
PyCorrFit Documentation

Release 1.1.1.dev13

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Welcome to the documentation of PyCorrFit (version 1.1.1.dev13), a data analysis software for fluorescence correlation spectroscopy (FCS).

In current biomedical research, fluorescence correlation spectroscopy (FCS) is applied to characterize molecular dynamic processes in vitro and in living cells. Commercial FCS setups only permit data analysis that is limited to a specific instrument by the use of in-house file formats or a finite number of implemented correlation model functions. PyCorrFit is a general-purpose FCS evaluation software that, amongst other formats, supports the established Zeiss ConfoCor3 `~.fcs` file format. PyCorrFit comes with several built-in model functions, covering a wide range of applications in standard confocal FCS. In addition, it contains equations dealing with different excitation geometries like total internal reflection (TIR).

1.1 Supported operating systems

- Windows 7 and higher
- Linux (Debian-based)
- Any other operating system with a Python 3.6 installation (via pip)

1.2 Supported filetypes

- ALV correlators (`~.ASC`)
- Correlator.com (Flex) correlators (`~.SIN`)
- Zeiss ConfoCor3 (`~.fcs`)
- PicoQuant (`~.pt3`) as implemented by Dominic Waithe (https://github.com/dwaithe/FCS_point_correlator)
- PyCorrFit (`~.csv`)
- PyCorrFit session (`~.pcfs`)

1.3 Fitting

- Pre-defined model functions (confocal FCS, TIR-FCS, triplet blinking, multiple components)
- Import of user-defined model functions
- Global fitting across multiple model functions or data sets
- Least squares fit using Levenberg-Marquard, Simplex, and more
- Weighted fitting with standard deviation

1.4 Tools and Features

- Averaging of curves
- Background correction
- Batch processing
- Overlay tool to identify outliers
- Fast simulation of model parameter behavior
- Session management
- High quality plot export using LaTeX (bitmap or vector graphics)

1.5 How to cite

Müller, P., Schwille, P., and Weidemann, T. *PyCorrFit - generic data evaluation for fluorescence correlation spectroscopy*. *Bioinformatics* 30(17):2532-2533 (2014). doi:[10.1093/bioinformatics/btu328](https://doi.org/10.1093/bioinformatics/btu328)

CHAPTER 2

Gallery

TODO:

- Automatically insert all images from the gallery folder.
- Add new screenshots.

3.1 Installation

- Windows installers for PyCorrFit are available at the [release page](#).
- On Debian-based systems, install via `apt-get install pycorffit`.
- If you have Python 3.6 installed, you may install PyCorrFit via `pip install pycorffit[GUI]`. After the installation, type `pycorffit` in a command shell to start PyCorrFit.

3.2 Documentation

The documentation is in the process of being transferred entirely to readthedocs.org. Currently, it is scattered across several places and it is most-likely outdated:

- Original LaTeX-based PDF file (outdated): https://github.com/FCS-analysis/PyCorrFit/wiki/PyCorrFit_doc.pdf
- Wiki pages: <https://github.com/FCS-analysis/PyCorrFit/wiki/>
- A tutorial: <https://github.com/FCS-analysis/PyCorrFit/wiki/Tutorial>
- How to write model functions: <https://github.com/FCS-analysis/PyCorrFit/wiki/Writing-model-functions>

4.1 General remarks

PyCorrFit has no funding and a vanishingly small developer community. My personal objective is to keep PyCorrFit operational on Linux and Windows which is currently limited by the free time I have available.

An active community is very important for an open source project such as PyCorrFit. You can help this community grow (and thus help improve PyCorrFit) in numerous ways:

1. Tell your colleagues and peers about PyCorrFit. One of them might be able to contribute to the project.
2. If you need a new feature in PyCorrFit, publicly announce a bounty for its implementation.
3. If your research heavily relies on FCS, please consider diverting some of your resources to the development of PyCorrFit.
4. You don't have to be a Python programmer to contribute. If you are familiar with reStructuredText or LaTeX, you might be able to help out with the online documentation.
5. Please cite: Müller et al. *Bioinformatics* 30(17): 2532–2533, 2014

If you are planning to contribute to PyCorrFit, please contact me via the PyCorrFit issue page on GitHub such that we may coordinate a pull request.

4.2 For documentation writers

To build this documentation, fork PyCorrFit, navigate to the *docs* (not *doc*) directory and run.

- `pip install -r requirements.txt` followed by
- `sphinx-build . _build`.

This will create the html documentation on your computer. Syntax warnings and errors will be displayed during the build (there should be none). After making your changes to your forked branch, create a pull request on GitHub.

If you only found a typo or wish to make text-only changes, you can also use the GitHub interface to edit the files (without testing the build step on your computer).

4.3 For developers

4.3.1 Running from source

It is recommended to work with [virtual environments](#).

Windows

The easiest way to run PyCorrFit from source on Windows is [Anaconda](#).

- `conda install matplotlib numpy pip scipy wxpython`
- `pip install cython wheel simplejson sympy lmfit`
- `pip install -e . # in the root directory of the repository`

Ubuntu 17.10

PyCorrFit requires wxPython $\geq 4.0.1$ which is not available as a binary wheel on PyPI and thus must be built from the `.tar.gz`. Install all dependencies (<https://github.com/wxWidgets/Phoenix/blob/master/README.rst>):

- `pip install cython matplotlib lmfit numpy scipy sympy`
- `sudo apt-get install -qq libgtk2.0 libgtk2.0-dev libwebkitgtk-dev dpkg-dev build-essential python3.6-dev libjpeg-dev libtiff-dev libsdl1.2-dev libnotify-dev freeglut3 freeglut3-dev libsm-dev libgtk-3-dev libwebkit2gtk-4.0-dev libxtst-dev libgstreamer-plugins-base1.0-dev`
- `pip install wxPython # this will take some time`
- `pip install -e . # in the root directory of the repository`

4.3.2 Testing

PyCorrFit is tested using `pytest`. If you have the time, please write test methods for your code and put them in the `tests` directory. You may run all tests by issuing:

```
python setup.py test
```

4.3.3 Pull request guidelines

Please fork PyCorrFit and create a pull request (PR) introducing your changes.

- A new PR should always be made into the `develop` branch.
- If a PR introduces a new functionality or fixes a bug, it should provide a test case, i.e. a new file or function in the `tests` directory (see [here](#) for examples). Note that currently there is no recipe for testing the graphical user interface code.
- New code should follow the [style guide for Python](#). Please use `flake8` to check the files you changed or created.

- New code should be documented well.
- Make sure to update the [changelog](#).

4.3.4 Windows test binaries

After each commit to the PyCorrFit repository, a binary installer is created by [Appveyor](#). Click on a build and navigate to ARTIFACTS (upper right corner right under the running time of the build). From there you can download the Windows installer for the commit.

List of changes in-between PyCorrFit releases.

5.1 version 1.1.2

- ci: Automated release to PyPI with appveyor and travis-ci
- fix: support lmfit \geq 0.9.11

5.2 version 1.1.1

- Fix plotting error with LaTeX (thanks @toubol) (#179)
- Update documentation

5.3 version 1.1.0

- BREAKING CHANGE: Move to Python3 (thanks @toubol) (#173)
- GUI:
 - Add option in Preferences to automatically close tools after usage
 - Add keyboard shortcuts (thanks @toubol)
- Fix entry point for GUI (#172)
- Refactor several asserts into raises

5.4 version 1.0.1

- Improved support for ALV “.ASC” file format (#169)
- NumPy 0.13 support for “.ptu” file reader
- Code cleanup:
 - Fetch latest available version from GitHub releases
 - New dependency for “simplejson” Python package
 - Move appveyor recipe to separate folder

5.5 version 1.0.0

- New confocal fitting models T+T+2D and T+T+3D
- Fix regression: .sin files could not be opened (#167)

5.6 version 0.9.9

- Remove admin-requirement during install (Windows)
- Support newer correlator.com .sin file format (experimental, #135)
- Add smart progress dialog for fitting (#155)
- Statistics: check “filename/title” by default (#151)
- Documentation: fix bad LaTeX commands (#163)

5.7 version 0.9.8

- Bugfixes:
 - Indexing error when saving sessions (#154)
 - Page number truncated in csv export (#159)
 - Export of csv files used incorrect normalization (#153)
 - Normalization parameter was not displayed in the ‘Info’ tool

5.8 version 0.9.7

- Second triplet time is now larger than first triplet time by default
- Remove a hack that causes a run through all pages e.g. when an average is created
- Bugfixes:
 - Opening sessions with user-defined models
 - Saving sessions with comments containing non-ASCII characters

- Windows build: Graphical plot export was misconfigured (added matplotlibrc patch in .spec file)

5.9 version 0.9.6

- Bugfixes:
 - Fixed minor wx sizer problems for the tools
 - Fixed ‘AttributeError’ in page.py if no weights are present
- New confocal fitting models (#111):
 - 3D+3D, 2D+2D, 3D+2D; no triplet
 - T+T+2D+2D, T+T+3D+2D; double triplet
 - T+3D+3D+3D, T+3D+3D+2D (#40, #59)
- Under the hood:
 - Separation of core and GUI modules
 - Include tests in distributions for PyPI
 - Improve automated testing on Windows and Mac OS
 - More constraint options for fitting

5.10 version 0.9.5

- Bugfixes
 - Closing the batch control window causes segfault bug (#142)
 - Closing page causes error when batch control is active (#143)
 - Plot normalization causes “Save Session” to fail (#144)
 - Plot normalization not loaded from session (#145)

5.11 version 0.9.4

- Batch control allows to select individual parameters (#108)
- Allow to exclude pages from batch fitting (#107)
- Bugfixes:
 - Fix ‘ValueError’ in parameter display
 - Possibly fixed error with ‘yaml.safe_dump’ on Mac OSx 10.8.5
 - Make sure background is lower than signal (#137)

5.12 version 0.9.3

- Fitting: migrate to lmfit
 - This introduces a new dependency for building PyCorrFit. (e.g. in Debian, the package “python-lmfit” is required)
 - Improved fitting behavior at parameter boundaries
 - Removed “Polak-Ribiere” fitting algorithm
 - Added “Sequential Linear Squares Programming” algorithm
- Heuristic fit (#109):
 - Detect parameters that are stuck during fitting
 - Fit each curve five times or less and check whether the fit converges.
 - If two diffusion time parameter exist in a model, always make sure that one parameter is the larger one. This feature can currently not be disabled (#110).
- Allow infinity (“inf” and “-inf”) parameters for models and boundaries.
- New model: confocal T+T+3D+3D
- Bugfixes:
 - Sessions saved with 64bit Windows were not opened (#136)
 - Old sessions and “KeyError: ‘chi2’”
 - Old session file extension was not recognized (#106)

5.13 version 0.9.2

- Bugfixes:
 - “Slider Simulation”/”Parm Range” broken (#133)
 - Computation of average intensity did not work correctly for unequally spaced traces
- Update .pt3 reader to version 8399ff7401
- Import traces of .pt3 files (experimental, #118) Warning: Absolute values for intensity might be wrong

5.14 version 0.9.1

- Tool ‘Overlay curves’: improve UI (#117)
- Tool ‘Statistics view’: improve UI (#113)
- Tool ‘Trace view’: display countrate (#121)
- Bugfixes:
 - Unicode errors in statistics tool (#131)
 - Load session errors with empty pages

5.15 version 0.9.0

- Improve parameter display (#52, #114)
- Display Chi2 on each page (#115)
- The displayed Chi2-value for non-weighted fits is now normalized to the expected values of the fit. The documentation has been updated accordingly.
- Add “All files” option in save dialogs (#97)
- Improved plot export dialog (#99)

5.16 version 0.8.9

- Improved support for “ALV-7004” files (#104)
- Increase resolution for image export
- Load weights from PyCorrFit csv files
- Tool ‘Overlay Curves’: show cropped correlation curves
- Tool ‘Trace view’: increase size of window (#93)
- Tool ‘Global fitting’: remove forced, joint weights
- Session comment dialog: more intuitive behavior (#116)
- Improve plot export (#95)
- Bugfixes:
 - Weighted fits at borders of fit interval were computed incorrectly due to integer division
 - Fitting algorithms did not work (#94)
 - Creating averages did not work (#123)
 - ASCII errors in statistics tool (#112)
- Under the hood:
 - Introduce new classes: Correlation, Fit, Trace
 - Code cleanup and rewrite to support planned features
 - In some cases support older versions of NumPy

5.17 version 0.8.8

- Improved support for “ALV-7004” files
- If you install the GUI with pip, you now need to include the ‘GUI’ requirement: ‘pip install pycorffit[GUI]’. The GUI depends on matplotlib and wxPython which is not required for scripting with the pycorffit module.
- Bugfix: missing version string on SuSe linux (#101)
- Under the hood:
 - Python entry point script replaces “bin/” script

- Windows build system hosted by appveyor.com
- MacOS X build system hosted by travis-ci.org
- New builds use wxPython3 (#85)
- Unicode support without ‘reload(sys)’
- Error messages are more verbose

5.18 version 0.8.7

- Removed unused fitting parameter `d_eva` from model 6022 and secured backwards compatibility.
- Improved support for ALV700X (#92)
- Bugfix: Corrected false display of Unicode characters on Windows
- Under the hood:
 - Code cleanup with pyflakes
 - Repo cleanup (#98)

5.19 version 0.8.6

- Bugfix: Opening .fcs files with only one AC curve works now
- Zip files with measurements may now contain subfolders
- Improved pt3-file support from https://github.com/dwaithe/FCS_point_correlator (#89)

5.20 version 0.8.5

- Fixed bug that made it impossible to load data (#88)
- Exceptions are now handled by wxPython
- Under the hood:
 - Pythonic repository structure
 - Relative imports
 - Windows build machine is now Windows 7
 - Removed strict dependency on matplotlib

5.21 version 0.8.4

- Support for PicoQuant data file format Many thanks to Dominic Waithe (@dwaithe)
- Improved compatibility with Zeiss .fcs file format
- PyCorrFit is now dependent on Cython
- The module ‘openfile’ is now available from within Python

- Installer for Windows

5.22 version 0.8.3

- New .pcfs (PyCorrFit Session) file format (#60)
- Additional fitting algorithms: Nelder-Mead, BFGS, Powell, Polak-Ribiere (#71)
- Improvements
 - Massive speed-up when working with large data sets (#77)
 - Plot export: legend position and displayed parameters (#54)
 - Average tool: traces may now start at time points != 0
 - Statistics tool: display on smaller screens
 - ALV data files: updated parser to identify curve types and segment traces
 - Zeiss ConfoCor3 data files: some files could not be opened due to dummy AC curves
 - Models: default parameters were changed to prevent unstable fits
 - Software: notification dialogs for missing modules or other software
- Bugfixes
 - User could accidentally clear a session (#65)
 - wxPython plotting problem on MacOSx (#64)
 - Statistics view: some parameters were duplicated (#76)
 - Caught zero-division warnings (models with triplet component)
 - Corrected x-axis scaling of statistics view and trace view

5.23 version 0.8.2

- The documentation has been thoroughly reworked
- The user is now warned if he does not have a TeX distribution installed
- Improvements:
 - Complete support for installing PyCorrFit with virtualenv and pip (This is documented in the wiki)
 - Statistics tool now displays average and SD (#43)
- Bugfix: TeX did not work on Ubuntu due to missing imports

5.24 version 0.8.1

- Thanks to Alex Mestiashvili for providing initial setup.py files and for debianizing PyCorrFit (@mestia)
- Thanks to Thomas Weidemann for his contributions to the documentation (@weidemann)
- Bugfixes
 - Some ConfoCor files were not imported

- The cpp was not calculated correctly in case of background correction (#45)
- Enabled averaging of single pages (#58)
- Background correction for cross-correlation data is now computed (#46)
- Improvements of the user interface
 - The menus have been reordered (#47, #50)
 - The fitting panel has been optimized (#49)
 - the slider simulation got a reset button (#51)
 - The Help menu contains documentation and wiki (#56)
 - Model functions that are somehow redundant have been removed from the menu, but are still supported
 - The model doc strings were fully converted to Unicode
 - Several text messages were modified for better coherence
 - The background correction tool is more intuitive
 - Statistics panel improvements (#43)
 - Run information is included in the Data set title
 - The page counter starts at “1” instead of “0” (#44)
 - New handling of background correction (#46, #53)

5.25 version 0.8.0

- Filename/title of each tab now shows up in the notebook (#39)
- Statistics tool can plot parameters and page selection with the Overlay tool is possible (#31)

5.26 version 0.7.9

- Support for Mac OSX
- Enhancements:
 - Export file format (.csv) layout improved
 - Model function info text in UTF-8
 - Improved warning message when opening sessions from future versions
 - New feature lets user set the range for the fitting parameters
- Bugfixes:
 - Cleaned minor tracebacks and exceptions created by the frontend
 - Mac version now works as expected, but .app bundling failed
 - Latex plotting features now support more characters such as “[{}]^”

5.27 version 0.7.8

- Enhancements:
 - Averages can now be calculated from user-selected pages
 - Pages selected in the Overlay tool are now automatically set for computation of average and for global fitting
 - Source pages are now displayed in average title
 - Graph normalization with particle numbers is now possible
- Bugfixes:
 - Errors during fitting with weights equal to zero
 - Overlay tool displayed last curve after all pages have been removed
 - Global fit did not work with weights
- Session saving now uses 20 digits accuracy
- CSV export is now using tab-delimited data for easier Excel-import
- Added version checking for session management

5.28 version 0.7.7

- Fixed: Tools windows could not be closed (or moved on MS Windows)
- Fixed: .csv export failed in some cases where no weights were used
- Enhancement: The user is now asked before a page is closed
- Enhancement: Tool “Page Info” and in exported .csv files, variables and values are now separated by a tab stop instead of a “=”
- Fixed: Opening a session with an empty page failed in some cases
- Fixed: Tool “Statistics” missed to output the column “filename/title” if that key value is empty - replaced empty strings with “NoName”
- Enhancement: Tool “Overlay” now asks the user to check kept curves instead of showing the curves to be removed
- Enhancement: Tool “Overlay” now has a “Cancel” button

5.29 version 0.7.6

- Improved handling
 - Tools are now sorted according to a standard work-flow
 - Renamed “Curve selection” to “Overlay tool” - this is more intuitive
 - Tools will now stay open or may be opened when there are no open pages (#25)
 - Filenames and runs are now displayed on each page (also added filename/title tag) (#23)
 - Notebook: moved close button to each tab to prevent accidental closing of tabs

- Improved tool “Statistics” (#21)
 - Fixed the case where “useless” data was produced - instead we write “NaN” data, removed warning message accordingly
 - Row-wise ordering according to page numbers (#22)
 - Column-wise ordering is now more intuitive (Fitted parameters with errors first)
 - Some columns are now checked by default
 - PyCorrFit remembers checked parameters for a page (not saved in session)
- Improved tool “Overlay” (#23)
 - New feature: Overlay shows run number of each file (upon import), the run (or index) of an experimental file is unique to PyCorrFit
 - Upon import, filenames and runs are displayed
 - In a session, the filename/title is displayed
- Web address of PyCorrFit changed from “fcstools.dyndns.org/pycorrfit” to “pycorrfit.craban.de”
- Minor bugfixes: Batch control, Global fitting, import dialog

5.30 version 0.7.5

- Added model functions to documentation.
- Weights from fitting are now exported in .csv files.
- Rework of info panel for fitting
- Cleared unintuitive behavior of session saving: The fitting parameters were read from the frontend. This could have led to saving false fit meta data.
- During fitting, units are now displayed as “human readable” (#17).
- Slider simulation now also uses human readable units (#17).
- Secured support for Ubuntu 12.10 and 13.04
- Fixed: new line (n) characters for LaTeX plotting on Windows

5.31 version 0.7.4

- New tool: Colorful curve selection
- Import data: Curve selection possible
- Average: Crop average according to current page.
- Fixed: Page now displays Chi-squared of global fit.
- Fixed: Chi-squared and parameters of global fitting are now stored in sessions.

5.32 version 0.7.3

- Issue closed. External weights from averages saved in session (#11).
- Solved minor bugs
- Added estimation of errors of fit (Issue #12/#14)
- Fixed: Some .fcs files containing averages were not imported.

5.33 version 0.7.2

- Bugfix: Issue #10; we now have a goodness of the fit, if weighted fitting is performed
- Bugfix: Weights for fitting not properly calculated ($\sqrt{\text{std}}$).
- Bugfix: Batch control IndexError with Info window opened
- Tool Statistics: Sort values according to page numbers
- Tool global: Added weighted fitting
- Residuals: According to weighted fitting, weighted residuals are plotted
- Average: Variances from averaging can be used for weighted fitting

5.34 version 0.7.1

- Feature: Added Python shell
- Bugfix: Saving image was not performed using WXAgg
- Bugfix: Notebook pages were drag'n'dropable
- Update function now works in its own thread
- Code cleanup: documentation of model functions
- Added program icon

5.35 version 0.7.0

- File import dialog was enhanced (#4, #5 - subsequently #7, #8):
 - Now there is only one “load data” dialog in the file menu
 - The model function is chosen for each type of data that is to be imported (AC, CC, etc.)
- Bugfix: Channel selection window causes crash on file import (#1).
- Bugfix: Hidden feature changes fixed parameters during fitting (#2).
- Feature: Convert TIR model function parameters λ and NA to σ (#3).
- Code cleanup: Opening data files is now handled internally differently.

5.36 version 0.6.9

- Initial GitHub commit

CHAPTER 6

Indices and tables

- `genindex`
- `modindex`
- `search`