Pycorrelate Documentation

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Contents

Pycorrelate computes fast and accurate cross-correlation over arbitrary time lags. Cross-correlations can be calculated on "uniformly-sampled" signals or on "point-processes", such as photon timestamps. Pycorrelate allows computing cross-correlation at log-spaced lags covering several orders of magnitude. This type of cross-correlation is commonly used in physics or biophysics for techniques such as *fluorescence correlation spectroscopy* (FCS) or *dynamic light scattering* (DLS).

Two types of correlations are implemented:

- ucorrelate: the classical text-book linear cross-correlation between two signals defined at **uniformly spaced** intervals. Only positive lags are computed and a max lag can be specified. Thanks to the limit in the computed lags, this function can be much faster than numpy.correlate.
- pcorrelate: cross-correlation of discrete events in a point-process. In this case input arrays can be timestamps or positions of "events", for example **photon arrival times**. This function implements the algorithm in Laurence et al. Optics Letters (2006). This is a generalization of the multi-tau algorithm which retains high execution speed while allowing arbitrary time-lag bins.

Pycorrelate is implemented in Python 3 and operates on standard numpy arrays. Execution speed is optimized using numba.

- Free software: GNU General Public License v3
- Documentation: https://pycorrelate.readthedocs.io.

CHAPTER 1

Documentation

1.1 Installation

1.1.1 Stable release

To install Pycorrelate, run this command in your terminal:

```
$ pip install pycorrelate
```

This is the preferred method to install Pycorrelate, as it will always install the most recent stable release.

If you don't have pip installed, this Python installation guide can guide you through the process.

1.1.2 From sources

The sources for Pycorrelate can be downloaded from the Github repo.

You can either clone the public repository:

```
$ git clone git://github.com/tritemio/pycorrelate
```

Or download the tarball:

```
$ curl  -OL https://github.com/tritemio/pycorrelate/tarball/master
```

Once you have a copy of the source, you can install it with:

```
$ python setup.py install
```

1.2 Usage

Imports:

```
import numpy as np
import pycorrelate as pyc
```

Create two arrays *t* and *u* of discrete events, exponentially correlated:

```
np.random.seed(1)
size = 10**4
t = np.sort(np.random.randint(0, 10**5, size=size))
u = np.sort(t + np.random.exponential(scale=10, size=t.size).astype(np.int64))
```

Compute correlation:

```
lags = np.arange(0, 201)
G = pyc.pcorrelate(t, u, lags)
```

G contains the cross-correlation of *t* and *u* at the defined *lags*.

For more examples see *Pycorrelate examples*.

1.3 API Reference

Quick links:

- `pcorrelate()`
- `pnormalize()`
- `make_loglags()`
- `ucorrelate()`

1.3.1 List of Pycorrelate functions

Functions to compute linear correlation on discrete signals (uniformly sampled in time) **or** on point-processes (e.g. timestamps of events).

`pycorrelate.pycorrelate.`**`make_loglags`**(*exp_min*, *exp_max*, *points_per_base*, *base=10*)

Make a log-spaced array useful as lag bins for cross-correlation.

This function conveniently creates an arrays on lag-bins to be used with `pcorrelate()`.

Parameters

- **exp_min** (*int*) – exponent of the minimum value
- **exp_max** (*int*) – exponent of the maximum value
- **points_per_base** (*int*) – number of points per base (i.e. in a decade when *base = 10*)
- **base** (*int*) – base of the exponent. Default 10.

Returns Array of log-spaced values with specified range and spacing.

Example

Compute log10-spaced bins with 2 bins per decade, starting from 10^1 and stopping at 10^3:

```
>>> make_loglags(-1, 3, 2)
array([  1.00000000e-01,   3.16227766e-01,   1.00000000e+00,
         3.16227766e+00,   1.00000000e+01,   3.16227766e+01,
         1.00000000e+02,   3.16227766e+02,   1.00000000e+03])
```

See also:

pcorrelate()

`pycorrelate.pycorrelate.`**`pcorrelate`**

Compute correlation of two arrays of discrete events (Point-process).

The input arrays need to be values of a point process, such as photon arrival times or positions. The correlation is efficiently computed on an arbitrary array of lag-bins. As an example, bins can be uniformly spaced in log-space and span several orders of magnitudes. (you can use *make_loglags()* to creat log-spaced bins). This function implements the algorithm described in (Laurence 2006).

Parameters

- **t** (*array*) – first array of "points" to correlate. The array needs to be monothonically increasing.
- **u** (*array*) – second array of "points" to correlate. The array needs to be monothonically increasing.
- **bins** (*array*) – bin edges for lags where correlation is computed.
- **normalize** (*bool*) – if True, normalize the correlation function as typically done in FCS using *pnormalize()*. If False, return the unnormalized correlation function.

Returns Array containing the correlation of *t* and *u*. The size is *len(bins) - 1*.

See also:

make_loglags() to genetate log-spaced lag bins.

`pycorrelate.pycorrelate.`**`pnormalize`**

Normalize point-process cross-correlation function.

This normalization is usually employed for fluorescence correlation spectroscopy (FCS) analysis. The normalization is performed according to (Laurence 2006). Basically, the input argument *G* is multiplied by:

$$\frac{T-\tau}{n(\{i \ni t_i \le T-\tau\})n(\{j \ni u_j \ge \tau\})}$$

where *n({})* is the operator counting the elements in a set, *t* and *u* are the input arrays of the correlation, τ is the time lag and *T* is the measurement duration.

Parameters

- **G** (*array*) – raw cross-correlation to be normalized.
- **t** (*array*) – first input array of "points" used to compute *G*.
- **u** (*array*) – second input array of "points" used to compute *G*.
- **bins** (*array*) – array of bins used to compute *G*. Needs to have the same units as input arguments *t* and *u*.

Returns Array of normalized values for the cross-correlation function, same size as the input argument *G*.

`pycorrelate.pycorrelate.`**`ucorrelate`**

Compute correlation of two signals defined at uniformly-spaced points.

The correlation is defined only for positive lags (including zero). The input arrays represent signals defined at uniformily-spaced points. This function is equivalent to `numpy.correlate()`, but can efficiently compute correlations on a limited number of lags.

Note that binning point-processes with uniform bins, provides signals that can be passed as argument to this function.

Parameters

- **tx** (*array*) – first signal to be correlated
- **ux** (*array*) – second signal to be correlated
- **maxlag** (*int*) – number of lags where correlation is computed. If None, computes all the lags where signals overlap *min(tx.size, tu.size) - 1*.

Returns Array contained the correlation at different lags. The size of this array is equal to the input argument *maxlag* (if defined) or to *min(tx.size, tu.size) - 1*.

Example

Correlation of two signals *t* and *u*:

```
>>> t = np.array([1, 2, 0, 0])
>>> u = np.array([0, 1, 1])
>>> pycorrelate.ucorrelate(t, u)
array([2, 3, 0])
```

The same result can be obtained with numpy swapping *t* and *u* and restricting the results only to positive lags:

```
>>> np.correlate(u, t, mode='full')[t.size - 1:]
array([2, 3, 0])
```

1.4 Pycorrelate examples

This notebook shows howto use `pycorrelate` as well as comparisons with other implementations.

```
In [1]: import numpy as np
        import h5py
```

```
In [2]: # Tweak here matplotlib style
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        mpl.rcParams['font.sans-serif'].insert(0, 'Arial')
        mpl.rcParams['font.size'] = 14
        %config InlineBackend.figure_format = 'retina'
        %matplotlib inline
```

```
In [3]: import pycorrelate as pyc
```

1.4.1 Load Data

We start by downloading some timestamps data:

```
In [4]: url = 'http://files.figshare.com/2182601/0023uLRpitc_NTP_20dT_0.5GndCl.hdf5'
        pyc.utils.download_file(url, save_dir='data')
```

```
URL:  http://files.figshare.com/2182601/0023uLRpitc_NTP_20dT_0.5GndCl.hdf5
File: 0023uLRpitc_NTP_20dT_0.5GndCl.hdf5

File already on disk: data/0023uLRpitc_NTP_20dT_0.5GndCl.hdf5
Delete it to re-download.
```

```
In [5]: fname = './data/' + url.split('/')[-1]
        h5 = h5py.File(fname)
        unit = 12.5e-9
```

```
In [6]: num_ph = int(3e6)
        detectors = h5['photon_data']['detectors'][:num_ph]
        timestamps = h5['photon_data']['timestamps'][:num_ph]
        t = timestamps[detectors == 0]
        u = timestamps[detectors == 1]
```

```
In [7]: t.shape, u.shape, t[0], u[0]
```

```
Out[7]: ((839592,), (1844370,), 146847, 188045)
```

```
In [8]: t.max()*unit, u.max()*unit
```

```
Out[8]: (599.99944191249995, 599.99847228750002)
```

Timestamps need to be monotonic, let's test it:

```
In [9]: assert (np.diff(t) > 0).all()
        assert (np.diff(u) > 0).all()
```

1.4.2 Log-scale bins (base 10)

Here we compute the cross-correlation on log10-spaced bins.

First we compute the array of lag bins using the function make_loglags:

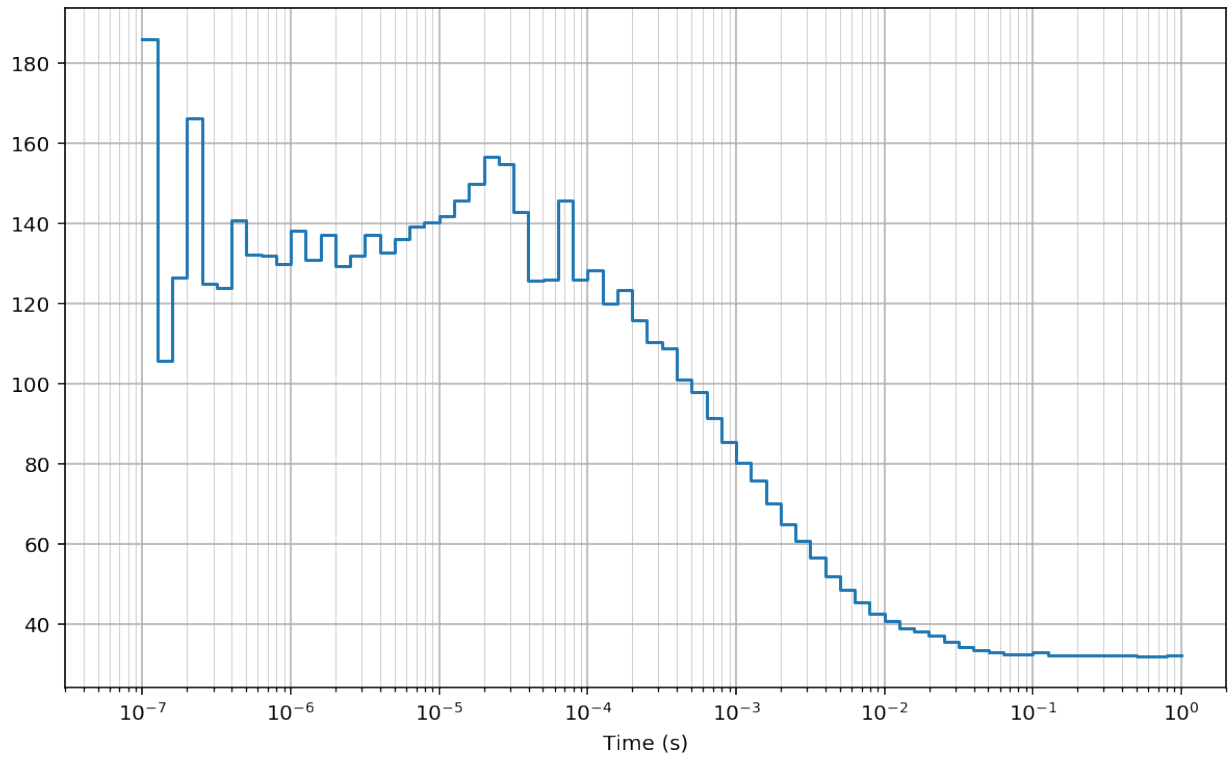
```
In [10]: # compute lags in sec. then convert to timestamp units
         bins = pyc.make_loglags(-7, 0, 10) / unit
```

Then, we compute the cross-correlation using the function pcorrelate:

```
In [11]: G = pyc.pcorrelate(t, u, bins)
```

```
In [12]: fig, ax = plt.subplots(figsize=(10, 6))
         plt.plot(bins*unit, np.hstack((G[:1], G)), drawstyle='steps-pre')
         plt.xlabel('Time (s)')
         #for x in bins[1:]: plt.axvline(x*unit, lw=0.2)  # to mark bins
         plt.grid(True); plt.grid(True, which='minor', lw=0.3)
         plt.xscale('log')
         plt.xlim(30e-9, 2)
```

```
Out[12]: (3e-08, 2)
```



1.4.3 Log-scale bins (base 2)

Here we compute the same cross-correlation on log2-spaced bins.

First we compute the array of lag bins using the function make_loglags:

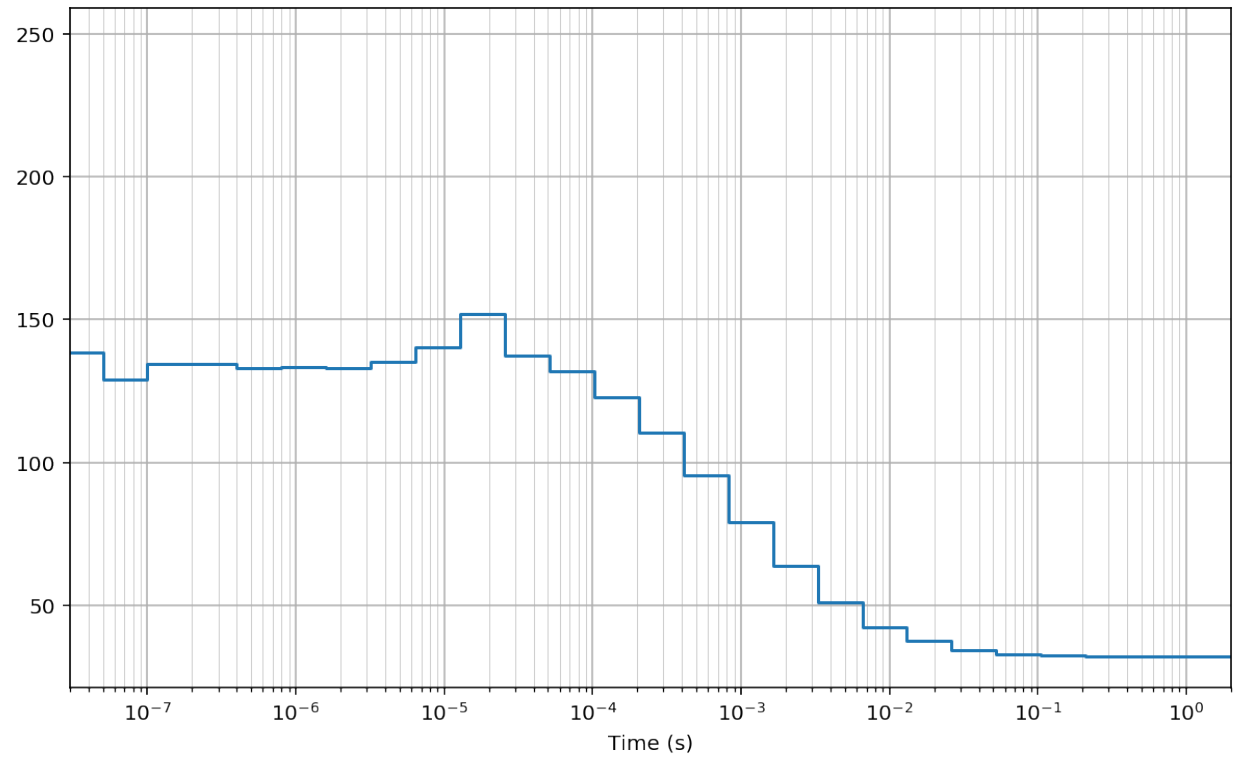
```
In [13]: # compute lags directly in timestamp units
         bins = pyc.make_loglags(-1, 28, 1, base=2).astype('int')
```

Then, we compute the cross-correlation using the function pcorrelate:

```
In [14]: G = pyc.pcorrelate(t, u, bins)
```

```
In [15]: fig, ax = plt.subplots(figsize=(10, 6))
         plt.plot(bins*unit, np.hstack((G[:1], G)), drawstyle='steps-pre')
         plt.xlabel('Time (s)')
         #for x in bins[1:]: plt.axvline(x*unit, lw=0.2)  # to mark bins
         plt.grid(True); plt.grid(True, which='minor', lw=0.3)
         plt.xscale('log')
         plt.xlim(30e-9, 2)
```

```
Out[15]: (3e-08, 2)
```



1.4.4 Multi-tau bins

Finally, we compute the cross-correlation on arbitrarly-spaced bins. Similar to the multi-tau bins, here we use constant bin size for a number of bins (`n_group`), then we double the bin size and we keep it constant for another `n_group` and so on:

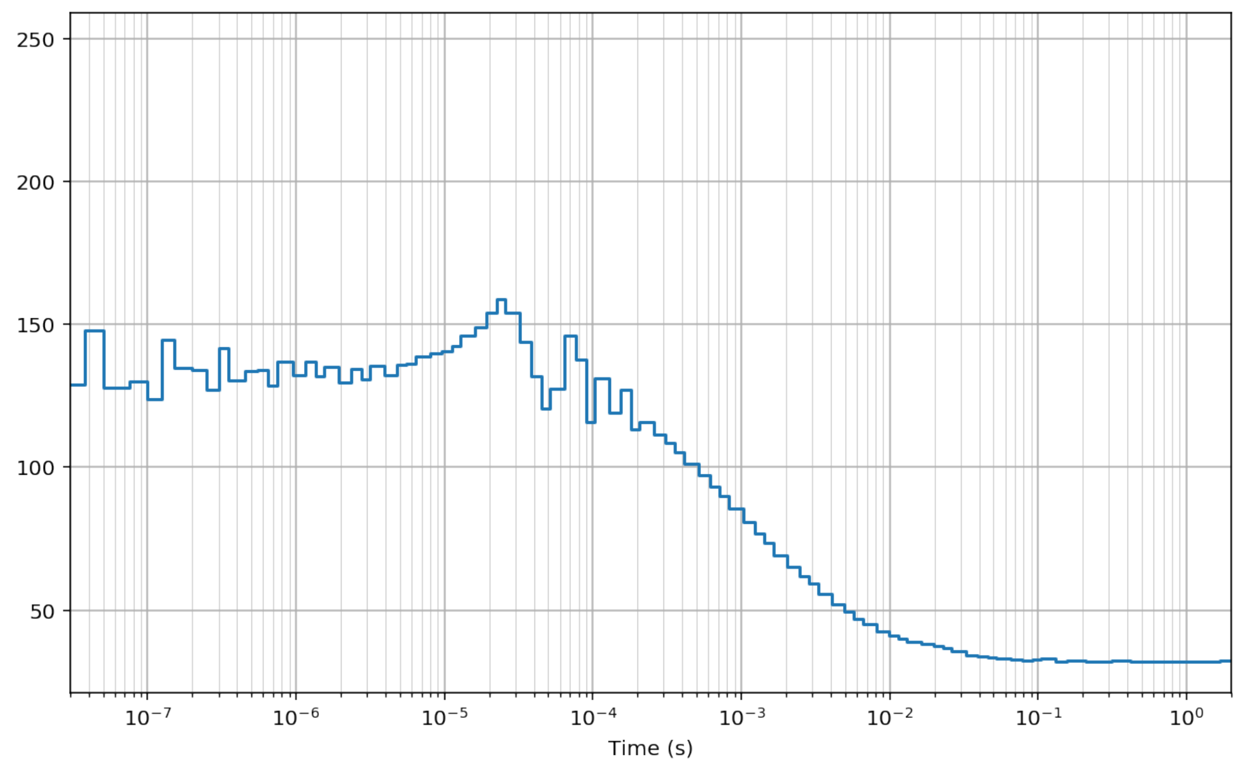
```
In [16]: n_group = 4
         bin_widths = []
         for i in range(26):
             bin_widths += [2**i]*n_group
         np.array(bin_widths)
         bins = np.hstack(([0], np.cumsum(bin_widths)))
```

Then, we compute the cross-correlation using the function pcorrelate:

```
In [17]: G = pyc.pcorrelate(t, u, bins)
```

```
In [18]: fig, ax = plt.subplots(figsize=(10, 6))
         plt.plot(bins*unit, np.hstack((G[:1], G)), drawstyle='steps-pre')
         plt.xlabel('Time (s)')
         #for x in bins[1:]: plt.axvline(x*unit, lw=0.2)  # to mark bins
         plt.grid(True); plt.grid(True, which='minor', lw=0.3)
         plt.xscale('log')
         plt.xlim(30e-9, 2)
```

```
Out[18]: (3e-08, 2)
```



1.4.5 Test: comparison with np.histogram

For testing alternative (slower) implementations we use smaller input arrays:

```
In [19]: tt = t[:5000]
         uu = u[:5000]
```

The algoritm implemented in `pycorrelate.pcorrelate` can be re-written in a very simple way using `numpy.histogram`:

```
In [20]: # compute lags in sec. then convert to timestamp units
         bins = pyc.make_loglags(-7, 0, 10) / unit
```

```
In [21]: Y = np.zeros(bins.size - 1, dtype=np.int64)
         for ti in tt:
             Yc, _ = np.histogram(uu - ti, bins=bins)
             Y += Yc
         G = Y / np.diff(bins)
```

```
In [22]: assert (G == pyc.pcorrelate(tt, uu, bins)).all()
```

Test passed! Here we demonstrated that the logic of the algorithm is implemented as described in the paper (and in the few lines of code above).

1.4.6 Tests: comparison with np.correlate

The comparison with `np.correlate` is a little tricky. First we need to bin our input to create timetraces that can be correlated by linear convolution. For testing purposes, let's choice some timetrace bins:

```
In [23]: binwidth = 50e-6
         bins_tt = np.arange(0, tt.max()*unit, binwidth) / unit
         bins_uu = np.arange(0, uu.max()*unit, binwidth) / unit
```

```
In [24]: bins_tt.max()*unit, bins_tt.size
```

```
Out[24]: (4.137249999999999, 82746)
```

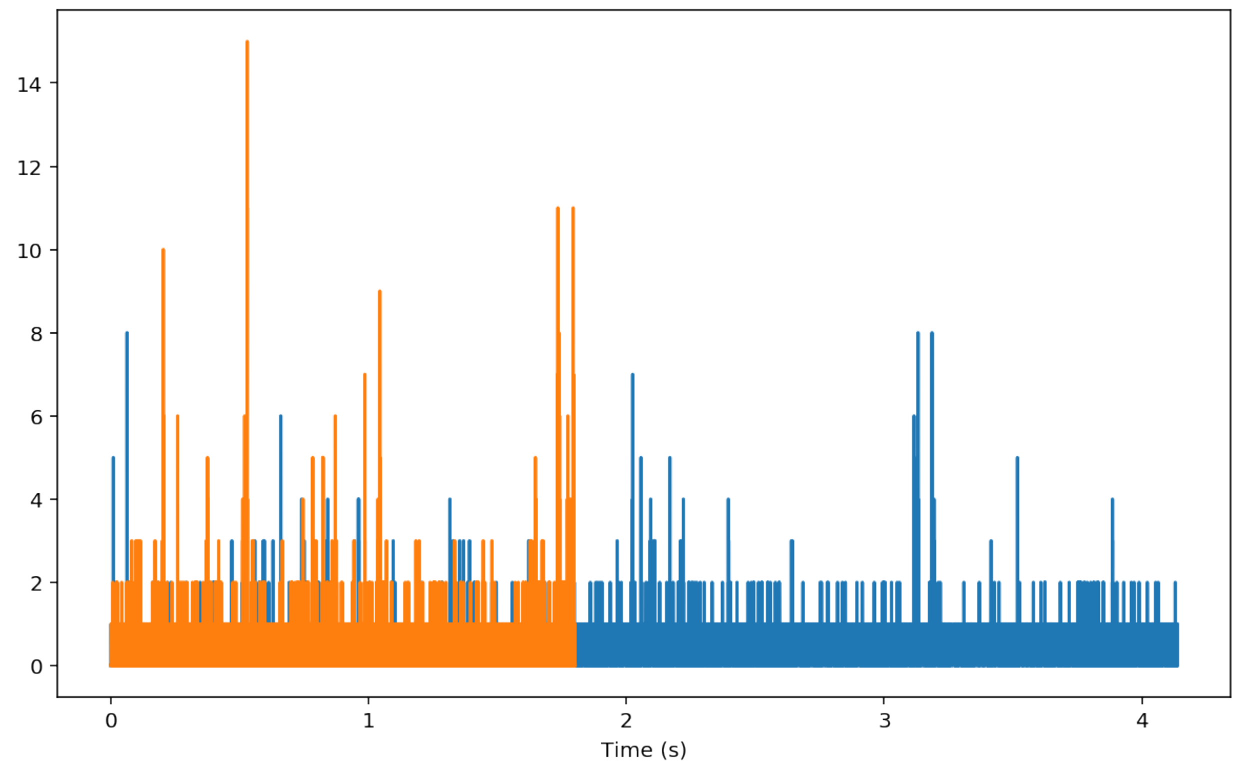
```
In [25]: bins_uu.max()*unit, bins_uu.size
```

```
Out[25]: (1.8020999999999998, 36043)
```

```
In [26]: tx, _ = np.histogram(tt, bins=bins_tt)
         ux, _ = np.histogram(uu, bins=bins_uu)

         plt.figure(figsize=(10, 6))
         plt.plot(bins_tt[1:]*unit, tx)
         plt.plot(bins_uu[1:]*unit, ux)
         plt.xlabel('Time (s)')
```

```
Out[26]: Text(0.5,0,'Time (s)')
```



The plots above are the two curves we are going to feed to `np.correlate`:

```
In [27]: C = np.correlate(ux, tx, mode='full')
```

We need to trim the result to obtain a proper alignment with the 0-time lag:

```
In [28]: Gn = C[tx.size-1:]  # trim to positive time lags
```

Now, we can check that both `numpy.correlate` and `pycorrelate.ucorrelate` give the same result:

```
In [29]: Gu = pyc.ucorrelate(tx, ux)
         assert (Gu == Gn).all()
```

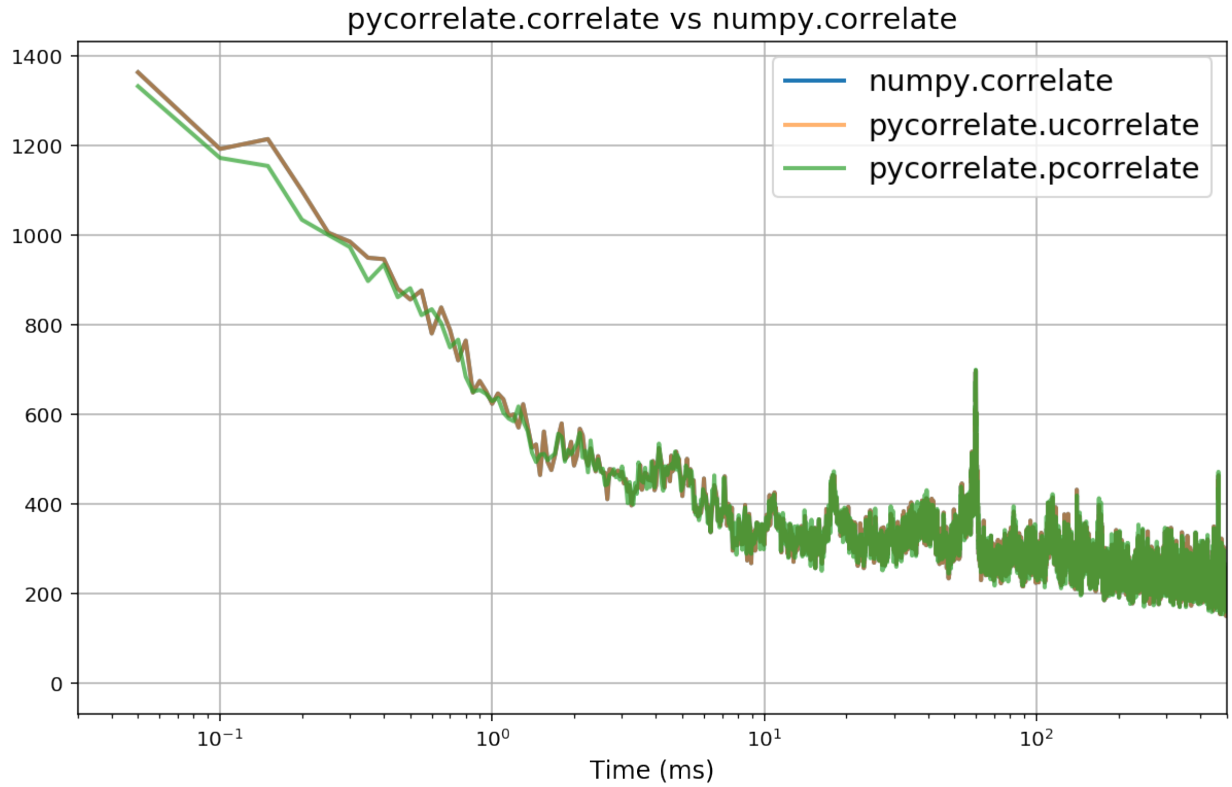
Now, let's compute the correlation also with `pycorrelate.pcorrelate`:

```
In [30]: maxlag_sec = 3.9
         lagbins = (np.arange(0, maxlag_sec, binwidth) / unit).astype('int64')
```

```
In [31]: Gp = pyc.pcorrelate(tt, uu, lagbins) * int(binwidth / unit)
```

Let's plot a comparison:

```
In [32]: fig, ax = plt.subplots(figsize=(10, 6))
         Gn_t = np.arange(1, Gn.size+1) * binwidth * 1e3
         Gu_t = np.arange(1, Gu.size+1) * binwidth * 1e3
         Gp_t = lagbins[1:] * unit * 1e3
         plt.plot(Gn_t, Gn, alpha=1, lw=2, label='numpy.correlate')
         plt.plot(Gu_t, Gu, alpha=0.6, lw=2, label='pycorrelate.ucorrelate')
         plt.plot(Gp_t, Gp, alpha=0.7, lw=2, label='pycorrelate.pcorrelate')
         plt.xlabel('Time (ms)', fontsize='large')
         plt.grid(True)
         plt.xlim(30e-3, 500)
         plt.xscale('log')
         plt.title('pycorrelate.correlate vs numpy.correlate', fontsize='x-large')
         plt.legend(loc='best', fontsize='x-large');
```



1.4.7 Conclusion

- `numpy.correlate` and `pycorrelate.ucorrelate` give identical results, with the latter being much faster. Note that the inputs are swapped between the two functions.
- `pycorrelate.ucorrelate` and `pycorrelate.pcorrelate` agree when using uniform time-lag bins.

1.5 Simple FCS example

This notebook shows howto compute and fit an FCS curve using `pycorrelate`.

1.5.1 Initial imports

```
In [1]: import numpy as np
        import h5py
```

```
In [2]: # Tweak here matplotlib style
        %matplotlib inline
        %config InlineBackend.figure_format = 'retina'
        import matplotlib.pyplot as plt
        import matplotlib as mpl
        mpl.rcParams['font.sans-serif'].insert(0, 'Arial')
        mpl.rcParams['font.size'] = 14
```

```
In [3]: import pycorrelate as pyc
        pyc.__version__
```

```
Out[3]: '0.3'
```

```
In [4]: import lmfit
        lmfit.__version__
```

```
Out[4]: '0.9.7'
```

1.5.2 Load Data

We start downloading a sample dataset of a smFRET "measurement" with a single CW excitation laser and two detectors donor (D) and acceptor (A) (the data is actually a simulation performed with PyBroMo).

```
In [5]: url = 'http://files.figshare.com/4917046/smFRET_44f3da_P_20_s0_20_s20_D_6.0e11_6.0e11_E_75_30
        pyc.utils.download_file(url, save_dir='data')
```

```
URL:  http://files.figshare.com/4917046/smFRET_44f3da_P_20_s0_20_s20_D_6.0e11_6.0e11_E_75_30_EmTot_20
File: smFRET_44f3da_P_20_s0_20_s20_D_6.0e11_6.0e11_E_75_30_EmTot_200k_200k_BgD1500_BgA800_t_max_600s

File already on disk: data/smFRET_44f3da_P_20_s0_20_s20_D_6.0e11_6.0e11_E_75_30_EmTot_200k_200k_BgD15
Delete it to re-download.
```

```
In [6]: fname = './data/' + url.split('/')[-1]
        h5 = h5py.File(fname)
        unit = h5['photon_data']['timestamps_specs']['timestamps_unit'][()]
        unit
```

```
Out[6]: 4.9999999999999998e-08
```

We can check that there are only two detectors:

```
In [7]: np.unique(h5['photon_data']['detectors'][:])
```

```
Out[7]: array([0, 1], dtype=uint8)
```

Then load the timestamps in two arrays `t` and `u`:

```
In [8]: detectors = h5['photon_data']['detectors'][:]
        timestamps = h5['photon_data']['timestamps'][:]
        t = timestamps[detectors == 0]
        u = timestamps[detectors == 1]
```

```
In [9]: t.shape, u.shape, t[0], u[0]
```

```
Out[9]: ((1152331,), (755468,), 50, 128800)
```

```
In [10]: t.max()*unit, u.max()*unit
```

```
Out[10]: (599.99934099999996, 599.99989349999998)
```

Timestamps need to be monotonic:

```
In [11]: assert (np.diff(t) >= 0).all()
         assert (np.diff(u) >= 0).all()
```

1.5.3 Compute CCF

To avoid afterpulsing, we can compute the cross-correlation function (CCF) between D and A channels.

We first create the lag bins array with the make_loglags() function:

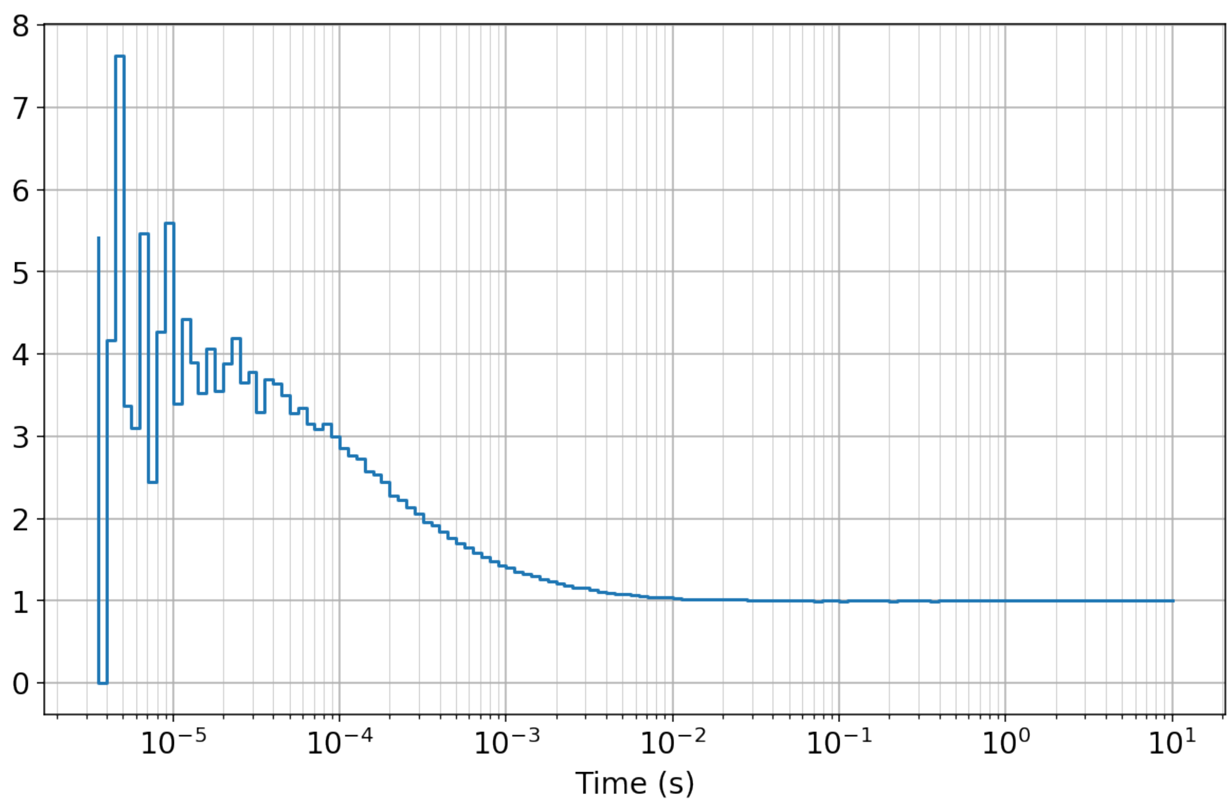
```
In [12]: # compute lags in sec. then convert to timestamp units
         bins_per_dec = 20
         bins = pyc.make_loglags(-6, 1, bins_per_dec)[bins_per_dec // 2:] / unit
```

Then, we compute the cross-correlation with pcorrelate:

```
In [13]: Gn = pyc.pcorrelate(t, u, bins, normalize=True)
```

Plotting the CCF function `Gn` we observe the typical diffusion shape:

```
In [14]: fig, ax = plt.subplots(figsize=(10, 6))
         plt.semilogx(bins[1:]*unit, Gn, drawstyle='steps-pre')
         plt.xlabel('Time (s)')
         plt.grid(True); plt.grid(True, which='minor', lw=0.3);
```



1.5.4 Fit FCS model

The next step is fitting the computed CCF with a model. For freely-diffusing species under confocal excitation (and no photo-physics) the simplest model is the 2D model (i.e. the PSF z dimension is neglected):

$$G(\tau) = 1 + A_0 \left(1 + \frac{\tau}{\tau_D}\right)^{-1}$$

The full 3D model is just slightly more complicated:

$$G(\tau) = 1 + A_0 \left(1 + \frac{\tau}{\tau_D}\right)^{-1} \left[1 + \left(\frac{r}{z}\right)^2 \frac{\tau}{\tau_D}\right]^{-1/2}$$

There is a link between A_0 and concentration. Neglecting background, $A_0 = 1/N$ where N is the mean number of molecules in the excitation volume. The background makes $A_0 < 1/N$. For full expression see Orrit 2002.

Here, for the sake of the example, we will just fit the simple 2D model.

Let's start defining the model functions and the array of time-lags:

```
In [15]: def diffusion_2d(timelag, tau_diff, A0):
             return 1 + A0 * 1/(1 + timelag/tau_diff)

         def diffusion_3d(timelag, tau_diff, A0, waist_z_ratio=0.1):
             return (1 + A0 * 1/(1 + timelag/tau_diff) *
                     1/np.sqrt(1 + waist_z_ratio**2 * timelag/tau_diff))
```

```
In [16]: tau = 0.5 * (bins[1:] + bins[:-1]) * unit
```

Now we build a "fitting model" with lmfit and use it to fit the CCF curve `Gn`:

```
In [17]: model = lmfit.Model(diffusion_2d)
         params = model.make_params(A0=1, tau_diff=1e-3)
         params['A0'].set(min=0.01, value=1)
         params['tau_diff'].set(min=1e-6, value=1e-3)
         #params['waist_z_ratio'].set(value=1/6, vary=False)  # 3D model only

         weights = np.ones_like(Gn)
         #weights = np.log(np.sqrt(G*np.diff(bins)))  # and example of using weights
         fitres = model.fit(Gn, timelag=tau, params=params, method='least_squares',
                            weights=weights)
         print('\nList of fitted parameters for %s: \n' % model.name)
         fitres.params.pretty_print(colwidth=10, columns=['value', 'min', 'max'])
```

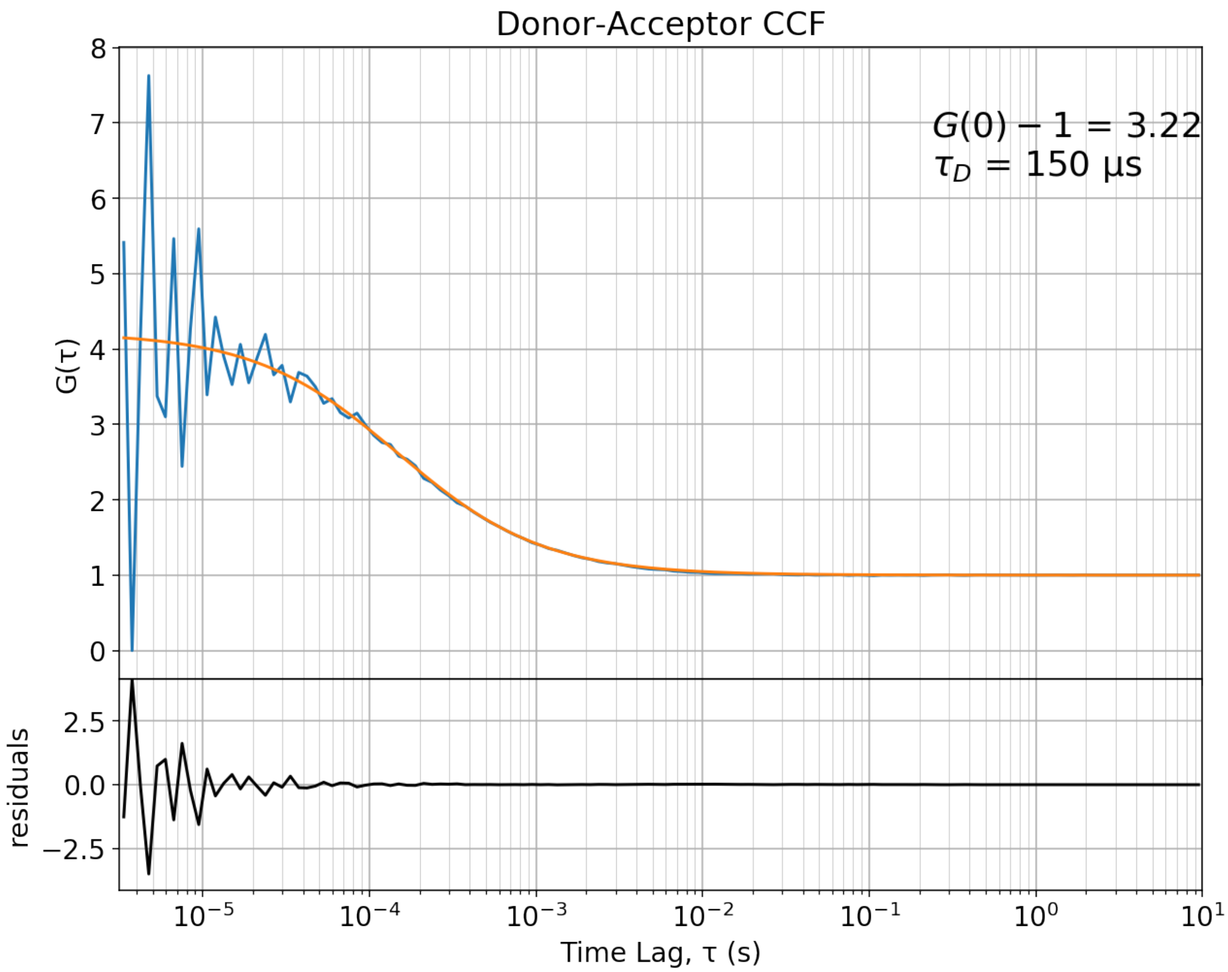
```
List of fitted parameters for Model(diffusion_2d):

Name          Value        Min        Max
A0            3.219       0.01        inf
tau_diff  0.0001495      1e-06        inf
```

Finally, we plot fit results and residuals:

```
In [18]: fig, ax = plt.subplots(2, 1, figsize=(10, 8), sharex=True,
                                gridspec_kw={'height_ratios': [3, 1]})
         plt.subplots_adjust(hspace=0)
         ax[0].semilogx(tau, Gn)
         for a in ax:
             a.grid(True); a.grid(True, which='minor', lw=0.3)
         ax[0].plot(tau, fitres.best_fit)
         ax[1].plot(tau, fitres.residual*weights, 'k')
         ym = np.abs(fitres.residual*weights).max()
```

```
ax[1].set_ylim(-ym, ym)
ax[1].set_xlim(bins[0]*unit, bins[-1]*unit);
tau_diff_us = fitres.values['tau_diff'] * 1e6
msg = ((r'$G(0)-1$ = {A0:.2f}'+'\n'+r'$\tau_D$ = {tau_diff_us:.0f} μs')
        .format(A0=fitres.values['A0'], tau_diff_us=tau_diff_us))
ax[0].text(.75, .9, msg,
           va='top', ha='left', transform=ax[0].transAxes, fontsize=18);
ax[0].set_ylabel('G(τ)')
ax[1].set_ylabel('residuals')
ax[0].set_title('Donor-Acceptor CCF')
ax[1].set_xlabel('Time Lag, τ (s)');
```



The flatness of the residual indicates a good fit. If you followed so far, you should be able to extent this example to use more complex models when needed.

1.6 Theory

1.6.1 Cross-correlation of point processes

In fluorescence correlation spectroscopy (FCS) the (normalized) cross-correlation function (CCF) of two continuous signals $I_1(t)$ and $I_2(t)$ is defined as:

$$G(\tau) = \frac{\langle I_1(t)\ I_2(t)\rangle}{\langle I_1(t)\rangle\langle I_2(t)\rangle}$$

The auto-correlation function (ACF) is just a special case where $I_1(t) = I_2(t)$.

In actual experiments, signals are not continuous but come from single-photon detectors that produce a pulse for each photon. These pulses are usually timestamped with ~10ns resolution. The series of photon arrival times is used as input for ACF or CCF computations.

In principle, timestamps can be binned to produce a discrete-time signal. In signal processing, the (non-normalized) cross-correlation of two real discrete-time signals $\{A_i\}$ and $\{B_i\}$ is defined as

$$c[k] = \sum_{i=0}^{N} A[i]\ B[i+k].$$

The previous formula is implemented by `ucorrelate()` and numpy.correlate.

Binning timestamps to obtain timetraces would be very inefficient for FCS analysis where time-lags spans may orders of magnitude. It is much more efficient to directly compute the cross-correlation function from timestamps. The popular multi-tau algorithm allows computing the correlation directly from timestamps on a fixed arrangement of quasi-log-spaced bins. More generally, Laurence algorithm (Laurence et al. Optics Letters (2006)) allows computing cross-correlation from timestamps on arbitrary bins of time-lags, with similar performances as the multi-tau. Computing cross-correlation $C(\tau)$ from timestamps is fundamentally a counting tasks. Given two timestamps arrays *t* and *u* and considering the k-th time-lag bin $[\tau_k, \tau_{k+1})$, $C(k)$ is the number of pairs where:

$$\tau_k \le t_i - u_j < \tau_{k+1}$$

for all the possible *i* and *j* combinations.

$$C(k) = \frac{n(\{(i,j) \ni t_i < u_i - \Delta\tau_k\})}{\Delta\tau_k} \tag{1.1}$$

where *n({})* is the operator counting the elements in a set, $\Delta\tau_k$ is the duration of the k-th time-lag bin and T is the measurement duration. For FCS we normally want the normalized CCF, that is:

$$G(k) = \frac{n(\{(i,j) \ni t_i < u_i - \Delta\tau_k\})}{n(\{i \ni t_i \le T - \Delta\tau_k\})\, n(\{j \ni u_j \ge \Delta\tau_k\})} \frac{(T - \Delta\tau_k)}{\Delta\tau_k} \tag{1.2}$$

Eq. (1.1) and (1.2) are implemented by `pcorrelate()`, where the argument *normalize* allows choosing between the normalized and unnormalized version.

Note: In *Laurence 2006* the expression for *G(k)* (there called $C_{AB}(\tau)$) does not include the $\Delta\tau_k$ in the denominator due to a typo.

References

- Laurence, T. A., Fore, S., Huser, T. (2006). Fast, flexible algorithm for calculating photon correlations. *Optics Letters* , *31* (6), 829–831. https://doi.org/10.1364/OL.31.000829

- Petra Schwille and Elke Haustein, Fluorescence Correlation Spectroscopy An Introduction to its Concepts and Applications
- Haustein, E., Schwille, P. (2003). Ultrasensitive investigations of biological systems by fluorescence correlation spectroscopy. *Methods*, *29* (2), 153–166. https://doi.org/10.1016/S1046-2023(02)00306-7

1.7 Contributing

Contributions are welcome, and they are greatly appreciated! Every little bit helps, and credit will always be given.

You can contribute in many ways:

1.7.1 Types of Contributions

Report Bugs

Report bugs at https://github.com/tritemio/pycorrelate/issues.

If you are reporting a bug, please include:

- Your operating system name and version.
- Any details about your local setup that might be helpful in troubleshooting.
- Detailed steps to reproduce the bug.

Fix Bugs

Look through the GitHub issues for bugs. Anything tagged with "bug" and "help wanted" is open to whoever wants to implement it.

Implement Features

Look through the GitHub issues for features. Anything tagged with "enhancement" and "help wanted" is open to whoever wants to implement it.

Write Documentation

Pycorrelate could always use more documentation, whether as part of the official Pycorrelate docs, in docstrings, or even on the web in blog posts, articles, and such.

Submit Feedback

The best way to send feedback is to file an issue at https://github.com/tritemio/pycorrelate/issues.

If you are proposing a feature:

- Explain in detail how it would work.
- Keep the scope as narrow as possible, to make it easier to implement.
- Remember that this is a volunteer-driven project, and that contributions are welcome :)

1.7.2 Get Started!

Ready to contribute? Here's how to set up *pycorrelate* for local development.

1. Fork the *pycorrelate* repo on GitHub.
2. Clone your fork locally:

```
$ git clone git@github.com:your_name_here/pycorrelate.git
```

3. Install your local copy into a virtualenv. Assuming you have virtualenvwrapper installed, this is how you set up your fork for local development:

```
$ mkvirtualenv pycorrelate
$ cd pycorrelate/
$ python setup.py develop
```

4. Create a branch for local development:

```
$ git checkout -b name-of-your-bugfix-or-feature
```

   Now you can make your changes locally.

5. When you're done making changes, check that your changes pass tests (not yet, see #3), and that notebooks runs without errors.
6. Commit your changes and push your branch to GitHub:

```
$ git add .
$ git commit -m "Your detailed description of your changes."
$ git push origin name-of-your-bugfix-or-feature
```

7. Submit a pull request through the GitHub website.

1.7.3 Pull Request Guidelines

Before you submit a pull request, check that it meets these guidelines:

1. The pull request should include tests (for now see #3).
2. If the pull request adds functionality, the docs should be updated. Put your new functionality into a function with a docstring, and add the feature to the list in README.rst.
3. The pull request should work for Python 3.5+. Check https://travis-ci.org/tritemio/pycorrelate/pull_requests and make sure that the tests pass for all supported Python versions.

1.7.4 Tips

To run a subset of tests (not yet, see #3):

```
$ py.test tests.test_pycorrelate
```

1.8 Credits

1.8.1 Development Lead

- Antonino Ingargiola <tritemio@gmail.com>

1.8.2 Contributors

None yet. Why not be the first?

1.9 History

1.9.1 0.2.1 (2017-11-15)

- Added normalization for FCS curves (see pnormalize).
- Added example notebook showing how to fit a simple FCS curve
- Renamed ucorrelate argument from *maxlags* to *maxlag*.
- Added theory page in the documentation, showing the exact formula used for CCF calculations.

1.9.2 0.1.0 (2017-07-23)

- First release on PyPI.

1.10 Indices and tables

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