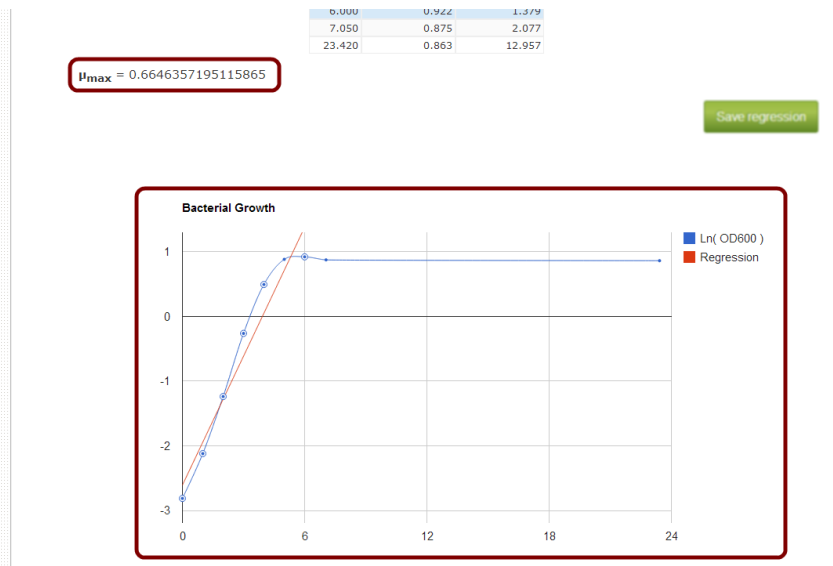
Save regression

#### 4. Live preview

The chart below the table shows a live preview of the linear regression, as well as the max for the regression.

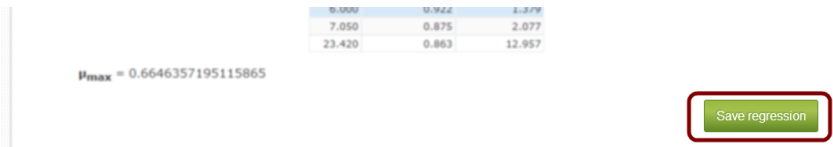
$$y = a + \mu_{max} \cdot x$$

The preview is updated as the selected points change.



5. Save the regression

Click on "Save regression" button



## 5 Modeling Extensions

### 5.1 Overview

This is a Octave/Matlab package that provides methods for non-linear parameter estimation for a REST application. It reads a web query string and returns a JSON file with the results.

### 5.2 Download

Model extensions can be downloaded at [https://github.com/averissimo/model\\_blackbox](https://github.com/averissimo/model_blackbox)

### 5.3 Technical Overview

This package source code is divided in:

- Models in *models* directory that separates
- Algebraic models in *models/algebraic*
- Differential models (ODE) in *models/differential*
- In each sub-directory a different model is defined by 3 different functions: *model* / *estimator* / *simulator*
- Auxiliary functions in the *toolbox* directory that contains:
- Auxiliary functions in the *toolbox/src* directory
- SBTOOLBOX2 models structure that uses *toolbox/estimators*, *toolbox/models*, and *toolbox/simulators* directories
- Compile model script that pre-compiles the SBTOOLBOX2 models as MEX executables

### 5.4 Models

Model Extensions currently implements dynamic models that can implement algebraic or differential (ODE) equations.

The package already has some implemented models that are described in literature:

- **Baranyi** – *Baranyi J., Roberts T.A. and McClure P.J. (1993a). A non-autonomous differential equation to model bacterial growth. Food Microbiol. 10, 43-59;*
- **Gompertz, Logistics, Richards and Schnute** – *M. H. Zwietering, I. Jongenburger, F. M. Rombouts, and K. van t Riet. Modeling of the bacterial growth curve. Applied and Environmental Microbiology, 56(6):1875-1881, June 1990;*

- **LENP type Ib** – *Roberts, C. J., Kinetics of Irreversible Protein Aggregation: Analysis of Extended LumryEyring Models and Implications for Predicting Protein Shelf Life. J. Phys. Chem. B 2003, 107 (5), 1194-1207;*
- **Live Cell Growth** – *Milotti et al, Interplay between distribution of live cells and growth dynamics of solid tumours, Sci Rep., 2, December 2012.*

As an example, the “Baranyi” algebraic model (baranyia) will use the following equation, described as F(t) with auxiliary function F2(t)

$$F2(t) = ( 1 ./ mu ) .* log( exp(-v .* t) + exp(-h0) - exp(-v .* t - h0) );$$

$$F(t) = y0 + mu .* t + F2 - (1 ./ m) * log( 1 + ( exp( m .* mu .* t + F2) - 1 ) ./ exp(m .* (ymax - y0) ) );$$

For a differential model, such as the “LENP type Ib”, a differential equation, such as:

$$dxdt = -2 .* fr_ .* fr_ .* k11_ .* ( n_ / 2 ) .* x .* x;$$

note:  $x = x$  and only the right side of the equation should be included in the definition.

## 5.5 Requirements

This Octave/Matlab package is a blackbox application for parameter estimation and model simulation.

It supports three different backends:

- Octave (optim package)
- Matlab (optimization toolbox)
- Matlab (SBTOOLBOX2 toolbox)

We recommend to use either Octave or Matlab own toolboxes, as the SBTOOLBOX2 might become unstable if the data scale is increased.

The models in the models base directory are compatible with both Octave and Matlab.

### 5.5.1 Requirements for Octave-based models

- Octave environment (tested with 3.6.2)
- Optim package [octave.sourceforge.net/optim](http://octave.sourceforge.net/optim)

### 5.5.2 Requirements for Matlab-based models

- Matlab environment
- Optimization toolbox
- Compiler toolbox

### 5.5.3 Requirements for SBTOOLBOX2-based models

- Matlab environment
- Compiler toolbox
- SBTOOLBOX2 toolbox [sbtoolbox2.org](http://sbtoolbox2.org)
- SBPD toolbox [sbtoolbox2.org](http://sbtoolbox2.org)

## 5.6 Structure

The usage of any model is dependant of having three files:

- model: where the model's equation is defined
- estimator : .m file that defines the necessary steps to estimate parameters
- simulator : .m file that simulates a curve with given parameters

These files allow to generate a cgi script for the model that can be accessed online or in a local computer

## 5.7 Create a new model blackbox

### 5.7.1 Octave / Matlab model

1. Clone the repository;
2. Navigate to the models folder;
3. Navigate to the algebraic or differential folder, depending on the model type. If it is defined as an algebraic equation or as an differential, choose the right folder;
4. Copy the TEMPLATE folder and name it to the model name;
5. Open each of the .m files and change it accordingly;
  - model: write the equation, if it is a differential equation don't forget the initial condition;
  - estimator: change the 'model' variable to the name of the model;
  - simulator: change how the parameters are set in alphabetical order and the 'model' variable.

### 5.7.2 Compile for octave

Navigate to the base dir and run:

```
make octave
```

### 5.7.3 Compile for matlab

Navigate to the base dir add to the Makefile file a target using any of the existing as a template:

```
make %model_name%
```

### 5.7.4 Compile for SBTOOLBOX2 model

1. Create a SBTOOLBOX2 model (SBModel) and copy it the directory:

```
source/models/
```

2. compile the model calling the compile\_model.m function, ex:

```
compile_model('models/baranyi')
```

3. copy the following files to the same directory and name it after the model, preserving the suffix (just to help organizing the files' function

```
source/estimators/TEMPLATE_est.m
```

```
source/simulators/TEMPLATE_sim.m
```

4. change the source code to reflect the name of the model by replacing all the occurrences of Gompertz to "Yourmodel"

**IMPORTANT: the first letter must be Uppercase**

5. in the simulators/Yourmodel\_sim.m you must change the code to handle the model's parameters

6. add the makefile target following the existing templates

7. run

```
make yourmodel_est yourmodel_sim clean
```

## 5.8 Test the model

You can simulate the query by calling in Octave/Matlab the respective function with the arguments: \* simulate flag: if 1 then it will use te test data defined at the top of the function \* draw plot: draws a plot of the results

## 5.9 Deploy

These functions can be deployed as cgi scripts through a REST API and return a JSON response. The parameters can be passed in the url or as POST.

The main requirement is a web server such as Apache or Nginx

### 5.9.1 Octave

To deploy a model using Octave, it is only required to have Octave installed (tested with 3.6.1) and have the toolbox on path.

It is necessary to deactivate octave verbose output. When using a linux server we recommend the use of a shebang script (see the “bin” folder)

```
#!/bin/sh
exec octave --silent --no-window-system $@
```

The package allows to generate all the cgi scripts by running the following command in the root directory:

```
make octave
```

This will create a estimator and a simulator cgi scripts for all models inside the “models” directory.

See Requirements for Octave-based models above

### 5.9.2 Matlab or SBTOOLBOX2

The process to deploy Matlab models (both Matlab or SBTOOLBOX2) is a bit different, as the user needs to compile the model as a standalone application before.

For this the Compiler Toolbox is required to generate executable files. There are already makefile targets for existing models that can be used as templates.

As an example, to deploy the baranyi algebraic models as Matlab cgi scripts, the following command should be issued:

```
make baranyia
```

The makefile will generate a standalone that only needs the Matlab libraries to run.

See Requirements for Matlab-based models above for matlab models, or the Requirements for SBTOOLBOX2-based models for SBTOOLBOX2 models



## 6 Questions and Sugestions

Contact the team at [svinga@kdbio.inesc-id.pt](mailto:svinga@kdbio.inesc-id.pt)