TIMPGUI: A graphical user interface for the package TIMP

Joris J. Snellenburg
Department of Physics and Astronomy, Vrije Universiteit Amsterdam, The Netherlands
jsnel@few.vu.nl

Supported by The Netherlands Organisation for Scientific Research (NWO) grant 635.000.014
**TIMP** is a package for fitting **superposition models** that has been applied to measurements arising in

- time (and/or temperature, polarization, pH)-resolved spectroscopy
- fluorescence lifetime imaging microscopy (FLIM)
- time-resolved mass spectrometry data

This data can often be described as a (ragged) matrix representing possibly multiple experimental conditions.

<table>
<thead>
<tr>
<th>time (ns)</th>
<th>wavelength (nm)</th>
<th>amplitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>349</td>
<td>0.8</td>
</tr>
<tr>
<td>0.4</td>
<td>382</td>
<td>0.6</td>
</tr>
<tr>
<td>0.6</td>
<td>415</td>
<td>0.8</td>
</tr>
<tr>
<td>0.8</td>
<td>448</td>
<td>1.0</td>
</tr>
</tbody>
</table>

![3D graph showing the relationship between time, wavelength, and amplitude]
Parameter estimation problem

from the data

need to solve inverse problem to obtain a (parametric) description of components in time and in wavelength

\[ \Psi = C(\theta)E^T \]
in modeling data arising time-resolved spectroscopy, microscopy and mass spectrometry experiments, often need to

- test many different models
- evaluate the estimated parameters for physical interpretability
- explore the data and fit interactivity

**TIMP** is designed for easy model postulation, optimization and validation . . .

but . . . the interface has some disadvantages that are best explained by example
Example analysis of time-resolved spectroscopy data

Sum square error: 6930989843
Residual standard error: 512.2677 on 26412 degrees of freedom

Parameters: kinpar
dataset 1: 0.0021461974

Parameters: irfpar
dataset 1: 253.58303599

Example analysis of time-resolved spectroscopy data

Concentrations
time

Spectra

Normalized spectra

Residuals Dataset 1

LSV Residuals

RSV Residuals

SV Val Residuals

LSV Data

RSV Data

SingVal Data

350 550 650
wavelength

-0.3 0 0.3
amplitude

5 10 15
wavelength
In order to provide:

- possibilities for model specification via a graphical user interface (GUI)
- cross-platform software, to allow collaboration between Linux/Unix, MS Windows, and Mac OS users
- possibilities for interactive exploration of data and fit

we developed the java-based graphical user interface TIMPGUI

- built on top of the Netbeans platform
- calls TIMP via JRI from RoSuDa
- persistant storage of models and fitting options via XML files

The results are also best explained by example …
LIVE DEMO SCREENSHOT: specification of model
LIVE DEMO SCREENSHOT: specification of fitting options
LIVE DEMO SCREENSHOT: selection of data, model and fitting options
LIVE DEMO SCREENSHOT: interactive validation of results
Conclusions and outlook

- package TIMP fits superposition models to data arising in physics and chemistry
- a java-based GUI has been developed to facilitate interactive model specification, optimization and validation with TIMP
- TIMPGUI is in very active development and will continue to be extended

outlook:

- develop further TIMPGUI options
- publicly release source code
  - source is currently available by request to those willing to participate in testing
Acknowledgments

Katharine M. Mullen, Vrije Universiteit Amsterdam

Sergey Laptenok, Belarusian State University and Wageningen University

Ivo H. M. van Stokkum, Vrije Universiteit Amsterdam