
dclab Documentation

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This is dclab, a Python library for the post-measurement analysis of real-time deformability cytometry (RT-DC) datasets. This is the documentation of dclab version 0.31.0.

1.1 Installation

To install dclab, use one of the following methods:

- **from PyPI:** `pip install dclab[all]`
- **from sources:** `pip install .[all]`

The extra key `[all]` installs all possible dependencies in any context of RT-DC data analysis. You might prefer to only install a subset of these:

- `pip install dclab`: for the basic dclab functionalities
- `pip install dclab[dcor]`: to *access online data* from DCOR
- `pip install dclab[lme4]`: for *linear mixed effects model analysis* using R/lme4
- `pip install dclab[ml]`: for *machine-learning applications*
- `pip install dclab[tdms]`: for the (outdated) .tdms file format
- `pip install dclab[export]`: for .avi and .fcs export

You may also combine these dependencies, i.e. `pip install dclab[dcor,ml]` for DCOR and machine-learning support.

In addition, dclab already comes with code from [OpenCV](#) (computation of moments) and [scikit-image](#) (computation of contours and points in polygons) to reduce the list of dependencies (these libraries are not required by dclab).

Note that if you are installing from source or if no binary wheel is available for your platform and Python version, [Cython](#) will be installed to build the required dclab extensions. If this process fails, please request a binary wheel for your platform (e.g. Windows 64bit) and Python version (e.g. 3.6) by creating a new [issue](#).

1.2 Use cases

If you are a frequent user of RT-DC, you might run into problems that cannot (yet) be addressed with the graphical user interface [Shape-Out](#). Here is a list of use cases that would motivate an installation of dclab.

- You would like to convert old .tdms-based datasets to the new .rtdc file format, because of enhanced speed in Shape-Out and reduced disk usage. What you are looking for is the command line program *dclab-tdms2rtdc* that comes with dclab. It allows to batch-convert multiple measurements at a time. Note that you should keep the original .tdms files backed-up somewhere, because there might be future improvements or bug fixes from which you would like to benefit. Please note that [DCKit](#) offers a graphical user interface for batch conversion from .tdms to .rtdc.
- You would like to apply a simple set of filters (e.g. polygon filters that you exported from within Shape-Out) to every new measurement you take and apply a custom data analysis pipeline to the filtered data. This is a straight-forward Python coding problem with dclab. After reading the basic usage section below, please have a look at the [polygon filter reference](#).
- You would like to do advanced statistics or combine your RT-DC analysis with other fancy approaches such as machine-learning. It would be too laborious to do the analysis in Shape-Out, export the data as text files, and then open them in your custom Python script. If your initial analysis step with Shape-Out only involves tasks that can be automated, why not use dclab from the beginning?
- You simulated RT-DC data and plan to import them in Shape-Out for testing. Once you have loaded your data as a numpy array, you can instantiate an *RTDC_Dict* class and then use the *Export* class to create an .rtdc data file.

If you are still unsure about whether to use dclab or not, you might want to look at the [example section](#). If you need advice, do not hesitate to [create an issue](#).

1.3 Basic usage

Experimental RT-DC datasets are always loaded with the `new_dataset` method:

```
import numpy as np
import dclab

# .tdms file format
ds = dclab.new_dataset("/path/to/measurement/Online/M1.tdms")
# .rtdc file format
ds = dclab.new_dataset("/path/to/measurement/M2.rtdc")
# DCOR data
ds = dclab.new_dataset("fb719fb2-bd9f-817a-7d70-f4002af916f0")
```

The object returned by `new_dataset` is always an instance of `RTDCBase`. To show all available features, use:

```
print(ds.features)
```

This will list all scalar features (e.g. “area_um” and “deform”) and all non-scalar features (e.g. “contour” and “image”). Scalar features can be filtered by editing the configuration of `ds` and calling `ds.apply_filter()`:

```
# register filtering operations
amin, amax = ds["area_um"].min(), ds["area_um"].max()
ds.config["filtering"]["area_um min"] = (amax + amin) / 2
ds.config["filtering"]["area_um max"] = amax
ds.apply_filter() # this step is important!
```

This will update the binary array `ds.filter.all` which can be used to extract the filtered data:

```
area_um_filtered = ds["area_um"][ds.filter.all]
```

It is also possible to create a hierarchy child of this dataset that only contains the filtered data.

```
ds_child = dclab.new_dataset(ds)
```

The hierarchy child `ds_child` is dynamic, i.e. when the filters in `ds` change, then `ds_child` also changes after calling `ds_child.apply_filter()`.

Non-scalar features do not support fancy indexing (i.e. `ds["image"][ds.filter.all]` will not work. Use a for-loop to extract them.

```
for ii in range(len(ds)):
    image = ds["image"][ii]
    mask = ds["mask"][ii]
    # this is equivalent to ds["bright_avg"][ii]
    bright_avg = np.mean(image[mask])
    print("average brightness of event {}: {:.1f}".format(ii, bright_avg))
```

If you need more information to get started on your particular problem, you might want to check out the *examples section* and the *advanced scripting section*.

1.4 Citing dclab

If you use dclab in a scientific publication, please cite it with:

Paul Müller and others (2015), dclab version X.X.X: Python library for the post-measurement analysis of real-time deformability cytometry data sets [Software]. Available at <https://github.com/ZELLMECHANIK-DRESDEN/dclab>.

Command-line interface

2.1 dclab-compress

Create a compressed version of an .rtdc file. This can be used for saving disk space (loss-less compression). The data generated during an experiment is usually not compressed.

```
usage: dclab-compress [-h] INPUT OUTPUT
```

required arguments:

- INPUT Input path (.rtdc file)
- OUTPUT Output path (.rtdc file)

2.2 dclab-condense

Reduce an RT-DC measurement to its scalar-only features (i.e. without *contour*, *image*, *mask*, or *trace*). All available ancillary features are computed.

```
usage: dclab-condense [-h] INPUT OUTPUT
```

required arguments:

- INPUT Input path (.tdms or .rtdc file)
- OUTPUT Output path (.rtdc file)

2.3 dclab-join

Join two or more RT-DC measurements. This will produce one larger .rtdc file. The meta data of the dataset that was recorded earliest will be used in the output file. Please only join datasets that were recorded in the same measurement run.

```
usage: dclab-join [-h] -o OUTPUT [INPUT [INPUT ...]]
```

required arguments:

- INPUT Input paths (.tdms or .rtdc files)
- OUTPUT Output path (.rtdc file)

2.4 dclab-repack

Repack an .rtdc file. The difference to dclab-compress is that no logs are added. Other logs can optionally be stripped away. Repacking also gets rid of old clutter data (e.g. previous metadata stored in the HDF5 file).

```
usage: dclab-repack [-h] [--strip-logs] INPUT OUTPUT
```

required arguments:

- INPUT Input path (.rtdc file)
- OUTPUT Output path (.rtdc file)

optional arguments:

- `--strip-logs` (*disabled by default*) Do not copy any logs to the output file.

2.5 dclab-split

Split an RT-DC measurement file (.tdms or .rtdc) into multiple smaller .rtdc files.

```
usage: dclab-split [-h] [--path_out PATH_OUT] [--split-events SPLIT_EVENTS]
                  [--include-empty-boundary-images]
                  PATH_IN
```

required arguments:

- PATH_IN Input path (.tdms or .rtdc file)

optional arguments:

- `--path_out` (*default: PATH_IN*) Output directory (defaults to same directory)
- `--split-events` (*default: 10000*) Maximum number of events in each output file
- `--include-empty-boundary-images` (*disabled by default*) In old versions of Shape-In, the first or last images were sometimes not stored in the resulting .avi file. In dclab, such images are represented as zero-valued images. Set this option, if you wish to include these events with empty image data.

2.6 dclab-tdms2rtdc

Convert RT-DC .tdms files to the hdf5-based .rtdc file format. Note: Do not delete original .tdms files after conversion. The conversion might be incomplete.

```
usage: dclab-tdms2rtdc [-h] [--compute-ancillary-features]
                       [--include-empty-boundary-images]
                       TDMS_PATH RTDC_PATH
```


required arguments:

- TDMS_PATH Input path (tdms file or folder containing tdms files)
- RTDC_PATH Output path (file or folder), existing data will be overridden

optional arguments:

- `--compute-ancillary-features` (*disabled by default*) Compute features, such as volume or emodulus, that are otherwise computed on-the-fly. Use this if you want to minimize analysis time in e.g. Shape-Out. CAUTION: ancillary feature recipes might be subject to change (e.g. if an error is found in the recipe). Disabling this option maximizes compatibility with future versions and allows to isolate the original data.
- `--include-empty-boundary-images` (*disabled by default*) In old versions of Shape-In, the first or last images were sometimes not stored in the resulting .avi file. In dclab, such images are represented as zero-valued images. Set this option, if you wish to include these events with empty image data.

2.7 dclab-verify-dataset

Check experimental datasets for completeness. Note that old measurements will most likely fail this verification step. This program is used to enforce data integrity with future implementations of RT-DC recording software (e.g. Shape-In).

```
usage: dclab-verify-dataset [-h] PATH
```

required arguments:

- PATH Path to experimental dataset

3.1 Dataset overview plot

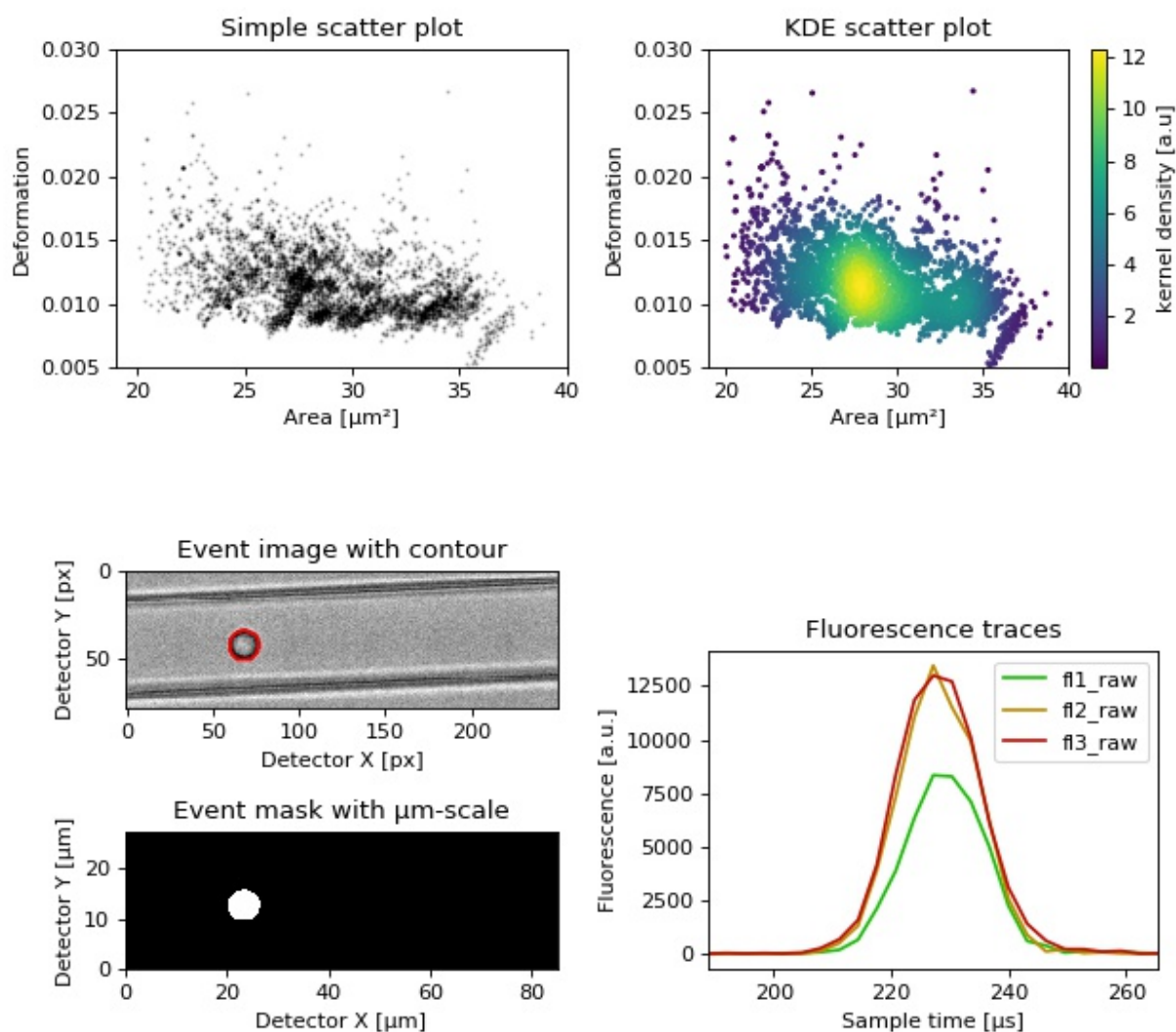
This example demonstrates basic data visualization with dclab and matplotlib. To run this script, download the reference dataset *calibration_beads.rtdc* [RHMGI9] and place it in the same directory.

You will find more examples in the *advanced usage* section of this documentation.

overview_plot.py

```
1 import matplotlib.pyplot as plt
2 import numpy as np
3
4 import dclab
5
6 # Dataset to display
7 DATASET_PATH = "calibration_beads.rtdc"
8 # Features for scatter plot
9 SCATTER_X = "area_um"
10 SCATTER_Y = "deform"
11 # Event index to display
12 EVENT_INDEX = 100
13
14 xlabel = dclab.dfn.get_feature_label(SCATTER_X)
15 ylabel = dclab.dfn.get_feature_label(SCATTER_Y)
16
17 ds = dclab.new_dataset(DATASET_PATH)
18
19 fig = plt.figure(figsize=(8, 7))
20
21
22 ax1 = plt.subplot(221, title="Simple scatter plot")
23 ax1.plot(ds[SCATTER_X], ds[SCATTER_Y], "o", color="k", alpha=.2, ms=1)
24 ax1.set_xlabel(xlabel)
25 ax1.set_ylabel(ylabel)
```

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```

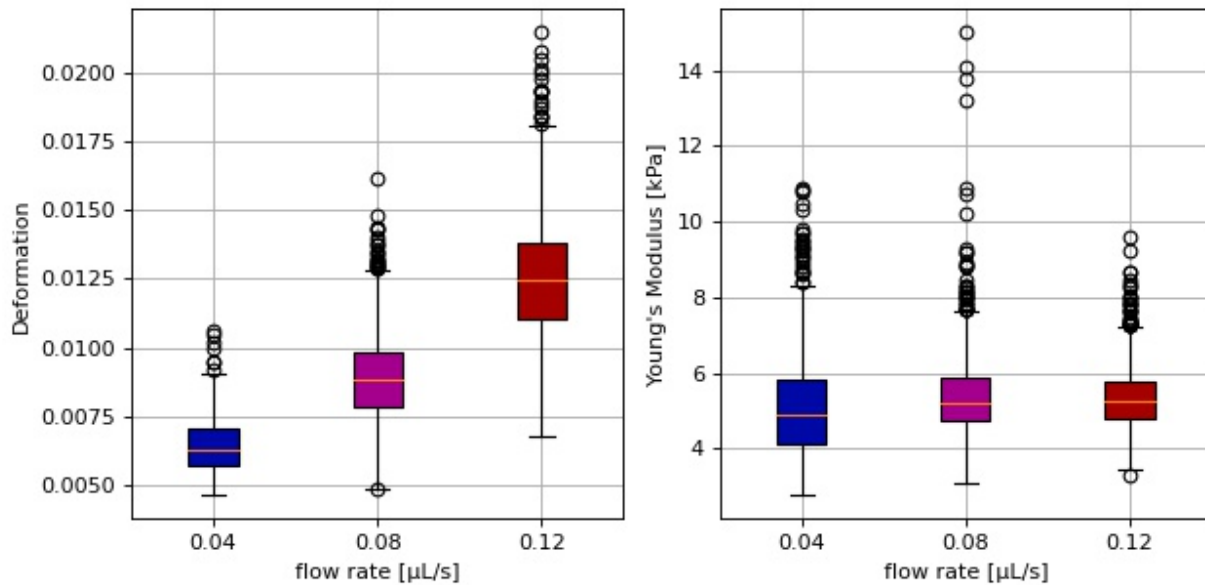
26 ax1.set_xlim(19, 40)
27 ax1.set_ylim(0.005, 0.03)
28
29 ax2 = plt.subplot(222, title="KDE scatter plot")
30 sc = ax2.scatter(ds[SCATTER_X], ds[SCATTER_Y],
31                 c=ds.get_kde_scatter(xax=SCATTER_X,
32                                     yax=SCATTER_Y,
33                                     kde_type="multivariate"),
34                 s=3)
35 plt.colorbar(sc, label="kernel density [a.u]", ax=ax2)
36 ax2.set_xlabel(xlabel)
37 ax2.set_ylabel(ylabel)
38 ax2.set_xlim(19, 40)
39 ax2.set_ylim(0.005, 0.03)
40
41 ax3 = plt.subplot(425, title="Event image with contour")
42 ax3.imshow(ds["image"][EVENT_INDEX], cmap="gray")
43 ax3.plot(ds["contour"][EVENT_INDEX][:, 0],
44         ds["contour"][EVENT_INDEX][:, 1],
45         c="r")
46 ax3.set_xlabel("Detector X [px]")
47 ax3.set_ylabel("Detector Y [px]")
48
49 ax4 = plt.subplot(427, title="Event mask with μm-scale")
50 pxsize = ds.config["imaging"]["pixel size"]
51 ax4.imshow(ds["mask"][EVENT_INDEX],
52           extent=[0, ds["mask"].shape[2] * pxsize,
53                  0, ds["mask"].shape[1] * pxsize],
54           cmap="gray")
55 ax4.set_xlabel("Detector X [μm]")
56 ax4.set_ylabel("Detector Y [μm]")
57
58 ax5 = plt.subplot(224, title="Fluorescence traces")
59 flsamples = ds.config["fluorescence"]["samples per event"]
60 flrate = ds.config["fluorescence"]["sample rate"]
61 fltime = np.arange(flsamples) / flrate * 1e6
62 # here we plot "fl?_raw"; you may also plot "fl?_med"
63 ax5.plot(fltime, ds["trace"]["f11_raw"][EVENT_INDEX],
64         c="#15BF00", label="f11_raw")
65 ax5.plot(fltime, ds["trace"]["f12_raw"][EVENT_INDEX],
66         c="#BF8A00", label="f12_raw")
67 ax5.plot(fltime, ds["trace"]["f13_raw"][EVENT_INDEX],
68         c="#BF0C00", label="f13_raw")
69 ax5.legend()
70 ax5.set_xlim(ds["f11_pos"][EVENT_INDEX] - 2*ds["f11_width"][EVENT_INDEX],
71             ds["f11_pos"][EVENT_INDEX] + 2*ds["f11_width"][EVENT_INDEX])
72 ax5.set_xlabel("Event time [μs]")
73 ax5.set_ylabel("Fluorescence [a.u.]")
74
75 plt.tight_layout()
76
77 plt.show()

```

3.2 Young's modulus computation from data on DCOR

This example reproduces the lower right subplot of figure 10 in [Her17]. It illustrates how the Young's modulus of elastic beads can be retrieved correctly (independent of the flow rate, with correction for pixelation and shear-thinning) using the area-deformation look-up table implemented in dclab (right plot). For comparison, the flow-rate-dependent deformation is also shown (left plot).

The dataset is loaded directly from DCOR and thus an active internet connection is required for this example.



emodulus_dcor.py

```

1 import dclab
2 import matplotlib.pyplot as plt
3
4 # The dataset is also available on figshare
5 # (https://doi.org/10.6084/m9.figshare.12721436.v1), but we
6 # are accessing it through the DCOR API, because we do not
7 # have the time to download the entire dataset. The dataset
8 # name is figshare-12721436-v1. These are the resource IDs:
9 ds_loc = ["e4d59480-fa5b-c34e-0001-46a944afc8ea",
10          "2cea205f-2d9d-26d0-b44c-0a11d5379152",
11          "2cd67437-a145-82b3-d420-45390f977a90",
12          ]
13 ds_list = [] # list of opened datasets
14 labels = [] # list of flow rate labels
15
16 # load the data
17 for loc in ds_loc:
18     ds = dclab.new_dataset(loc)
19     labels.append("{:.2f}".format(ds.config["setup"]["flow rate"]))
20     # emodulus computation
21     ds.config["calculation"]["emodulus medium"] = ds.config["setup"]["medium"]
22     ds.config["calculation"]["emodulus model"] = "elastic sphere"
23     ds.config["calculation"]["emodulus temperature"] = \
24         ds.config["setup"]["temperature"]

```

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```

25     # filtering
26     ds.config["filtering"]["area_ratio min"] = 1.0
27     ds.config["filtering"]["area_ratio max"] = 1.1
28     ds.config["filtering"]["deform min"] = 0
29     ds.config["filtering"]["deform max"] = 0.035
30     # This option will remove "nan" events that appear in the "emodulus"
31     # feature. If you are not working with DCOR, this might lead to a
32     # longer computation time, because all available features are
33     # computed locally. For data on DCOR, this computation already has
34     # been done.
35     ds.config["filtering"]["remove invalid events"] = True
36     ds.apply_filter()
37     # Create a hierarchy child for convenience reasons
38     # (Otherwise we would have to do e.g. ds["deform"][ds.filter.all]
39     # everytime we need to access a feature)
40     ds_list.append(dclab.new_dataset(ds))
41
42     # plot
43     fig = plt.figure(figsize=(8, 4))
44
45     # box plot for deformation
46     ax1 = plt.subplot(121)
47     ax1.set_ylabel(dclab.dfn.get_feature_label("deform"))
48     data_deform = [di["deform"] for di in ds_list]
49     # Uncomment this line if you are not filtering invalid events (above)
50     # data_deform = [d[~np.isnan(d)] for d in data_deform]
51     bplot1 = ax1.boxplot(data_deform,
52                          vert=True,
53                          patch_artist=True,
54                          labels=labels,
55                          )
56
57     # box plot for Young's modulus
58     ax2 = plt.subplot(122)
59     ax2.set_ylabel(dclab.dfn.get_feature_label("emodulus"))
60     data_emodulus = [di["emodulus"] for di in ds_list]
61     # Uncomment this line if you are not filtering invalid events (above)
62     # data_emodulus = [d[~np.isnan(d)] for d in data_emodulus]
63     bplot2 = ax2.boxplot(data_emodulus,
64                          vert=True,
65                          patch_artist=True,
66                          labels=labels,
67                          )
68
69     # colors
70     colors = ["#0008A5", "#A5008D", "#A50100"]
71     for bplot in (bplot1, bplot2):
72         for patch, color in zip(bplot['boxes'], colors):
73             patch.set_facecolor(color)
74
75     # axes
76     for ax in [ax1, ax2]:
77         ax.grid()
78         ax.set_xlabel("flow rate [pL/s]")
79
80     plt.tight_layout()
81     plt.show()

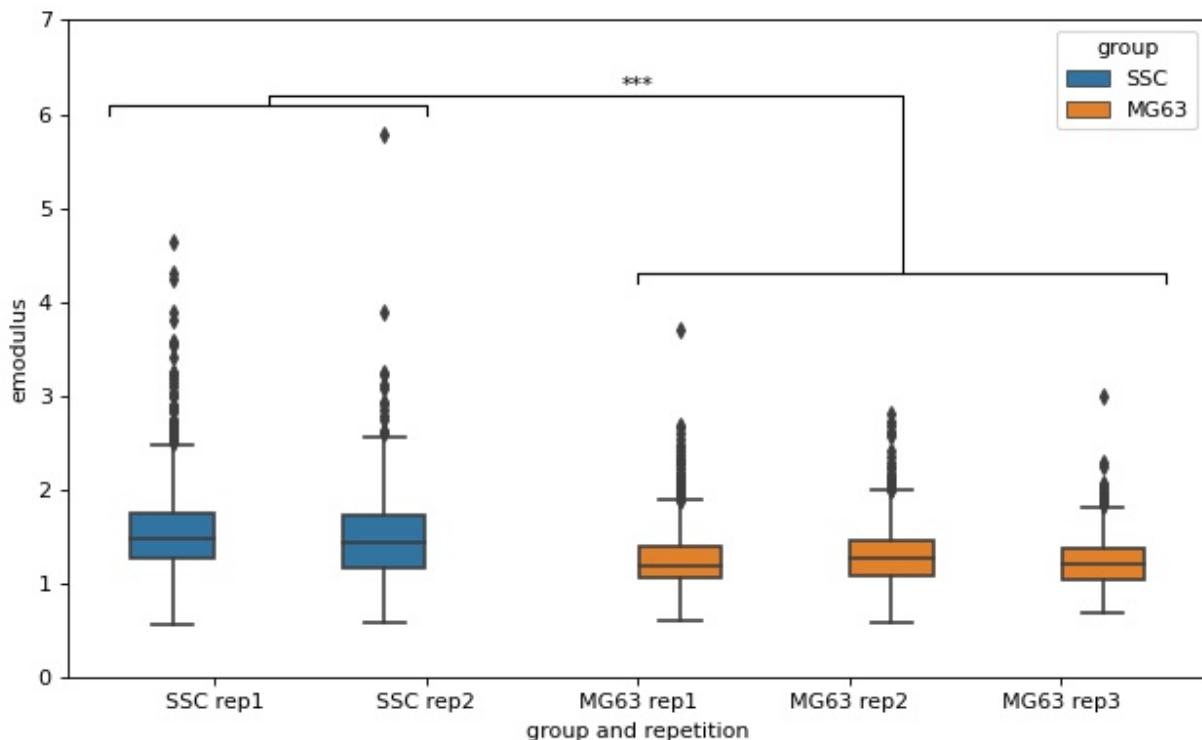
```

3.3 lme4: Linear mixed-effects models

We would like to quantify the difference between human skeletal stem cells (SSC) and the human osteosarcoma cell line MG-63 (which is often used as a model system for SSCs) using a likelihood ratio test based on LMM.

This example illustrates a basic LMM analysis. The data are loaded from DCOR ([XRM+20], [DCOR:figshare-11662773-v2](https://dcor.mpl.mpg.de/dataset/figshare-11662773-v2)). We treat SSC as our “treatment” and MG-63 as our “control” group. These are just names that remind us that we are comparing one type of sample against another type.

We are interested in the p-value, which is 0.01256 for deformation. We repeat the analysis with area (0.0002183) and Young’s modulus (0.0002771). The p-values indicate that MG-63 (mean elastic modulus 1.26 kPa) cells are softer than SSCs (mean elastic modulus 1.54 kPa). The figure reproduces the last subplot of figure 6b in [HMMO18].



lme4_lmer.py

```
1 import dclab
2 from dclab import lme4
3
4 import pandas as pd
5 import seaborn as sns
6 import matplotlib.pyplot as plt
7
8
9 # https://dcor.mpl.mpg.de/dataset/figshare-11662773-v2
10 # SSC_16uls_rep1_20150611.rtdc
11 ds_ssc_rep1 = dclab.new_dataset("86cc5a47-364b-cf58-f9e3-cc114dd38e55")
12 # SSC_16uls_rep2_20150611.rtdc
13 ds_ssc_rep2 = dclab.new_dataset("ab95c914-0311-6a46-4eba-8fabca7d27d6")
14 # MG63_pure_16uls_rep1_20150421.rtdc
15 ds_mg63_rep1 = dclab.new_dataset("42cb33d4-2f7c-3c22-88e1-b9102d64d7e9")
```

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```

16 # MG63_pure_16uls_rep2_20150422.rtdc
17 ds_mg63_rep2 = dclab.new_dataset("a4a98fcb-1de1-1048-0efc-b0a84d4ab32e")
18 # MG63_pure_16uls_rep3_20150422.rtdc
19 ds_mg63_rep3 = dclab.new_dataset("0a8096ce-ea7a-e36d-1df3-42c7885cd71c")
20
21 datasets = [ds_ssc_rep1, ds_ssc_rep2, ds_mg63_rep1, ds_mg63_rep2, ds_mg63_rep3]
22 for ds in datasets:
23     # perform filtering
24     ds.config["filtering"]["area_ratio min"] = 0
25     ds.config["filtering"]["area_ratio max"] = 1.05
26     ds.config["filtering"]["area_um min"] = 120
27     ds.config["filtering"]["area_um max"] = 550
28     ds.config["filtering"]["deform min"] = 0
29     ds.config["filtering"]["deform max"] = 0.1
30     ds.apply_filter()
31     # enable computation of Young's modulus
32     ds.config["calculation"]["emodulus medium"] = "CellCarrier"
33     ds.config["calculation"]["emodulus model"] = "elastic sphere"
34     ds.config["calculation"]["emodulus temperature"] = 23.0
35
36 # setup lme4 analysis
37 rlme4 = lme4.Rlme4(model="lmer")
38 rlme4.add_dataset(ds_ssc_rep1, group="treatment", repetition=1)
39 rlme4.add_dataset(ds_ssc_rep2, group="treatment", repetition=2)
40 rlme4.add_dataset(ds_mg63_rep1, group="control", repetition=1)
41 rlme4.add_dataset(ds_mg63_rep2, group="control", repetition=2)
42 rlme4.add_dataset(ds_mg63_rep3, group="control", repetition=3)
43
44 # perform analysis for deformation
45 for feat in ["area_um", "deform", "emodulus"]:
46     res = rlme4.fit(feature=feat)
47     print("Results for {}".format(feat))
48     print("  p-value", res["anova p-value"])
49     print("  mean of MG-63", res["fixed effects intercept"])
50     print("  fixed effect size", res["fixed effects treatment"])
51
52 # prepare for plotting
53 df = pd.DataFrame()
54 for ds in datasets:
55     group = ds.config["experiment"]["sample"].split()[0]
56     rep = ds.config["experiment"]["sample"].split()[-1]
57     dfi = pd.DataFrame.from_dict(
58         {"area_m": ds["area_um"][ds.filter.all],
59          "deform": ds["deform"][ds.filter.all],
60          "emodulus": ds["emodulus"][ds.filter.all],
61          "group and repetition": [group + " " + rep] * ds.filter.all.sum(),
62          "group": [group] * ds.filter.all.sum(),
63         })
64     df = df.append(dfi)
65
66 # plot
67 fig = plt.figure(figsize=(8, 5))
68 ax = sns.boxplot(x="group and repetition", y="emodulus", data=df, hue="group")
69 # note that `res` is still the result for "emodulus"
70 numstars = sum([res["anova p-value"] < .05,
71                 res["anova p-value"] < .01,
72                 res["anova p-value"] < .001,

```

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```

73         res["anova p-value"] < .0001])
74 # significance bars
75 h = .1
76 y1 = 6
77 y2 = 4.2
78 y3 = 6.2
79 ax.plot([-0.5, -0.5, 1, 1], [y1, y1+h, y1+h, y1], lw=1, c="k")
80 ax.plot([2, 2, 4.5, 4.5], [y2, y2+h, y2+h, y2], lw=1, c="k")
81 ax.plot([.25, .25, 3.25, 3.25], [y1+h, y1+2*h, y1+2*h, y2+h], lw=1, c="k")
82 ax.text(2, y3, "*" * numstars, ha='center', va='bottom', color="k")
83 ax.set_ylim(0, 7)
84
85 plt.tight_layout()
86 plt.show()

```

3.4 lme4: Generalized linear mixed-effects models with differential deformation

This example illustrates how to perform a differential feature (including reservoir data) GLMM analysis. The example data are taken from DCOR ([XRM+20], [DCOR:figshare-11662773-v2](https://figshare.com/figure/dcor-figshare-11662773-v2)). As in the *previous example*, we treat SSC as our “treatment” and MG-63 as our “control” group.

The p-value for the differential deformation is magnitudes lower than the p-value for the (non-differential) deformation in the previous example. This indicates that there is a non-negligible initial deformation of the cells in the reservoir.

lme4_glmer_diff.py

```

1 from dclab import lme4, new_dataset
2
3 # https://dcor.mpl.mpg.de/dataset/figshare-11662773-v2
4 datasets = [
5     # SSC channel
6     [new_dataset("86cc5a47-364b-cf58-f9e3-cc114dd38e55"), "treatment", 1],
7     [new_dataset("ab95c914-0311-6a46-4eba-8fabca7d27d6"), "treatment", 2],
8     # SSC reservoir
9     [new_dataset("761ab515-0416-ed8-5137-135c1682580c"), "treatment", 1],
10    [new_dataset("3b83d47b-d860-4558-51d6-dcc524f5f90d"), "treatment", 2],
11    # MG-63 channel
12    [new_dataset("42cb33d4-2f7c-3c22-88e1-b9102d64d7e9"), "control", 1],
13    [new_dataset("a4a98fcb-1de1-1048-0efc-b0a84d4ab32e"), "control", 2],
14    [new_dataset("0a8096ce-ea7a-e36d-1df3-42c7885cd71c"), "control", 3],
15    # MG-63 reservoir
16    [new_dataset("56c449bb-b6c9-6df7-6f70-6744b9960980"), "control", 1],
17    [new_dataset("387b5ac9-1cc6-6cac-83d1-98df7d687d2f"), "control", 2],
18    [new_dataset("7ae49cd7-10d7-ef35-a704-72443bb32da7"), "control", 3],
19 ]
20
21 # perform filtering
22 for ds, _, _ in datasets:
23     ds.config["filtering"]["area_ratio min"] = 0
24     ds.config["filtering"]["area_ratio max"] = 1.05
25     ds.config["filtering"]["area_um min"] = 120
26     ds.config["filtering"]["area_um max"] = 550
27     ds.config["filtering"]["deform min"] = 0

```

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```

28     ds.config["filtering"]["deform max"] = 0.1
29     ds.apply_filter()
30
31     # perform LMM analysis for differential deformation
32     # setup lme4 analysis
33     rlme4 = lme4.Rlme4(feature="deform")
34     for ds, group, repetition in datasets:
35         rlme4.add_dataset(ds, group=group, repetition=repetition)
36
37     # LMM
38     lmer_result = rlme4.fit(model="lmer")
39     print("LMM p-value", lmer_result["anova p-value"]) # 0.00000351
40
41     # GLMM with log link function
42     glmer_result = rlme4.fit(model="glmer+loglink")
43     print("GLMM p-value", glmer_result["anova p-value"]) # 0.000868

```

3.5 ML: Using RT-DC data with tensorflow

We use tensorflow to distinguish between beads and cells using scalar features only. The example data is taken from a [reference dataset on DCOR](#). The classification accuracy using only the inputs `area_ratio`, `area_um`, `bright_sd`, and `deform` reaches values above 95%.

Warning: This example neglects a lot of important aspects of machine learning with RT-DC data (e.g. brightness normalization) and it is a very easy task (beads are smaller than cells). Thus, this example should only be considered as a technical guide on how tensorflow can be used with RT-DC data.

Note: What happens when you add "bright_avg" to the features list? Can you explain the result?

Apparently, debris in the cell dataset is classified as beads. We could have gotten around that by filtering the input data before inference. In addition, some beads get classified as cells as well. This is a result of the limited features used for training/inference. Under normal circumstances, you would investigate other features in order to improve the model prediction.

ml_tensorflow.py

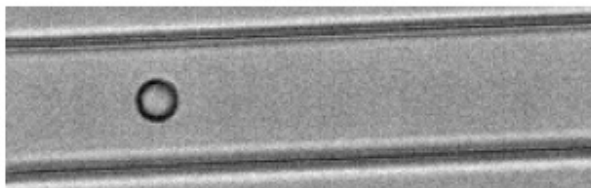
```

1  import matplotlib.pyplot as plt
2  import numpy as np
3  import tensorflow as tf
4  from dclab.ml import tf_dataset
5
6  tf.random.set_seed(42) # for reproducibility
7
8  # https://dcor.mpl.mpg.de/dataset/figshare-7771184-v2
9  dcor_ids = ["fb719fb2-bd9f-817a-7d70-f4002af916f0",
10             "f7fa778f-6abd-1b53-ae5f-9ce12601d6f8"]
11  labels = [0, 1] # 0: beads, 1: cells
12  features = ["area_ratio", "area_um", "bright_sd", "deform"]
13
14  # obtain train and test datasets

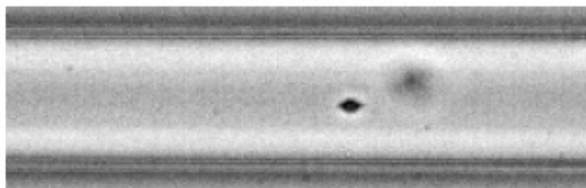
```

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bead (correct)



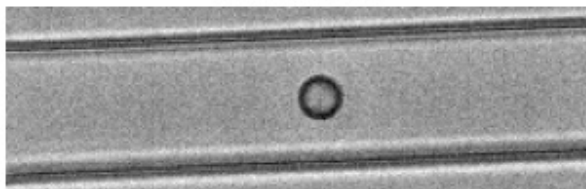
bead (wrong)



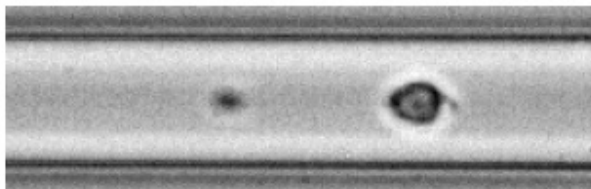
cell (correct)



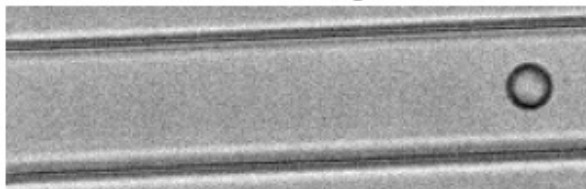
cell (wrong)



cell (correct)



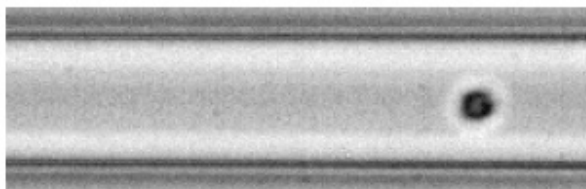
cell (wrong)



bead (correct)



bead (wrong)



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```

15 train, test = tf_dataset.assemble_tf_dataset_scalars(
16     dc_data=dcor_ids, # can also be list of paths or datasets
17     labels=labels,
18     feature_inputs=features,
19     split=.8)
20
21 # build the model
22 model = tf.keras.Sequential(
23     layers=[
24         tf.keras.layers.Input(shape=(len(features),)),
25         tf.keras.layers.Dense(128, activation='relu'),
26         tf.keras.layers.Dense(32),
27         tf.keras.layers.Dropout(0.2),
28         tf.keras.layers.Dense(2)
29     ],
30     name="scalar_features"
31 )
32
33 # fit the model to the training data
34 loss_fn = tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True)
35 model.compile(optimizer='adam', loss=loss_fn, metrics=['accuracy'])
36 model.fit(train, epochs=5)
37
38 # show accuracy using test data (loss: 0.1139 - accuracy: 0.9659)
39 model.evaluate(test, verbose=2)
40
41 # predict classes of the test data
42 probability_model = tf.keras.Sequential([model, tf.keras.layers.Softmax()])
43 y_test = np.concatenate([y for x, y in test], axis=0)
44 predict = np.argmax(probability_model.predict(test), axis=1)
45
46 # take a few exemplary events from true and false classification
47 false_cl = np.where(predict != y_test)[0]
48 true_cl = np.where(predict == y_test)[0]
49 num_events = min(4, min(len(true_cl), len(false_cl)))
50
51 false_images = tf_dataset.get_dataset_event_feature(
52     dc_data=dcor_ids,
53     feature="image",
54     tf_dataset_indices=false_cl[:num_events],
55     split_index=1,
56     split=.8)
57
58 true_images = tf_dataset.get_dataset_event_feature(
59     dc_data=dcor_ids,
60     feature="image",
61     tf_dataset_indices=true_cl[:num_events],
62     split_index=1,
63     split=.8)
64
65 fig = plt.figure(figsize=(8, 7))
66
67 for ii in range(num_events):
68     title_true = ("cell" if y_test[true_cl[ii]] else "bead") + " (correct)"
69     title_false = ("cell" if predict[false_cl[ii]] else "bead") + " (wrong)"
70     ax1 = plt.subplot(num_events, 2, 2*ii+1, title=title_true)
71     ax2 = plt.subplot(num_events, 2, 2*(ii + 1), title=title_false)

```

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```

72     ax1.axis("off")
73     ax2.axis("off")
74     ax1.imshow(true_images[ii], cmap="gray")
75     ax2.imshow(false_images[ii], cmap="gray")
76
77 plt.tight_layout()
78 plt.show()

```

3.6 ML: Creating built-in models for dclab

The *tensorflow example* already showcased a few convenience functions for machine learning implemented in dclab. In this example, we want to go even further and transform the predictions of an ML model into an *ancillary feature* (which is then globally available in dclab).

A few things are different from the other example:

- We rename `model` to `bare_model` to make a clear distinction between the actual ML model (from tensorflow) and the model wrapper (see *Using models in dclab*).
- We turn the two-class problem into a regression problem for one feature only. Consequently, the loss function changes to “binary crossentropy” and for some inexplicable reason we have to train for 20 epochs instead of the previously 5 to achieve convergence in accuracy.
- Finally, and this is the whole point of this example, we register the model as an ancillary feature and perform inference indirectly by simply accessing the `ml_score_cel` feature of the test dataset.

The plot shows the test fraction of the dataset. The x-axis is (arbitrarily) set to area. The y-axis shows the sigmoid (dclab automatically applies a sigmoid activation if it is not present in the final layer; see `dclab.ml.models.TensorflowModel.predict()`) of the model’s output logits.

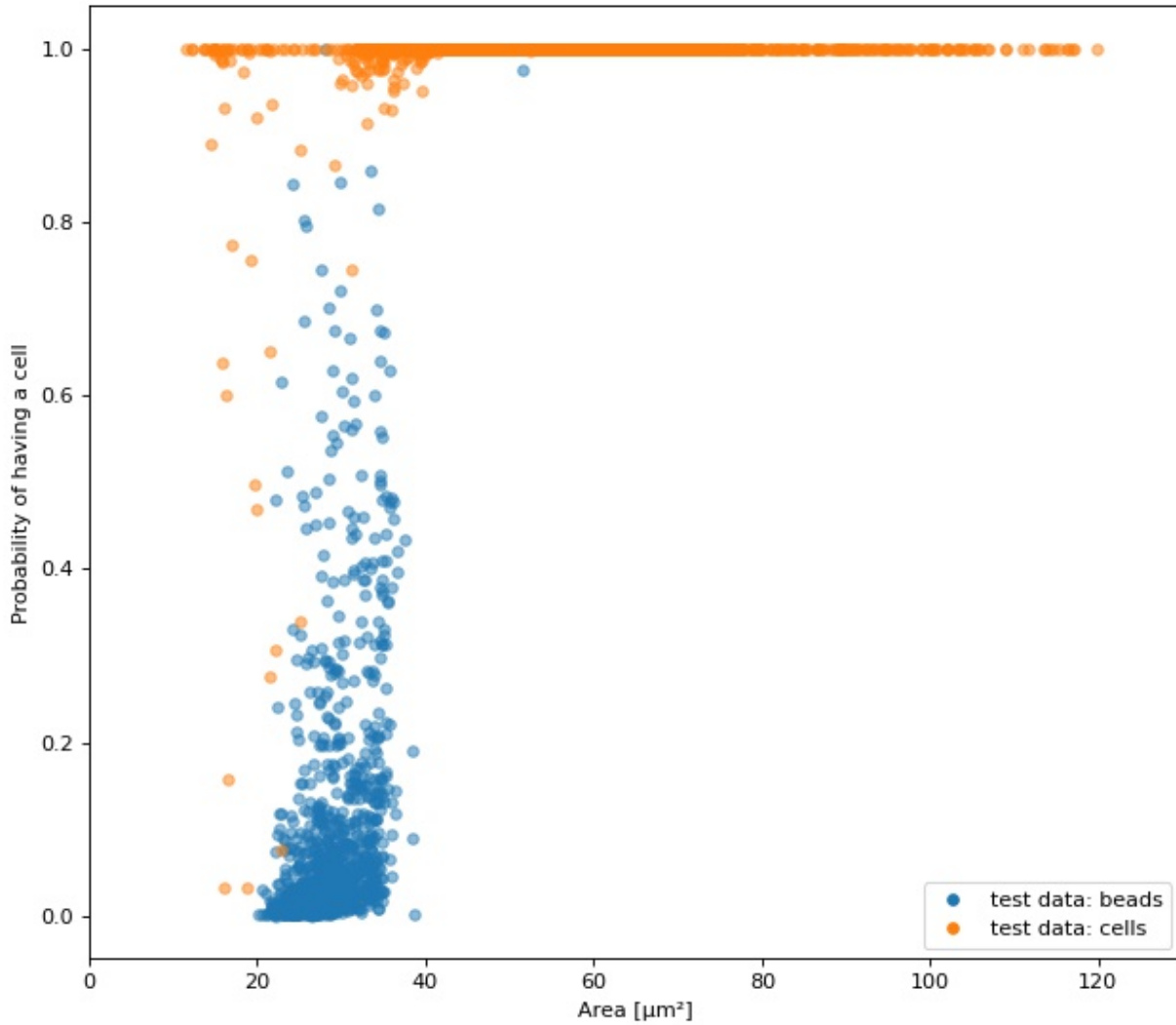
`ml_builtin.py`

```

1  import matplotlib.pyplot as plt
2  import numpy as np
3  import tensorflow as tf
4  import dclab.ml
5
6  tf.random.set_seed(42) # for reproducibility
7
8  # https://dcor.mpl.mpg.de/dataset/figshare-7771184-v2
9  dcor_ids = ["fb719fb2-bd9f-817a-7d70-f4002af916f0",
10             "f7fa778f-6abd-1b53-ae5f-9ce12601d6f8"]
11  labels = [0, 1] # 0: beads, 1: cells
12  features = ["area_ratio", "area_um", "bright_sd", "deform"]
13
14  tf_kw = {"dc_data": dcor_ids,
15          "split": .8,
16          "shuffle": True,
17          }
18
19  # obtain train and test datasets
20  train, test = dclab.ml.tf_dataset.assemble_tf_dataset_scalars(
21      labels=labels, feature_inputs=features, **tf_kw)
22
23  # build the model

```

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```

24 bare_model = tf.keras.Sequential(
25     layers=[
26         tf.keras.layers.Input(shape=(len(features),)),
27         tf.keras.layers.Dense(128),
28         tf.keras.layers.Dense(32),
29         tf.keras.layers.Dropout(0.3),
30         tf.keras.layers.Dense(1)
31     ],
32     name="scalar_features"
33 )
34
35 # fit the model to the training data
36 # Note that we did not add a "sigmoid" activation function to the
37 # final layer and are training with logits here. We also don't
38 # have to manually add it in a later step, because dclab will
39 # add it automatically (if it does not exist) before prediction.
40 loss_fn = tf.keras.losses.BinaryCrossentropy(from_logits=True)
41 bare_model.compile(optimizer='adam', loss=loss_fn, metrics=['accuracy'])
42 bare_model.fit(train, epochs=20)
43
44 # show accuracy using test data (loss: 0.0725 - accuracy: 0.9877)
45 bare_model.evaluate(test, verbose=2)
46
47 # register the ancillary feature "ml_score_cel" in dclab
48 dc_model = dclab.ml.models.TensorflowModel(
49     bare_model=bare_model,
50     inputs=features,
51     outputs=["ml_score_cel"],
52     output_labels=["Probability of having a cell"],
53     model_name="Distinguish between cells and beads",
54 )
55 dc_model.register()
56
57 # Now we are actually done already. The only thing left to do is to
58 # visualize the prediction for the test-fraction of our dataset.
59 # This involves a bit of data shuffling (obtaining the dataset indices
60 # from the "index" feature (which starts at 1 and not 0) and creating
61 # hierarchy children after applying the corresponding manual filters)
62 # which is less complicated than it looks.
63
64 # create dataset hierarchy children for bead and cell test data
65 bead_train_indices = dclab.ml.tf_dataset.get_dataset_event_feature(
66     feature="index", dc_data_indices=[0], split_index=0, **tf_kw)
67 ds_bead = dclab.new_dataset(dcor_ids[0])
68 ds_bead.filter.manual[np.array(bead_train_indices) - 1] = False
69 ds_bead.apply_filter()
70 ds_bead_test = dclab.new_dataset(ds_bead) # hierarchy child with test fraction
71
72 cell_train_indices = dclab.ml.tf_dataset.get_dataset_event_feature(
73     feature="index", dc_data_indices=[1], split_index=0, **tf_kw)
74 ds_cell = dclab.new_dataset(dcor_ids[1])
75 ds_cell.filter.manual[np.array(cell_train_indices) - 1] = False
76 ds_cell.apply_filter()
77 ds_cell_test = dclab.new_dataset(ds_cell) # hierarchy child with test fraction
78
79 fig = plt.figure(figsize=(8, 7))
80 ax = plt.subplot(111)

```

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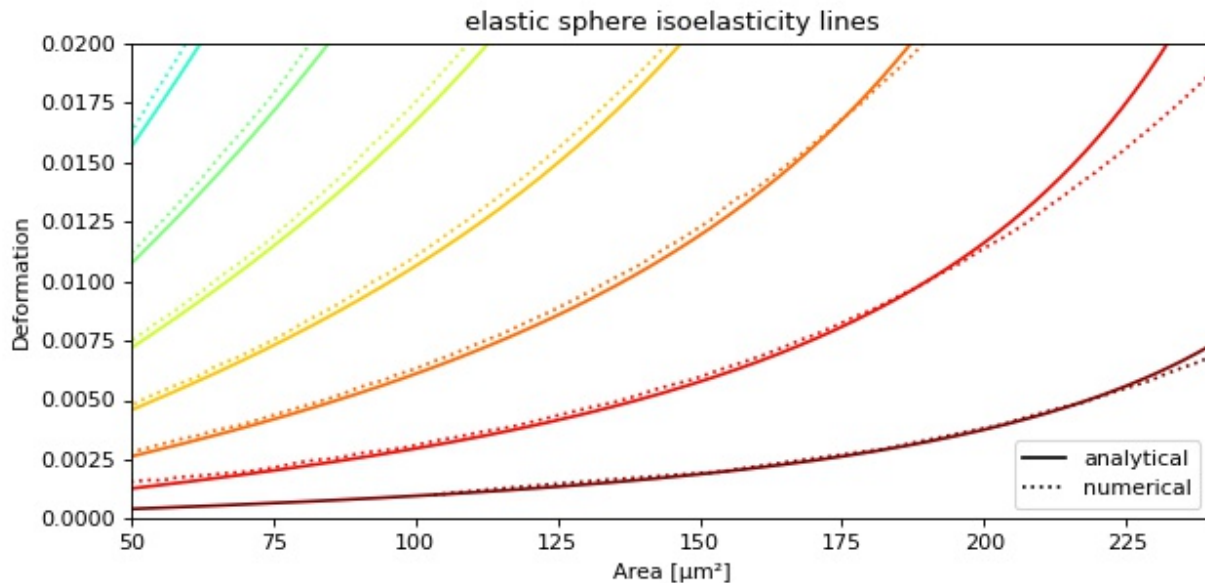
```

81 plt.plot(ds_bead_test["area_um"], ds_bead_test["ml_score_cel"], ".",
82          ms=10, alpha=.5, label="test data: beads")
83 plt.plot(ds_cell_test["area_um"], ds_cell_test["ml_score_cel"], ".",
84          ms=10, alpha=.5, label="test data: cells")
85 leg = plt.legend()
86 for lh in leg.legendHandles:
87     lh._legmarker.set_alpha(1)
88
89 ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
90 ax.set_ylabel(dclab.dfn.get_feature_label("ml_score_cel"))
91 ax.set_xlim(0, 130)
92
93 plt.tight_layout()
94 plt.show()

```

3.7 Plotting isoelastics

This example illustrates how to plot dclab isoelastics by reproducing figure 3 (lower left) of [MMM+17].



isoelastics.py

```

1  import matplotlib.pyplot as plt
2  import matplotlib.lines as mlines
3  from matplotlib import cm
4  import numpy as np
5
6  import dclab
7
8  # parameters for isoelastics
9  kwargs = {"col1": "area_um", # x-axis
10           "col2": "deform", # y-axis

```

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```

11     "channel_width": 20, # [um]
12     "flow_rate": 0.04, # [ul/s]
13     "viscosity": 15, # [mPa s]
14     "add_px_err": False # no pixelation error
15 }
16
17 isos = dclab.isoelastics.get_default()
18 analy = isos.get(method="analytical", **kwargs)
19 numer = isos.get(method="numerical", **kwargs)
20
21 plt.figure(figsize=(8, 4))
22 ax = plt.subplot(111, title="elastic sphere isoelasticity lines")
23 colors = [cm.get_cmap("jet")(x) for x in np.linspace(0, 1, len(analy))]
24 for aa, nn, cc in zip(analy, numer, colors):
25     ax.plot(aa[:, 0], aa[:, 1], color=cc)
26     ax.plot(nn[:, 0], nn[:, 1], color=cc, ls=":")
27
28 line = mlines.Line2D([], [], color='k', label='analytical')
29 dotted = mlines.Line2D([], [], color='k', ls=":", label='numerical')
30 ax.legend(handles=[line, dotted])
31
32 ax.set_xlim(50, 240)
33 ax.set_ylim(0, 0.02)
34 ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
35 ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
36
37 plt.tight_layout()
38 plt.show()

```

This section motivates the design of dclab and highlights useful built-in functionalities.

4.1 Notation

When coding with dclab, you should be aware of the following definitions and design principles.

4.1.1 Events

An event comprises all data recorded for the detection of one object (e.g. cell or bead) in an RT-DC measurement.

4.1.2 Features

A feature is a measurement parameter of an RT-DC measurement. For instance, the feature “index” enumerates all recorded events, the feature “deform” contains the deformation values of all events. There are scalar features, i.e. features that assign a single number to an event, and non-scalar features, such as “image” and “contour”. The following features are supported by dclab:

Scalar features

scalar features	description [units]
area_cvx	Convex area [px]
area_msd	Measured area [px]
area_ratio	Porosity (convex to measured area ratio)
area_um	Area [μm^2]
aspect	Aspect ratio of bounding box
bright_avg	Brightness average within contour [a.u.]

Continued on next page

Table 4.1 – continued from previous page

scalar features	description [units]
bright_sd	Brightness SD within contour [a.u.]
circ	Circularity
deform	Deformation
emodulus	Young's Modulus [kPa]
fl1_area	FL-1 area of peak [a.u.]
fl1_dist	FL-1 distance between two first peaks [μ s]
fl1_max	FL-1 maximum [a.u.]
fl1_max_ctc	FL-1 maximum, crosstalk-corrected [a.u.]
fl1_npeaks	FL-1 number of peaks
fl1_pos	FL-1 position of peak [μ s]
fl1_width	FL-1 width [μ s]
fl2_area	FL-2 area of peak [a.u.]
fl2_dist	FL-2 distance between two first peaks [μ s]
fl2_max	FL-2 maximum [a.u.]
fl2_max_ctc	FL-2 maximum, crosstalk-corrected [a.u.]
fl2_npeaks	FL-2 number of peaks
fl2_pos	FL-2 position of peak [μ s]
fl2_width	FL-2 width [μ s]
fl3_area	FL-3 area of peak [a.u.]
fl3_dist	FL-3 distance between two first peaks [μ s]
fl3_max	FL-3 maximum [a.u.]
fl3_max_ctc	FL-3 maximum, crosstalk-corrected [a.u.]
fl3_npeaks	FL-3 number of peaks
fl3_pos	FL-3 position of peak [μ s]
fl3_width	FL-3 width [μ s]
frame	Video frame number
g_force	Gravitational force in multiples of g
index	Event index (Dataset)
index_online	Event index (Online)
inert_ratio_cvx	Inertia ratio of convex contour
inert_ratio_prnc	Principal inertia ratio of raw contour
inert_ratio_raw	Inertia ratio of raw contour
ml_class	Most probable ML class
nevents	Total number of events in the same image
pc1	Principal component 1
pc2	Principal component 2
pos_x	Position along channel axis [μ m]
pos_y	Position lateral in channel [μ m]
size_x	Bounding box size x [μ m]
size_y	Bounding box size y [μ m]
temp	Chip temperature [$^{\circ}$ C]
temp_amb	Ambient temperature [$^{\circ}$ C]
tilt	Absolute tilt of raw contour
time	Event time [s]
userdef0	User defined 0
userdef1	User defined 1
userdef2	User defined 2
userdef3	User defined 3
userdef4	User defined 4

Continued on next page

Table 4.1 – continued from previous page

scalar features	description [units]
userdef5	User defined 5
userdef6	User defined 6
userdef7	User defined 7
userdef8	User defined 8
userdef9	User defined 9
volume	Volume [μm^3]

In addition to these scalar features, it is possible to define a large number of features dedicated to machine-learning, the “ml_score_???” features: The “?” can be a digit or a lower-case letter of the alphabet, e.g. “ml_score_rbc” or “ml_score_3a3”. If “ml_score_???” features are defined, then the ancillary “ml_class” feature, which identifies the most-probable feature for each event, becomes available.

Non-scalar features

non-scalar features	description [units]
contour	Binary event contour image
image	Gray scale event image
image_bg	Gray scale event background image
mask	Binary region labeling the event in the image
trace	Dictionary of fluorescence traces

Examples

deformation vs. area plot

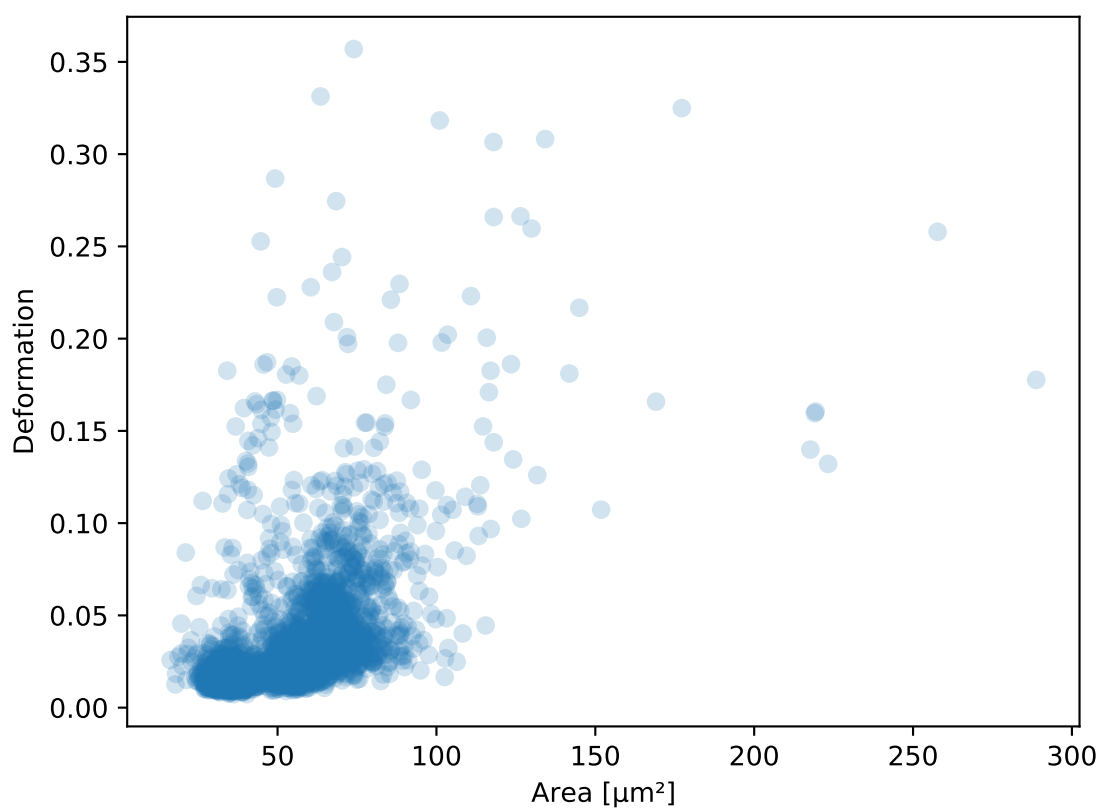
```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
ax = plt.subplot(111)
ax.plot(ds["area_um"], ds["deform"], "o", alpha=.2)
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
plt.show()
```

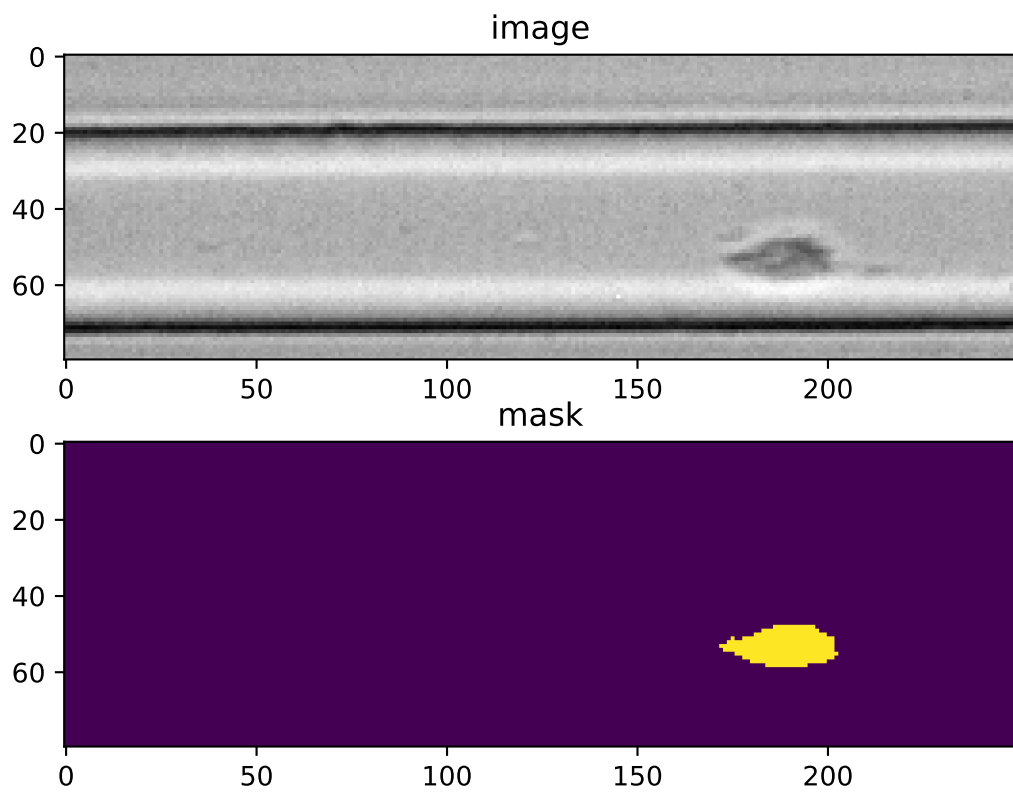
event image plot

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example_video.rtdc")
ax1 = plt.subplot(211, title="image")
ax2 = plt.subplot(212, title="mask")
ax1.imshow(ds["image"][6], cmap="gray")
ax2.imshow(ds["mask"][6])
```

4.1.3 Ancillary features

Not all features available in dclab are recorded online during the acquisition of the experimental dataset. Some of the features are computed offline by dclab, such as “volume”, “emodulus”, or scores from imported machine learning models (“ml_score_xxx”). These ancillary features are computed on-the-fly and are made available seamlessly through the same interface.





4.1.4 Filters

A filter can be used to gate events using features. There are min/max filters and 2D *polygon filters*. The following table defines the main filtering parameters:

filtering	parsed	description [units]
enable filters	<i>fbool</i>	Enable filtering
hierarchy parent	<i>str</i>	Hierarchy parent of the dataset
limit events	<i>fint</i>	Upper limit for number of filtered events
polygon filters	<i>fintlist</i>	Polygon filter indices
remove invalid events	<i>fbool</i>	Remove events with inf/nan values

Min/max filters are also defined in the *filters* section:

filtering	explanation
area_um min	Exclude events with area [μm^2] below this value
area_um max	Exclude events with area [μm^2] above this value
aspect max	Exclude events with an aspect ratio above this value
...	...

Examples

excluding events with large deformation

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")

ds.config["filtering"]["deform min"] = 0
ds.config["filtering"]["deform max"] = .1
ds.apply_filter()
dif = ds.filter.all

f, axes = plt.subplots(1, 2, sharex=True, sharey=True)
axes[0].plot(ds["area_um"], ds["bright_avg"], "o", alpha=.2)
axes[0].set_title("unfiltered")
axes[1].plot(ds["area_um"][dif], ds["bright_avg"][dif], "o", alpha=.2)
axes[1].set_title("Deformation <= 0.1")

for ax in axes:
    ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
    ax.set_ylabel(dclab.dfn.get_feature_label("bright_avg"))

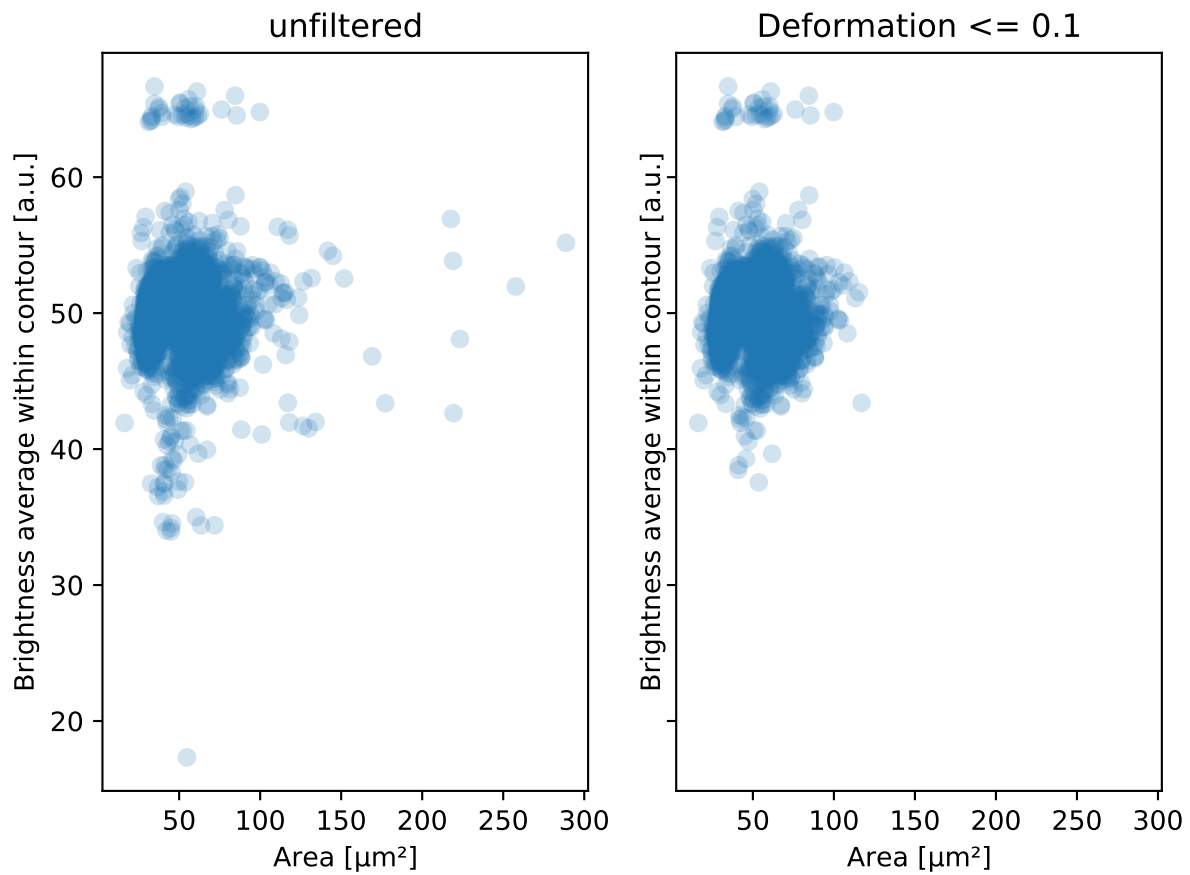
plt.tight_layout()
plt.show()
```

excluding random events

This is useful if you need to have a (sub-)dataset of a specified size. The downsampling is reproducible (the same points are excluded).

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
```

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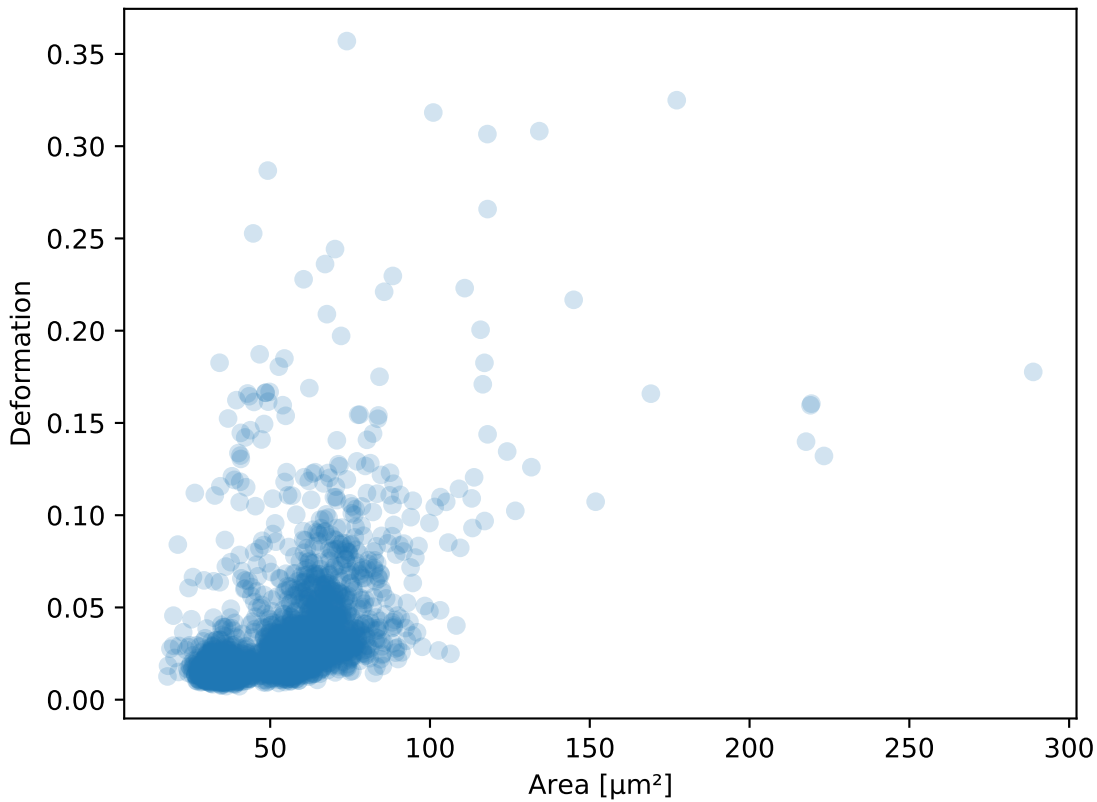
(continued from previous page)

```

ds.config["filtering"]["limit events"] = 4000
ds.apply_filter()
fid = ds.filter.all

ax = plt.subplot(111)
ax.plot(ds["area_um"][fid], ds["deform"][fid], "o", alpha=.2)
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
plt.show()

```



4.1.5 Experiment metadata

Every RT-DC measurement has metadata consisting of key-value-pairs. The following are supported:

experiment	parsed	description [units]
date	<i>str</i>	Date of measurement ('YYYY-MM-DD')
event count	<i>fint</i>	Number of recorded events
run index	<i>fint</i>	Index of measurement run
sample	<i>str</i>	Measured sample or user-defined reference
time	<i>str</i>	Start time of measurement ('HH:MM:SS[.S]')

fluorescence	parsed	description [units]
bit depth	<i>fint</i>	Trace bit depth
channel 1 name	<i>str</i>	FL1 description
channel 2 name	<i>str</i>	FL2 description
channel 3 name	<i>str</i>	FL3 description
channel count	<i>fint</i>	Number of active channels
channels installed	<i>fint</i>	Number of available channels
laser 1 lambda	<i>float</i>	Laser 1 wavelength [nm]
laser 1 power	<i>float</i>	Laser 1 output power [%]
laser 2 lambda	<i>float</i>	Laser 2 wavelength [nm]
laser 2 power	<i>float</i>	Laser 2 output power [%]
laser 3 lambda	<i>float</i>	Laser 3 wavelength [nm]
laser 3 power	<i>float</i>	Laser 3 output power [%]
laser count	<i>fint</i>	Number of active lasers
lasers installed	<i>fint</i>	Number of available lasers
sample rate	<i>float</i>	Trace sample rate [Hz]
samples per event	<i>fint</i>	Samples per event
signal max	<i>float</i>	Upper voltage detection limit [V]
signal min	<i>float</i>	Lower voltage detection limit [V]
trace median	<i>fint</i>	Rolling median filter size for traces

fmt_tdms	parsed	description [units]
video frame offset	<i>fint</i>	Missing events at beginning of video

imaging	parsed	description [units]
flash device	<i>str</i>	Light source device type
flash duration	<i>float</i>	Light source flash duration [μ s]
frame rate	<i>float</i>	Imaging frame rate [Hz]
pixel size	<i>float</i>	Pixel size [μ m]
roi position x	<i>float</i>	Image x coordinate on sensor [px]
roi position y	<i>float</i>	Image y coordinate on sensor [px]
roi size x	<i>fint</i>	Image width [px]
roi size y	<i>fint</i>	Image height [px]

online_contour	parsed	description [units]
bin area min	<i>fint</i>	Minium pixel area of binary image event
bin kernel	<i>fint</i>	Odd ellipse kernel size, binary image morphing
bin threshold	<i>fint</i>	Binary threshold for avg-bg-corrected image
image blur	<i>fint</i>	Odd sigma for Gaussian blur (21x21 kernel)
no absdiff	<i>fbool</i>	Avoid OpenCV ‘absdiff’ for avg-bg-correction

online_filter	parsed	description [units]
area_ratio max	float	Maximum porosity
area_ratio min	float	Minimum porosity
area_ratio soft limit	fbool	Soft limit, porosity
area_um max	float	Maximum area [μm^2]
area_um min	float	Minimum area [μm^2]
area_um soft limit	fbool	Soft limit, area [μm^2]
aspect max	float	Maximum aspect ratio of bounding box
aspect min	float	Minimum aspect ratio of bounding box
aspect soft limit	fbool	Soft limit, aspect ratio of bbox
deform max	float	Maximum deformation
deform min	float	Minimum deformation
deform soft limit	fbool	Soft limit, deformation
fl1_max max	float	Maximum FL-1 maximum [a.u.]
fl1_max min	float	Minimum FL-1 maximum [a.u.]
fl1_max soft limit	fbool	Soft limit, FL-1 maximum
fl2_max max	float	Maximum FL-2 maximum [a.u.]
fl2_max min	float	Minimum FL-2 maximum [a.u.]
fl2_max soft limit	fbool	Soft limit, FL-2 maximum
fl3_max max	float	Maximum FL-3 maximum [a.u.]
fl3_max min	float	Minimum FL-3 maximum [a.u.]
fl3_max soft limit	fbool	Soft limit, FL-3 maximum
size_x max	fint	Maximum bounding box size x [μm]
size_x min	fint	Minimum bounding box size x [μm]
size_x soft limit	fbool	Soft limit, bounding box size x
size_y max	fint	Maximum bounding box size y [μm]
size_y min	fint	Minimum bounding box size y [μm]
size_y soft limit	fbool	Soft limit, bounding box size y
target duration	float	Target measurement duration [min]
target event count	fint	Target event count for online gating

setup	parsed	description [units]
channel width	float	Width of microfluidic channel [μm]
chip region	lcstr	Imaged chip region (channel or reservoir)
flow rate	float	Flow rate in channel [$\mu\text{L/s}$]
flow rate sample	float	Sample flow rate [$\mu\text{L/s}$]
flow rate sheath	float	Sheath flow rate [$\mu\text{L/s}$]
identifier	str	Unique setup identifier
medium	str	Medium used
module composition	str	Comma-separated list of modules used
software version	str	Acquisition software with version
temperature	float	Mean chip temperature [$^{\circ}\text{C}$]

Example: date and time of a measurement

```
In [1]: import dclab

In [2]: ds = dclab.new_dataset("data/example.rtdc")

In [3]: ds.config["experiment"]["date"], ds.config["experiment"]["time"]
Out[3]: ('2017-07-16', '19:01:36')
```

4.1.6 Analysis metadata

In addition to metadata, dclab also supports a user-defined analysis configuration which is usually part of a specific analysis pipeline and thus not considered to be experimental metadata.

calculation	parsed	description [units]
crosstalk fl12	float	Fluorescence crosstalk, channel 1 to 2
crosstalk fl13	float	Fluorescence crosstalk, channel 1 to 3
crosstalk fl21	float	Fluorescence crosstalk, channel 2 to 1
crosstalk fl23	float	Fluorescence crosstalk, channel 2 to 3
crosstalk fl31	float	Fluorescence crosstalk, channel 3 to 1
crosstalk fl32	float	Fluorescence crosstalk, channel 3 to 2
emodulus medium	str	Medium used (e.g. CellCarrierB, water)
emodulus model	lcstr	Model for computing elastic moduli
emodulus temperature	float	Chip temperature [°C]
emodulus viscosity	float	Viscosity [Pa*s] if 'medium' unknown

4.2 RT-DC datasets

Knowing and understanding the *RT-DC dataset classes* is an important prerequisite when working with dclab. They are all derived from *RTDCBase* which gives access to features with a dictionary-like interface, facilitates data export or filtering, and comes with several convenience methods that are useful for data visualization. RT-DC datasets can be based on a data file format (*RTDC_TDMS* and *RTDC_HDF5*), accessed from an online repository (*RTDC_HDF5*), created from user-defined dictionaries (*RTDC_Dict*), or derived from other RT-DC datasets (*RTDC_Hierarchy*).

4.2.1 Basic usage

The convenience function `dclab.new_dataset()` takes care of determining the data format and returns the corresponding derived class.

```
In [1]: import dclab

In [2]: ds = dclab.new_dataset("data/example.rtdc")

In [3]: ds.__class__.__name__
Out[3]: 'RTDC_HDF5'
```

Working with other data

It is also possible to load other data into dclab from a dictionary.

```
In [4]: data = dict(deform=np.random.rand(100),
...:                area_um=np.random.rand(100))
...:

In [5]: ds_dict = dclab.new_dataset(data)

In [6]: ds_dict.__class__.__name__
Out[6]: 'RTDC_Dict'
```

Using filters

Filters are used to mask e.g. debris or doublets from a dataset.

```
# Restrict the deformation to 0.15
In [7]: ds.config["filtering"]["deform min"] = 0

In [8]: ds.config["filtering"]["deform max"] = .15

# Manually excluding events using array indices is also possible:
# `ds.filter.manual` is a 1D boolean array of size `len(ds)`
# where `False` values mean that the events are excluded.
In [9]: ds.filter.manual[[0, 400, 345, 1000]] = False

In [10]: ds.apply_filter()

# The boolean array `ds.filter.all` represents the applied filter
# and can be used for indexing.
In [11]: ds["deform"].mean(), ds["deform"][ds.filter.all].mean()
Out[11]: (0.0287258, 0.026486598)
```

Note that `ds.apply_filter()` must be called, otherwise `ds.filter.all` will not be updated.

Creating hierarchies

When applying filtering operations, it is sometimes helpful to use hierarchies for keeping track of the individual filtering steps.

```
In [12]: child = dclab.new_dataset(ds)

In [13]: child.config["filtering"]["area_um min"] = 0

In [14]: child.config["filtering"]["area_um max"] = 80

In [15]: grandchild = dclab.new_dataset(child)

In [16]: grandchild.apply_filter()

In [17]: len(ds), len(child), len(grandchild)
Out[17]: (5000, 4933, 4778)

In [18]: ds.filter.all.sum(), child.filter.all.sum(), grandchild.filter.all.sum()
Out[18]: (4933, 4778, 4778)
```

Note that calling `grandchild.apply_filter()` automatically calls `child.apply_filter()` and `ds.apply_filter()`. Also note that, as expected, the size of each hierarchy child is identical to the sum of the boolean filtering array from its hierarchy parent.

Scripting goodies

Here are a few useful functionalities for scripting with dclab.

```
# unique identifier of the RTDCBase instance (not reproducible)
In [19]: ds.identifier
Out[19]: 'mm-hdf5_3d641b9'
```

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```
# reproducible hash of the dataset
In [20]: ds.hash
Out [20]: '8ff19f702a236cbf91e13667e144e722'

# dataset format
In [21]: ds.format
Out [21]: 'hdf5'

# available features
In [22]: ds.features
Out [22]:
['area_cvx',
 'area_msd',
 'area_ratio',
 'area_um',
 'aspect',
 'bright_avg',
 'bright_sd',
 'circ',
 'deform',
 'frame',
 'index',
 'inert_ratio_cvx',
 'inert_ratio_raw',
 'nevents',
 'pos_x',
 'pos_y',
 'size_x',
 'size_y',
 'time']

# available scalar features
In [23]: ds.features_scalar
Out [23]:
['area_cvx',
 'area_msd',
 'area_ratio',
 'area_um',
 'aspect',
 'bright_avg',
 'bright_sd',
 'circ',
 'deform',
 'frame',
 'index',
 'inert_ratio_cvx',
 'inert_ratio_raw',
 'nevents',
 'pos_x',
 'pos_y',
 'size_x',
 'size_y',
 'time']

# test feature availability (success)
In [24]: "area_um" in ds
```

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```

Out[24]: True

# test feature availability (failure)
In [25]: "image" in ds
Out[25]: False

# accessing a feature and computing its mean
In [26]: ds["area_um"].mean()
Out[26]: 49.728645

# accessing the measurement configuration
In [27]: ds.config.keys()
Out[27]: dict_keys(['filtering', 'experiment', 'imaging', 'online_contour', 'setup'])

In [28]: ds.config["experiment"]
Out[28]:
{'date': '2017-07-16',
 'event count': 5000,
 'run index': 1,
 'sample': 'docs-data',
 'time': '19:01:36'}

# determine the identifier of the hierarchy parent
In [29]: child.config["filtering"]["hierarchy parent"]
Out[29]: 'mm-hdf5_3d641b9'

```

4.2.2 Statistics

The *statistics* module comes with a predefined set of methods to compute simple feature statistics.

```

In [30]: import dclab

In [31]: ds = dclab.new_dataset("data/example.rtdc")

In [32]: stats = dclab.statistics.get_statistics(ds,
.....:                                     features=["deform", "aspect"],
.....:                                     methods=["Mode", "Mean", "SD"])
.....:

In [33]: dict(zip(*stats))
Out[33]:
{'Mode Deformation': 0.016635261,
 'Mean Deformation': 0.0287258,
 'SD Deformation': 0.028740086,
 'Mode Aspect ratio of bounding box': 1.1091421916433233,
 'Mean Aspect ratio of bounding box': 1.2719607587337494,
 'SD Aspect ratio of bounding box': 0.2523385371130096}

```

Note that the statistics take into account the applied filters:

```

In [34]: ds.config["filtering"]["deform min"] = 0

In [35]: ds.config["filtering"]["deform max"] = .1

In [36]: ds.apply_filter()

```

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```
In [37]: stats2 = dclab.statistics.get_statistics(ds,
.....:                                     features=["deform", "aspect"],
.....:                                     methods=["Mode", "Mean", "SD"])
.....:

In [38]: dict(zip(*stats2))
Out[38]: {'Mode Deformation': 0.017006295,
'Mean Deformation': 0.02476519,
'SD Deformation': 0.015638638,
'Mode Aspect ratio of bounding box': 1.1232223188589807,
'Mean Aspect ratio of bounding box': 1.240720618624576,
'SD Aspect ratio of bounding box': 0.15993707940243287}
```

These are the available statistics methods:

```
In [39]: dclab.statistics.Statistics.available_methods.keys()
Out[39]: dict_keys(['Mean', 'Median', 'Mode', 'SD', 'Events', '%-gated', 'Flow rate'])
```

4.2.3 Export

The *RTDCBase* class has the attribute *RTDCBase.export* which allows to export event data to several data file formats. See *export* for more information.

```
In [40]: ds.export.tsv(path="export_example.tsv",
.....:                 features=["area_um", "deform"],
.....:                 filtered=True,
.....:                 override=True)
.....:

In [41]: ds.export.hdf5(path="export_example.rtdc",
.....:                  features=["area_um", "aspect", "deform"],
.....:                  filtered=True,
.....:                  override=True)
.....:
```

Note that data exported as HDF5 files can be loaded with dclab (reproducing the previously computed statistics - without filters).

```
In [42]: ds2 = dclab.new_dataset("export_example.rtdc")

In [43]: ds2["deform"].mean()
Out[43]: 0.02476519
```

4.3 Scatter plots

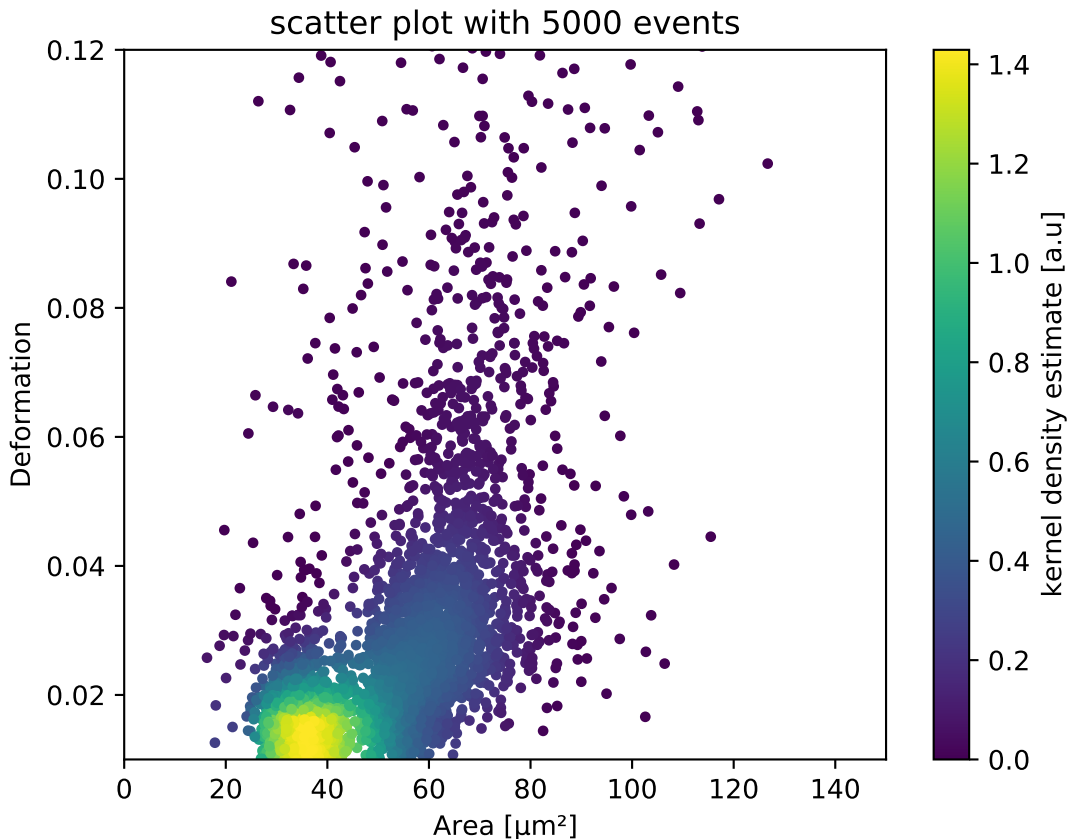
For data visualization, dclab comes with predefined *kernel density estimators (KDEs)* and an *event downsampling* module. The functionalities of both modules are made available directly via the *RTDCBase* class.

4.3.1 KDE scatter plot

The KDE of the events in a 2D scatter plot can be used to colorize events according to event density using the `RTDCBase.get_kde_scatter` function.

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
kde = ds.get_kde_scatter(xax="area_um", yax="deform")

ax = plt.subplot(111, title="scatter plot with {} events".format(len(kde)))
sc = ax.scatter(ds["area_um"], ds["deform"], c=kde, marker=".")
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
ax.set_xlim(0, 150)
ax.set_ylim(0.01, 0.12)
plt.colorbar(sc, label="kernel density estimate [a.u]")
plt.show()
```

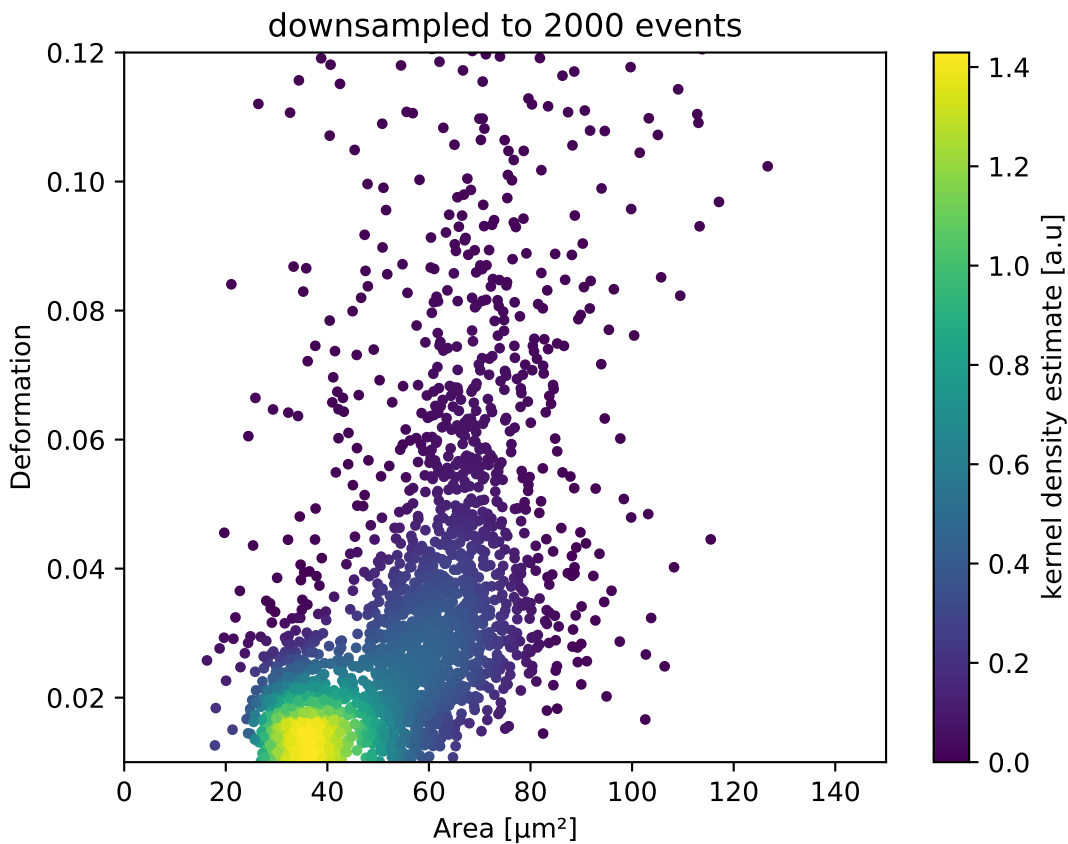


4.3.2 KDE scatter plot with event-density-based downsampling

To reduce the complexity of the plot (e.g. when exporting to scalable vector graphics (.svg)), the plotted events can be downsampled by removing events from high-event-density regions. The number of events plotted is reduced but the resulting visualization is almost indistinguishable from the one above.

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
xsamp, ysamp = ds.get_downsampled_scatter(xax="area_um", yax="deform",
↳downsample=2000)
kde = ds.get_kde_scatter(xax="area_um", yax="deform", positions=(xsamp, ysamp))

ax = plt.subplot(111, title="downsampled to {} events".format(len(kde)))
sc = ax.scatter(xsamp, ysamp, c=kde, marker=".")
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
ax.set_xlim(0, 150)
ax.set_ylim(0.01, 0.12)
plt.colorbar(sc, label="kernel density estimate [a.u]")
plt.show()
```



4.3.3 KDE estimate on a log-scale

Frequently, data is visualized on logarithmic scales. If the KDE is computed on a linear scale, then the result will look unaesthetic when plotted on a logarithmic scale. Therefore, the methods `get_downsampled_scatter`, `get_kde_contour`, and `get_kde_scatter` offer the keyword arguments `xscale` and `yscale` which can be set to “log” for prettier plots.

```

import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
kde_lin = ds.get_kde_scatter(xax="area_um", yax="deform", yscale="linear")
kde_log = ds.get_kde_scatter(xax="area_um", yax="deform", yscale="log")

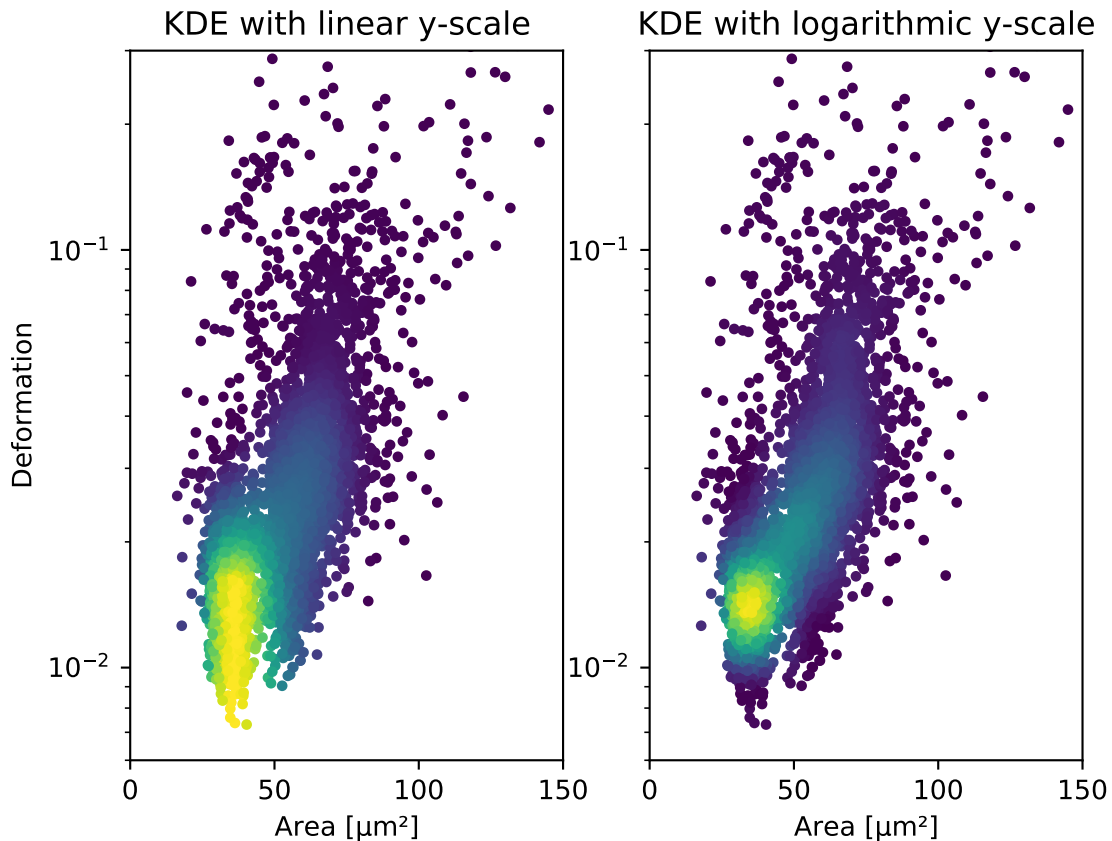
ax1 = plt.subplot(121, title="KDE with linear y-scale")
sc1 = ax1.scatter(ds["area_um"], ds["deform"], c=kde_lin, marker=".")

ax2 = plt.subplot(122, title="KDE with logarithmic y-scale")
sc2 = ax2.scatter(ds["area_um"], ds["deform"], c=kde_log, marker=".")

ax1.set_ylabel(dclab.dfn.get_feature_label("deform"))
for ax in [ax1, ax2]:
    ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
    ax.set_xlim(0, 150)
    ax.set_ylim(6e-3, 3e-1)
    ax.set_yscale("log")

plt.show()

```



4.3.4 Isoelasticity lines

In addition, dclab comes with predefined isoelasticity lines that are commonly used to identify events with similar elastic moduli. Isoelasticity lines are available via the *isoelastics* module.

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
kde = ds.get_kde_scatter(xax="area_um", yax="deform")

isodef = dclab.isoelastics.get_default()
iso = isodef.get_with_rtdcbase(method="numerical",
                              col1="area_um",
                              col2="deform",
                              dataset=ds)

ax = plt.subplot(111, title="isoelastics")
for ss in iso:
    ax.plot(ss[:, 0], ss[:, 1], color="gray", zorder=1)
sc = ax.scatter(ds["area_um"], ds["deform"], c=kde, marker=".", zorder=2)
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
ax.set_xlim(0, 150)
ax.set_ylim(0.01, 0.12)
plt.colorbar(sc, label="kernel density estimate [a.u]")
plt.show()
```

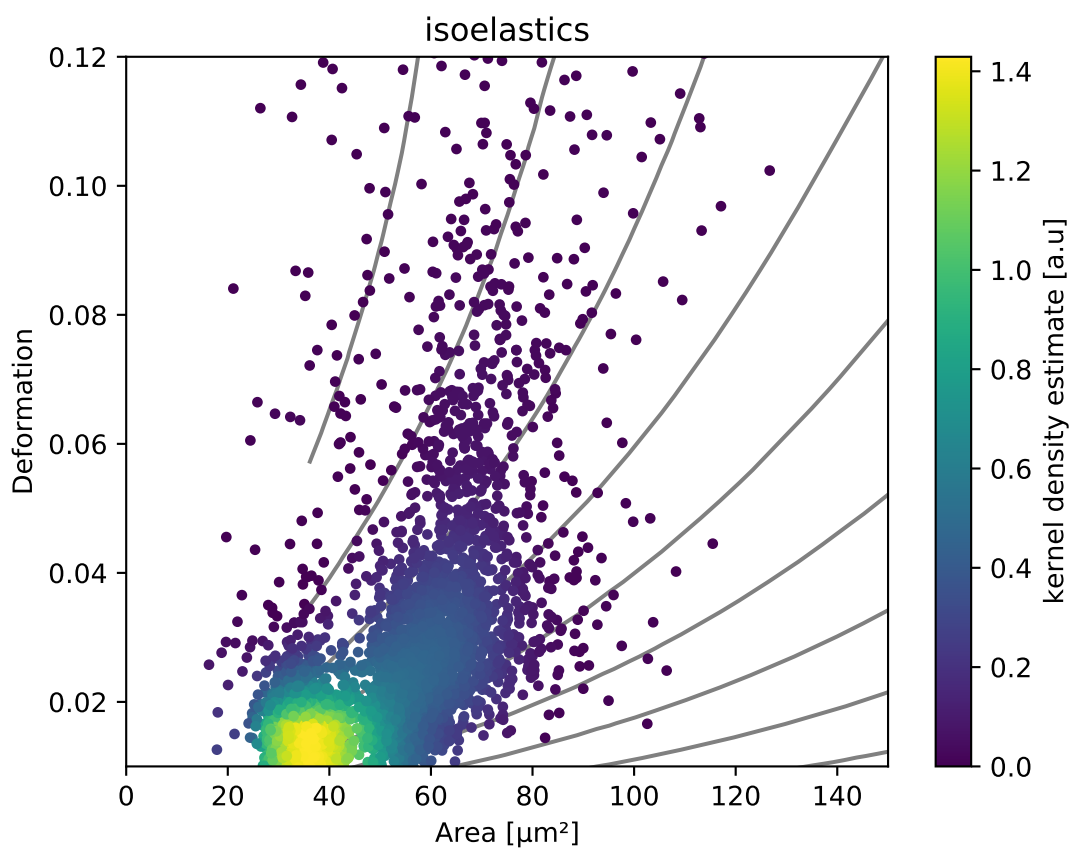
4.3.5 Contour plot with percentiles

Contour plots are commonly used to compare the kernel density between measurements. Kernel density estimates (on a grid) for contour plots can be computed with the function *RTDCBase.get_kde_contour*. In addition, it is possible to compute contours at data percentiles using *dclab.kde_contours.get_quantile_levels()*.

```
import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")
X, Y, Z = ds.get_kde_contour(xax="area_um", yax="deform")
Z /= Z.max()
quantiles = [.1, .5, .75]
levels = dclab.kde_contours.get_quantile_levels(density=Z,
                                                x=X,
                                                y=Y,
                                                xp=ds["area_um"],
                                                yp=ds["deform"],
                                                q=quantiles,
                                                )

ax = plt.subplot(111, title="contour lines")
sc = ax.scatter(ds["area_um"], ds["deform"], c="lightgray", marker=".", zorder=1)
cn = ax.contour(X, Y, Z,
               levels=levels,
               linestyles=["--", "-", "-"],
               colors=["blue", "blue", "darkblue"],
               linewidths=[2, 2, 3],
               zorder=2)
```

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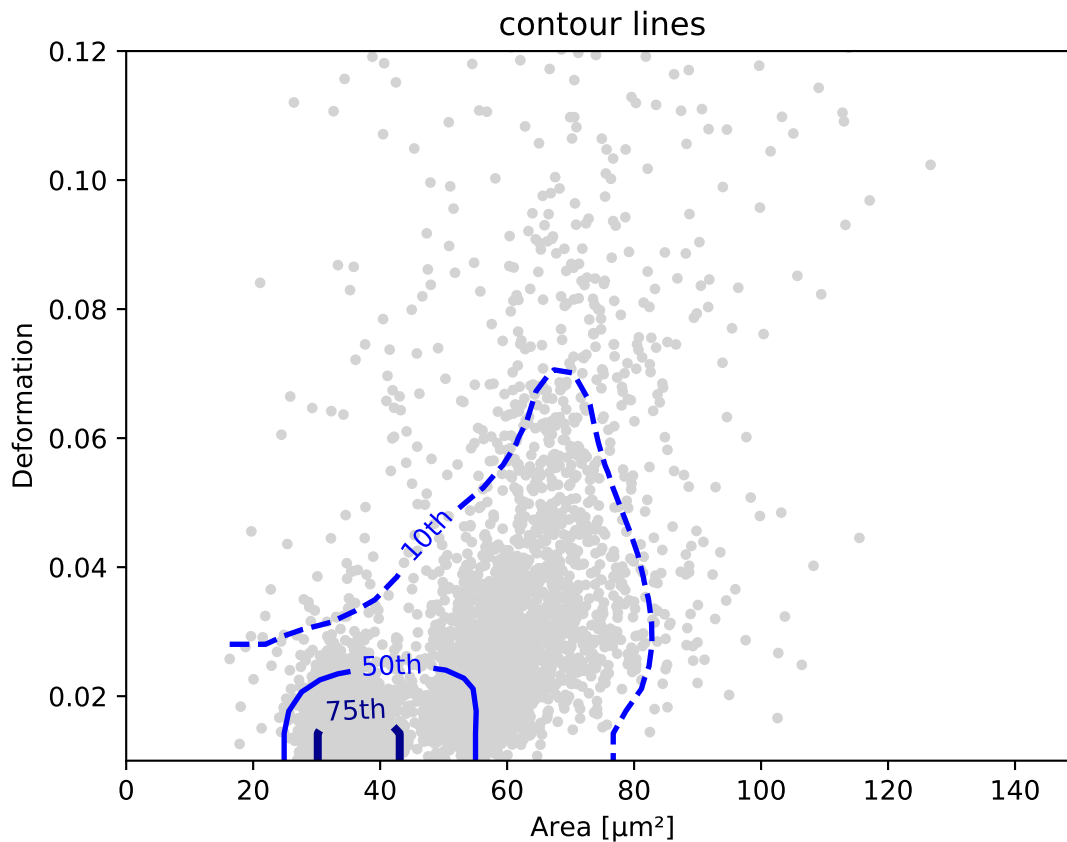


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```

ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
ax.set_xlim(0, 150)
ax.set_ylim(0.01, 0.12)
# label contour lines with percentiles
fmt = {}
for l, q in zip(levels, quantiles):
    fmt[l] = "{:.0f}th".format(q*100)
plt.clabel(cn, fmt=fmt)
plt.show()

```



Note that you may compute (and plot) the contour lines directly yourself using the function `dclab.kde_contours.find_contours_level()`.

4.3.6 Polygon filters / Shape-Out

Keep in mind that you can combine your dclab analysis pipeline with [Shape-Out](#). For instance, you can create and export *polygon filters* in Shape-Out and then import them in dclab.

```

import matplotlib.pyplot as plt
import dclab
ds = dclab.new_dataset("data/example.rtdc")

```

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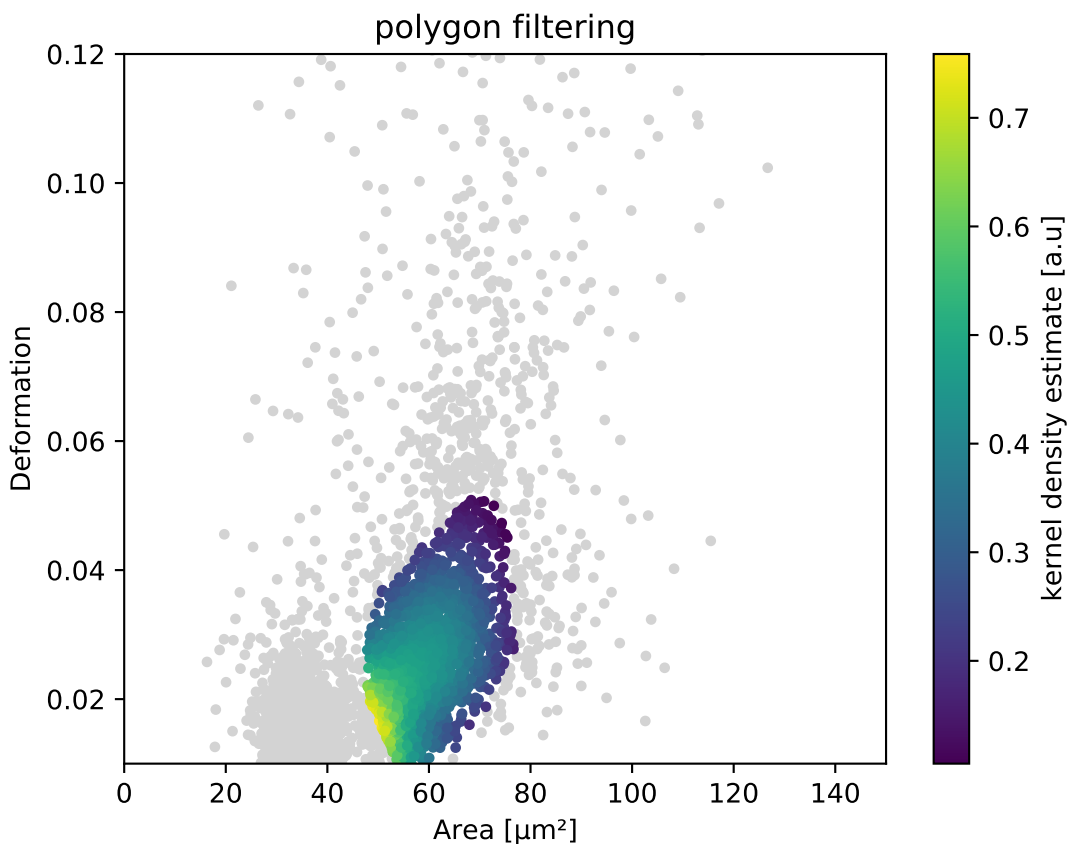
(continued from previous page)

```

kde = ds.get_kde_scatter(xax="area_um", yax="deform")
# load and apply polygon filter from file
pf = dclab.PolygonFilter(filename="data/example.poly")
ds.polygon_filter_add(pf)
ds.apply_filter()
# valid events
val = ds.filter.all

ax = plt.subplot(111, title="polygon filtering")
ax.scatter(ds["area_um"][~val], ds["deform"][~val], c="lightgray", marker=".")
sc = ax.scatter(ds["area_um"][val], ds["deform"][val], c=kde[val], marker=".")
ax.set_xlabel(dclab.dfn.get_feature_label("area_um"))
ax.set_ylabel(dclab.dfn.get_feature_label("deform"))
ax.set_xlim(0, 150)
ax.set_ylim(0.01, 0.12)
plt.colorbar(sc, label="kernel density estimate [a.u]")
plt.show()

```



4.4 Fluorescence traces

In RT-FDC, fluorescence data are stored alongside the regular image and scalar features. The fluorescence data consist of the trace data (fluorescence signal over time) and several scalar features (maximum, peak position, peak width,

etc.) for each fluorescence channel. The trace data are stored as *raw* and *median-filtered* traces, where *median-filtered* means that the *raw* data is filtered with a rolling median filter.

```
In [1]: import dclab

In [2]: ds = dclab.new_dataset("data/example_traces.rtdc")

# list the available traces in the dataset
In [3]: sorted(ds["trace"].keys())
Out[3]: ['fl1_median', 'fl1_raw', 'fl2_median', 'fl2_raw', 'fl3_median', 'fl3_raw']

# show fluorescence meta data
In [4]: ds.config["fluorescence"]
Out[4]:
{'bit depth': 16,
 'channel 1 name': '525/50',
 'channel 2 name': '593/46',
 'channel 3 name': '700/75',
 'channel count': 3,
 'channels installed': 3,
 'laser 1 lambda': 488.0,
 'laser 1 power': 8.0,
 'laser 3 lambda': 640.0,
 'laser 3 power': 100.0,
 'laser count': 2,
 'lasers installed': 3,
 'sample rate': 312500.0,
 'samples per event': 177,
 'signal max': 1.0,
 'signal min': -1.0,
 'trace median': 0}
```

Please note that the value of `trace median` is zero (no median filter applied), which tells us that the values of the *raw* and *median* trace data are identical. The example dataset is an excerpt from the [calibration beads dataset](#), with a total of three fluorescence channels used.

```
import matplotlib.pyplot as plt
import dclab

ds = dclab.new_dataset("data/example_traces.rtdc")
# event index to plot
idx = 8
# measuring time
samples = ds.config["fluorescence"]["samples per event"]
sample_rate = ds.config["fluorescence"]["sample rate"]
t = np.arange(samples) / sample_rate * 1e6

fig, axes = plt.subplots(nrows=3, sharex=True, sharey=True)

# fluorescence traces (colors manually chosen to represent filter set)
axes[0].plot(t, ds["trace"]["fl1_median"][idx], color="#16A422",
             label=ds.config["fluorescence"]["channel 1 name"])
axes[1].plot(t, ds["trace"]["fl2_median"][idx], color="#CE9720",
             label=ds.config["fluorescence"]["channel 2 name"])
axes[2].plot(t, ds["trace"]["fl3_median"][idx], color="#CE2026",
             label=ds.config["fluorescence"]["channel 3 name"])

# detected peak widths
```

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```

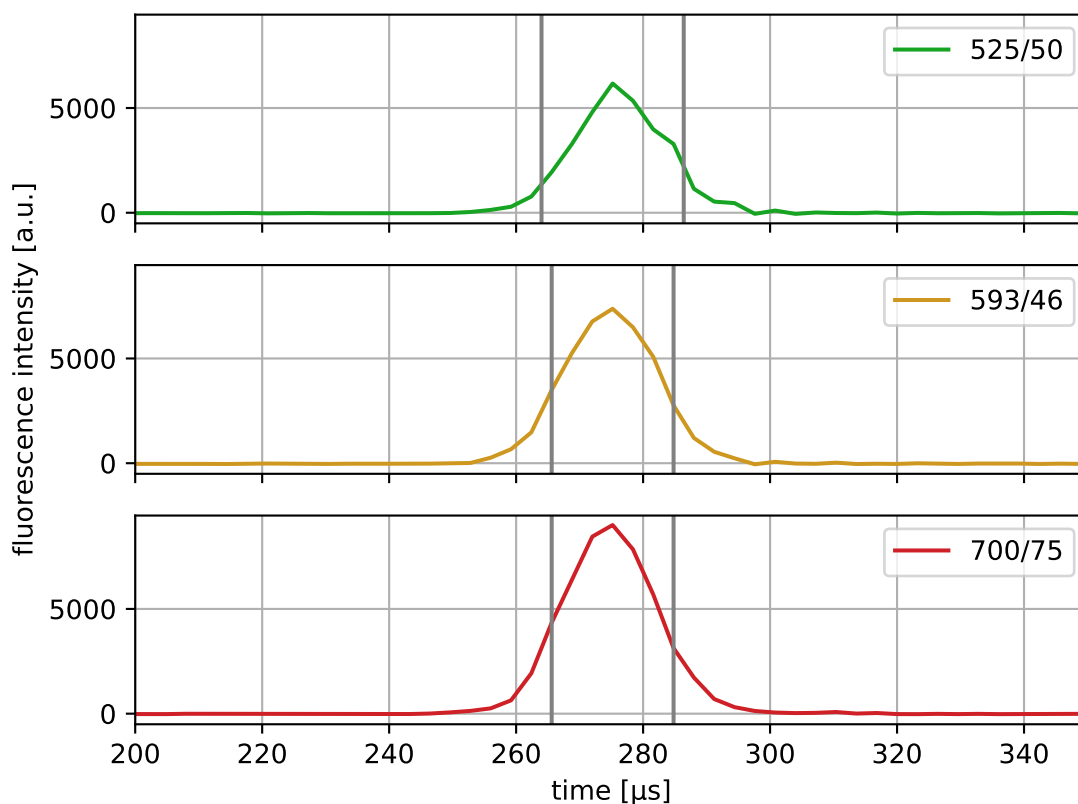
axes[0].axvline(ds["fl1_pos"][idx] + ds["fl1_width"][idx]/2, color="gray")
axes[0].axvline(ds["fl1_pos"][idx] - ds["fl1_width"][idx]/2, color="gray")
axes[1].axvline(ds["fl2_pos"][idx] + ds["fl2_width"][idx]/2, color="gray")
axes[1].axvline(ds["fl2_pos"][idx] - ds["fl2_width"][idx]/2, color="gray")
axes[2].axvline(ds["fl3_pos"][idx] + ds["fl3_width"][idx]/2, color="gray")
axes[2].axvline(ds["fl3_pos"][idx] - ds["fl3_width"][idx]/2, color="gray")

# axes labels
axes[1].set_ylabel("fluorescence intensity [a.u.]")
axes[2].set_xlabel("time [μs]")

for ax in axes:
    ax.set_xlim(200, 350)
    ax.grid()
    ax.legend()

plt.show()

```



Please note that the fluorescence traces are stored as integer values and have to be converted to μs using the meta data stored in `ds.config["fluorescence"]`. Also, notice how the scalar features are used for plotting the peak width.

4.5 Young’s modulus computation

The computation of the Young’s modulus uses a look-up table (LUT) that was derived from simulations based on the finite elements method (FEM) [MMM+17] and the analytical solution [MOG+15]. The LUT was generated with an incompressible (Poisson’s ratio of 0.5) linear elastic sphere model (an artificial viscosity was added to avoid division-by-zero errors) in an axis-symmetric channel (2D). Although the simulations were carried out in this cylindrical symmetry, they can be mapped onto a square cross-sectional channel by adjusting the channel radius to approximately match the desired flow profile. This was done with the spatial scaling factor 1.094 (see also supplement S3 in [MOG+15]). The original data used to generate the LUT are available on figshare [WMM+20].

All computations take into account:

- **scaling laws:** The original LUT was computed for a specific channel width L , flow rate Q , and viscosity η . If the experimental values of these parameters differ from those in the simulation, then they must be scaled before interpolating the Young’s modulus. The scale conversion rules can be derived from the characteristic length L and stress $\sigma = \eta \cdot Q/L^3$ [MOG+15]. For instance, the event area scales with $(L_{\text{exp}}/L_{\text{LUT}})^2$, the Young’s modulus scales with $\sigma_{\text{exp}}/\sigma_{\text{LUT}}$, and the deformation is not scaled as it has no units. Please note that the scaling laws were derived for linear elastic materials and may not be accurate for other materials (e.g. hyperelastic). The scaling laws are implemented in the submodule `dclab.features.emodulus.scale_linear`.
- **pixelation effects:** All features (including deformation and area) are computed from a pixelated contour. This has the effect that deformation is overestimated and area is underestimated (compared to features computed from a “smooth” contour). While a slight change in area does not have a significant effect on the interpolated Young’s modulus, a systematic error in deformation may lead to a strong underestimation of the Young’s modulus. A deeper analysis is visualized in the plot `pixelation_correction.png` which was created with `pixelation_correction.py`. Thus, before interpolation, the measured deformation must be corrected using a hard-coded correction function [Her17]. The pixelation correction is implemented in the submodule `dclab.features.emodulus.pxcorr`.
- **shear-thinning and temperature-dependence:** The viscosity of a medium usually is a function of temperature. In addition, complex media, such as 0.6% methyl cellulose (CellCarrier B), may also exhibit `shear-thinning`. The viscosity of such media decreases with increasing flow rates. Since the viscosity is required to apply the scaling laws (above), it must be corrected which is done using hard-coded correction functions [Her17]. The computation of viscosity is implemented in the submodule `dclab.features.emodulus.viscosity`.

Since the Young’s modulus is model-dependent, it is not made available right away as an *ancillary feature* (in contrast to e.g. event volume or average event brightness).

```
In [1]: import dclab

In [2]: ds = dclab.new_dataset("data/example.rtdc")

# "False", because we have not set any additional information.
In [3]: "emodulus" in ds
Out[3]: False
```

Additional information is required. There are three scenarios:

- A) The viscosity/Young’s modulus is computed individually from the chip temperature for **each** event. Required information:
 - The `temp` feature which holds the chip temperature of each event
 - The configuration key [calculation]: ‘emodulus medium’
 - The configuration key [calculation]: ‘emodulus model’
- B) Set a global viscosity. Use this if you have measured the viscosity of your medium (and know all there is to know about shear thinning [Her17]). Required information:

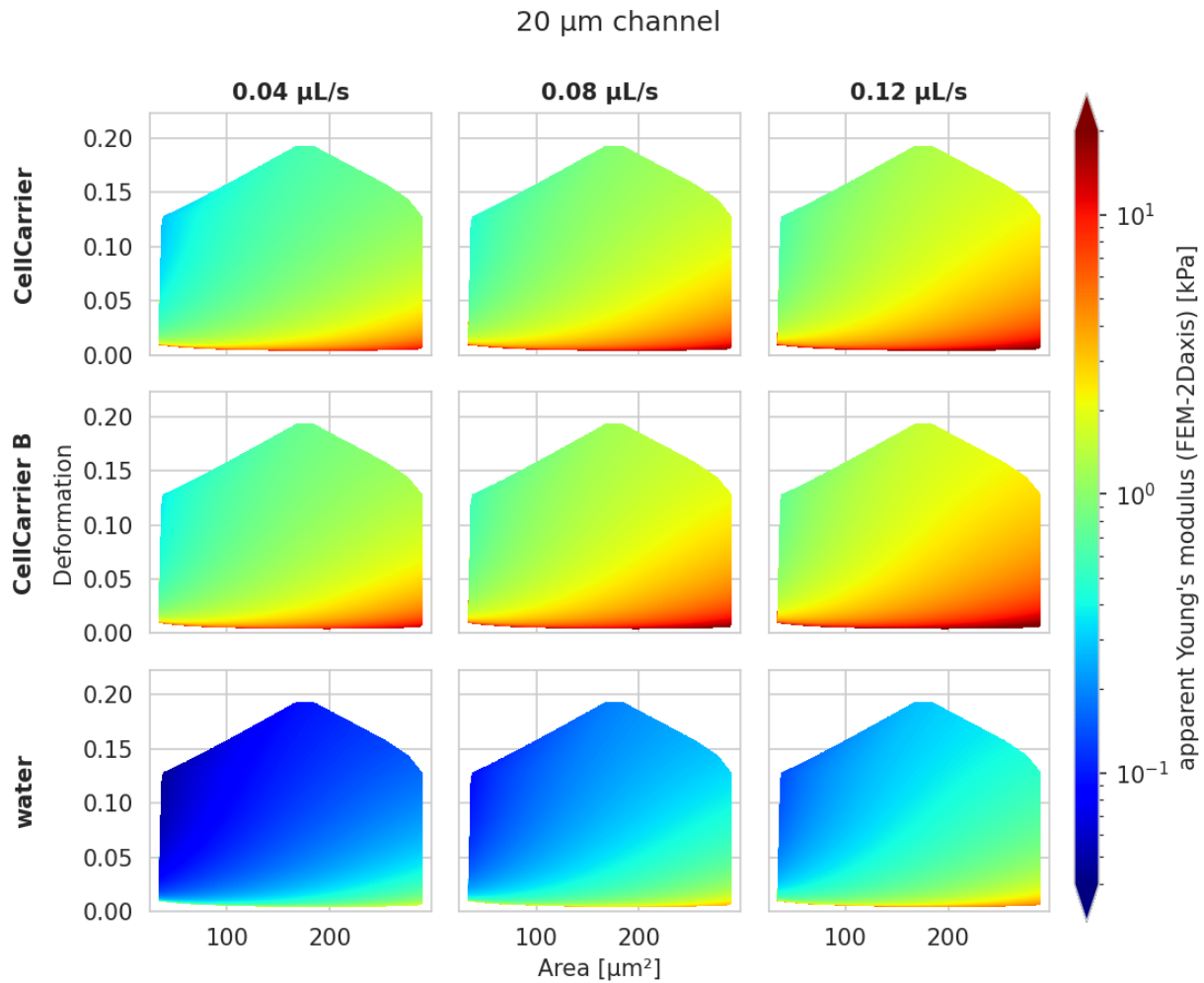


Fig. 4.1: Visualizations of the support and the values of the look-up table (LUT) used for determining the Young's modulus from deformation and cell area. The values of the Young's moduli in the regions shown depend on the channel size, the flow rate, the temperature, and the viscosity of the medium [MOG+15]. Here, they are computed for a 20 μm wide channel at 23°C with an effective pixel size of 0.34 μm . The data are corrected for pixelation effects according to [Her17].

- The configuration key [calculation]: ‘emodulus model’
- The configuration key [calculation]: ‘emodulus viscosity’

C) Compute the Young’s modulus using the viscosities of known media.

- The configuration key [calculation]: ‘emodulus medium’
- The configuration key [calculation]: ‘emodulus model’
- The configuration key [calculation]: ‘emodulus temperature’

Note that if ‘emodulus temperature’ is given, then this temperature is used, even if the *temp* feature exists (scenario A).

The key ‘emodulus model’ currently (2019) only supports the value ‘elastic sphere’. The key ‘emodulus medium’ must be one of the supported media defined in `dclab.features.emodulus.viscosity.KNOWN_MEDIA` and can be taken from [setup]: ‘medium’. The key ‘emodulus temperature’ is the mean chip temperature and could possibly be available in [setup]: ‘temperature’.

```
import matplotlib.pyplot as plt

import dclab

ds = dclab.new_dataset("data/example.rtdc")

# Add additional information. We cannot go for (A), because this example
# does not have the temperature feature (`temp` not in ds). We go for
# (C), because the beads were measured in a known medium.
ds.config["calculation"]["emodulus medium"] = ds.config["setup"]["medium"]
ds.config["calculation"]["emodulus model"] = "elastic sphere"
ds.config["calculation"]["emodulus temperature"] = 23.0 # a guess

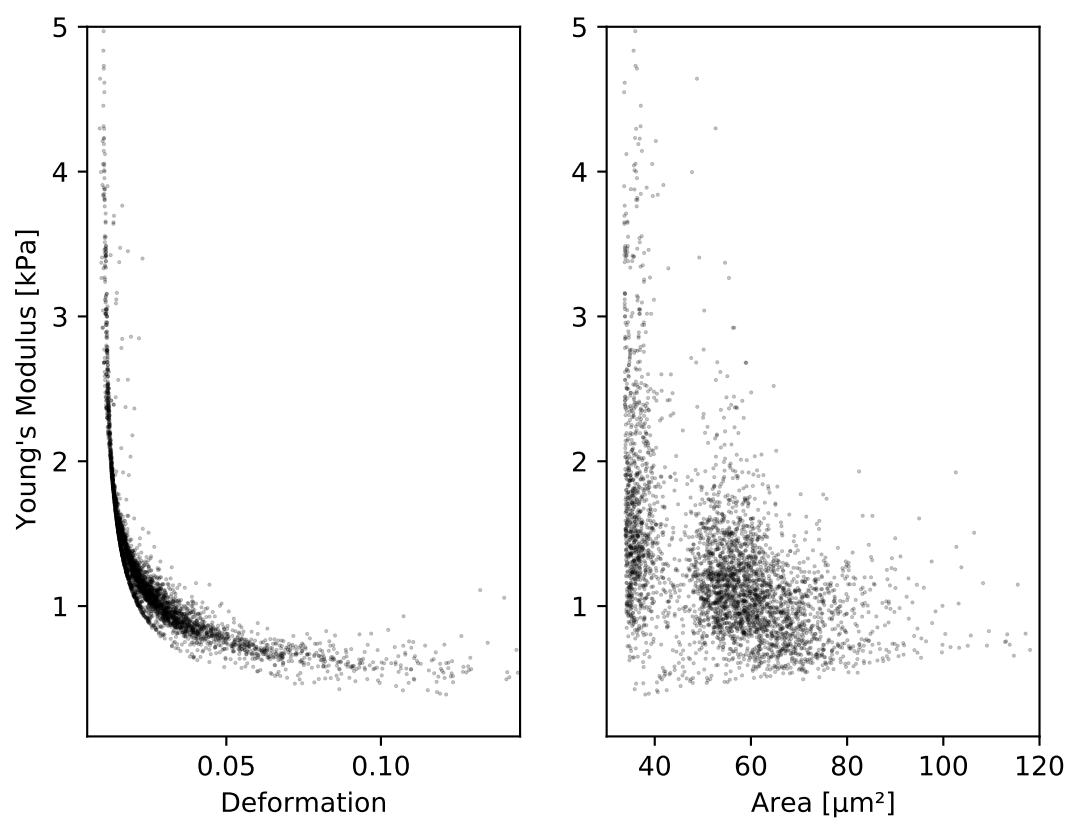
# Plot a few features
ax1 = plt.subplot(121)
ax1.plot(ds["deform"], ds["emodulus"], ".", color="k", markersize=1, alpha=.3)
ax1.set_ylim(0.1, 5)
ax1.set_xlim(0.005, 0.145)
ax1.set_xlabel(dclab.dfn.get_feature_label("deform"))
ax1.set_ylabel(dclab.dfn.get_feature_label("emodulus"))

ax2 = plt.subplot(122)
ax2.plot(ds["area_um"], ds["emodulus"], ".", color="k", markersize=1, alpha=.3)
ax2.set_ylim(0.1, 5)
ax2.set_xlim(30, 120)
ax2.set_xlabel(dclab.dfn.get_feature_label("area_um"))

plt.show()
```

4.6 Linear mixed-effects models

It is not straightforward to define a p-Value for RT-DC data (e.g. change in deformation for a treatment vs. its control). This is somewhat counter-intuitive, because one could assume that the large number of events in a single dataset should be enough to compare two datasets. However, Focus changes, chip-to-chip variations, etc. may generate systematic offsets which make a direct comparison (e.g. t-Test) impossible. Linear mixed effect models (LMM) allow to assign a significance to a treatment measurement compared to a control measurement (fixed effect) while considering the systematic bias in-between the measurement repetitions (random effect).



dclab offers LMM analysis as described in [HMMO18]. The LMM analysis is performed using the `lme4` R package.

4.6.1 Computing p-values with lme4 in dclab

dclab exposes two models from lme4:

- **linear mixed-effects models** (“lmer”): This is basically the simplest way of determining whether or not a treatment has an effect.
- **generalized linear mixed-effects models with a log-link function** (“glmer+loglink”): This model makes use of lme4’s generalized linear effects model (GLMM) `glmer` function with a log-link function (`family=Gamma(link='log')`). This is used for data that is log-normally distributed. Log-normal behaviour is quite common, especially in biology. When a physical parameter has a lower limit, and the measured values are close to that limit, the resulting distribution will be skewed, resembling a log-normal distribution. In case of RT-DC this is specially (but not only) true for deformation. Another example is area, which also has a lower limit of zero and may therefore have a skewed distribution. While GLMMs are designed to handle skewed data, it was shown that LMMs already deliver robust results, even for highly skewed data [GH06].

Warning: The decision whether to use LMM or GLMM is not particularly important. Ideally, both LMM and GLMM are consistent. However, never perform both analyses only to then pick the one with the lowest p-value. This is p-hacking! The analysis routine should be defined beforehand. If in doubt, stick to LMM.

An LMM analysis is straight-forward in dclab:

```
import dclab
from dclab import lme4

# Load the data
ds_rep1_ctl = dclab.new_dataset(...) # control measurement, 1st repetition
ds_rep1_trt = dclab.new_dataset(...) # treatment measurement, 1st repetition
ds_rep2_ctl = dclab.new_dataset(...) # control measurement, 2nd repetition
ds_rep2_trt = dclab.new_dataset(...) # treatment measurement, 2nd repetition

# Instantiate Rlme4
rlme4 = lme4.Rlme4(model="lmer", feature="deform")

# Add the datasets
rlme4.add_dataset(ds=ds_rep1_ctl, group="control", repetition=1)
rlme4.add_dataset(ds=ds_rep1_trt, group="treatment", repetition=1)
rlme4.add_dataset(ds=ds_rep2_ctl, group="control", repetition=2)
rlme4.add_dataset(ds=ds_rep2_trt, group="treatment", repetition=2)

# Perform the analysis
result = rlme4.fit()
print("p-value:", result["anova p-value"])
print("fixed effect:", result["fixed effects treatment"])
```

The `fit()` function returns the most important results and also exposes some of the underlying R objects (see `dclab.lme4.wrappr.Rlme4.fit()`). An LMM example is also given in the *example section*.

Note: If a treatment and a control share the same repetition number, it is implied that they are paired. For those measurements, lme4 will perform a paired test. In your experimental design you determine which measurements are paired, before doing any experiments. Pairing can be done e.g. for measurements done on the same day or on the same chip. In cases where you perform the control measurements on one day and the treatment measurements on

another day, you could still pair them. Just keep in mind that this could introduce systematic errors, if the measurement conditions (temperature, illumination, etc.) were not identical. Under no circumstances, choose a pairing that yields the lowest p-value (p-hacking).

Alternatively, you can also run an unpaired test by just giving each measurement a different repetition number. For example for 3x control and 3x treatment measurements, you could enumerate the repetition number from 1 to 6.

4.6.2 Differential feature analysis with reservoir data

The (G)LMM analysis is only applicable if the feature chosen is not pronounced visibly in the reservoir measurements. For instance, if a treatment results in a significant change in deformation already in the reservoir, then the p-value determined for the channel data might be underestimated (too many stars). In this case, the information of the reservoir measurement must be included by means of differential deformation [HMMO18]. The idea of differential deformation is to subtract the reservoir from the channel deformation. Since it is not possible to assign the events in the reservoir to the events in the channel (two different measurements), bootstrapping is employed which generates statistical representations of the two measurements that can then be subtracted from one another. Then, for the actual LMM analysis, only the differential deformation is used.

To perform a differential feature analysis, simply add the reservoir measurements to the `dclab.lme4.wrapr.Rlme4` class (they are recognized as reservoir measurements via their meta data).

```
# Load the data
ds_repl_ctl = dclab.new_dataset(...) # control measurement, 1st repetition (channel)
ds_repl_ctl_res = dclab.new_dataset(...) # control measurement, 1st repetition
↳ (reservoir)
[...]

# Instantiate Rlme4
rlme4 = lme4.Rlme4(model="lmer", feature="deform")

# Add the datasets
rlme4.add_dataset(ds=ds_repl_ctl, group="control", repetition=1)
rlme4.add_dataset(ds=ds_repl_ctl_res, group="control", repetition=1)
[...]

# Perform the analysis
result = rlme4.fit()
assert result["is differential"] # adding "reservoir" data forces differential
↳ analysis
```

Keep in mind that the analysis is now performed using the differential features and not the actual features (`result["is differential"]`). For more information, please see `dclab.lme4.wrapr.Rlme4.get_differential_dataset()` and `dclab.lme4.wrapr.bootstrapped_median_distributions()`. A full example, including GLMM and differential deformation, is given in the *example section*.

4.7 Accessing DCOR data

The deformability cytometry open repository (DCOR) allows you to upload and access RT-DC datasets online (internet connection required). The advantage is that you can access parts of the dataset (e.g. just two features) without downloading the entire data file (which includes image, contour, and traces information).

4.7.1 Public data

When you would previously download an entire dataset and do

```
import dclab
ds = dclab.new_dataset("/path/to/Downloads/calibration_beads.rtdc")
```

you can now skip the download and use the identifier (id) of a DCOR resource like so:

```
import dclab
ds = dclab.new_dataset("fb719fb2-bd9f-817a-7d70-f4002af916f0")
```

To determine the DCOR resource id, go to <https://dcor.mpl.mpg.de>, find the resource you are interested in, scroll down to the bottom, and copy the value from the **id** (not *package id* or *revision id*) field in (*Additional Information*). The DCOR format is documented in *DCOR (online) format*.

4.7.2 Private data

If you want to access private data, you need to pass your personal API Key:

```
import dclab
ds = dclab.new_dataset("fb719fb2-bd9f-817a-7d70-f4002af916f0",
                       api_key="XXXX-YYYY-ZZZZ")
```

You can find your API Key in the left panel of your profile page when logged in at <https://dcor.mpl.mpg.de>.

Alternatively, you can also set the API Key globally using

```
import dclab
from dclab.rtdc_dataset.fmt_dcor import APIHandler
APIHandler.add_api_key("XXXX-YYYY-ZZZZ")
ds = dclab.new_dataset("fb719fb2-bd9f-817a-7d70-f4002af916f0")
```

4.8 Machine learning

To simplify machine-learning (ML) tasks in the context of RT-DC, dclab offers a few convenience methods. This section describes the recommended way of implementing and distributing ML models based on RT-DC data. Please make sure that you have installed dclab with the *ml* extra (`pip install dclab[ml]`).

4.8.1 Using models in dclab

For RT-DC analysis, the most common task for ML is to determine the probability for a specific event (e.g. a cell) to belong to a specific class (e.g. red blood cell). Since RT-DC data always has a very specific format, it is worthwhile to standardize this regression/classification process.

In dclab, you are not directly using the *bare* models that you would e.g. get from tensorflow/keras. Instead, models are wrapped via a specific `dclab.ml.models.BaseModel` class that holds additional information about the features from which and to which a model maps. For instance, a model might have the inputs `deform` and `area_um` and make predictions regarding a defined output feature, e.g. `ml_score_rbc`. Output features for machine learning are always of the form `ml_score_xxx` where `x` can be any alphanumeric character (you are free to choose).

```
import dclab.ml
import tensorflow as tf

# do your magic
bare_model = tf.keras.Sequential(...)
bare_model.compile(...)
bare_model.fit(...)

# create a dclab model
dc_model = dclab.ml.models.TensorflowModel(
    bare_model=bare_model,
    inputs=["deform", "area_um"],
    outputs=["ml_score_rbc"],
    model_name="RBC identification",
    output_labels=["Red Blood Cells"])

# once you get here, you can use your model directly for inference
ds = dclab.new_dataset("path/to/a/dataset")
# `prediction` is a dictionary with the key "ml_score_rbc" mapping
# to a 1D ndarray of length `len(ds)`, holding the probability data.
prediction = dc_model.predict(ds)["ml_score_rbc"]
```

For user convenience, a model can also be registered with dclab as an *ancillary feature*.

```
dc_model.register()
prediction = ds["ml_score_rbc"] # same result as above
dc_model.unregister() # optional
```

If it is inconvenient for you to call the `register()` and `unregister` methods (e.g. when you would like to perform predictions for multiple models), then you can use `dc_model` in combination with the `with` statement:

```
with dc_model:
    prediction = ds["ml_score_rbc"] # same result as above
```

Please have a look at [this example](#) to see dclab models in action.

4.8.2 The .modc file format

The `.modc` file format is not a reinvention of the wheel. It is merely a wrapper around other ML file formats and describes which input features (e.g. `deform`, `area_um`, `image`, etc.) a machine learning method maps onto which output features (e.g. `ml_score_rbc`). A `.modc` file is just a `.zip` file containing an `index.json` file that lists all models. A model may be stored in multiple file formats (e.g. as a `tensorflow SavedModel` **and** as a Frozen Graph). Alongside the models, the `.modc` file format also contains human-readable versions of the output features, SHA256 checksums, and the creation date:

```
example.modc (ZIP file contents)
├── index.json
├── model_0
│   ├── another-format
│   │   └── another_formats_file.suffix
│   ├── tensorflow-SavedModel.tf
│   │   ├── assets
│   │   ├── saved_model.pb
│   │   ├── variables
│   │   └── variables.data-00000-of-00001
```

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```

└─ variables.index
└─ model_1
  └─ tensorflow-SavedModel.tf
    ├── assets
    ├── saved_model.pb
    ├── variables
    │   ├── variables.data-00000-of-00001
    │   └─ variables.index

```

The corresponding index.json file could look like this:

```

{
  "model count": 2,
  "models": [
    {
      "date": "2020-11-03 17:01",
      "formats": {
        "tensorflow-SavedModel": "tensorflow-SavedModel.tf",
        "library-OtherFormat": "another-format"
      },
      "index": 0,
      "input features": [
        "deform"
      ],
      "name": "Example Model 1",
      "output features": [
        "ml_score_low",
        "ml_score_hig"
      ],
      "output labels": [
        "Low",
        "High"
      ],
      "path": "model_0",
      "sha256": "ec11c73ae870da4551d9fa9cc73271566b8f2356f284d4c2cb02057ecb5bf6ce"
    },
    {
      "date": "2020-11-03 17:02",
      "formats": {
        "tensorflow-SavedModel": "tensorflow-SavedModel.tf"
      },
      "index": 1,
      "input features": [
        "area_um",
        "image"
      ],
      "name": "Example Model 2",
      "output features": [
        "ml_score_rbc",
        "ml_score_sad"
      ],
      "output labels": [
        "red boold cells",
        "sad cells"
      ],
      "path": "model_1",
      "sha256": "ac43c73ae870da4551d9fa9cc73271566b8f2356f284d4c2cb02057ecb5ba812"
    }
  ]
}

```

(continues on next page)

(continued from previous page)

```
}  
]  
}
```

The great advantage of such a file format is that users can transparently exchange machine learning methods and apply them in a reproducible manner to any RT-DC dataset using dclab or Shape-Out.

To save a machine learning model to a .modc file, you can use the *dclab.ml.save_modc* function:

```
dclab.ml.save_modc("path/to/file.modc", dc_model)
```

Conversely, you can load such a model at any time and use it for inference:

```
dc_model_loaded = dclab.ml.load_modc("path/to/file.modc")  
with dc_model_loaded:  
    prediction = ds["ml_score_rbc"] # same result as above
```

The methods for saving and loading .modc files are described in the *code reference*.

4.8.3 Helper functions

If you are working with *tensorflow*, you might find the functions in the *dclab.ml.tf_dataset* submodule helpful. Please also have a look at the *machine-learning examples*.

5.1 module-level methods

`dclab.new_dataset` (*data*, *identifier=None*, ***kwargs*)

Initialize a new RT-DC dataset

Parameters

- **data** – can be one of the following:
 - dict
 - .tdms file
 - .rtdc file
 - subclass of *RTDCBase* (will create a hierarchy child)
 - DCOR resource URL
- **identifier** (*str*) – A unique identifier for this dataset. If set to *None* an identifier is generated.
- **kwargs** (*dict*) – Additional parameters passed to the *RTDCBase* subclass

Returns **dataset** – A new dataset instance

Return type subclass of `dclab.rtdc_dataset.RTDCBase`

5.2 global definitions

These definitions are used throughout the dclab/Shape-In/Shape-Out ecosystem.

5.2.1 configuration

Valid configuration sections and keys are described in: *Analysis metadata* and *Experiment metadata*.

`dclab.dfn.CFG_ANALYSIS`

User-editable configuration for data analysis.

`dclab.dfn.CFG_METADATA`

Measurement-specific metadata.

`dclab.dfn.config_funcs`

Dictionary of dictionaries containing functions to convert input data to the predefined data type

`dclab.dfn.config_keys`

Dictionary with sections as keys and configuration parameter names as values

`dclab.dfn.config_types`

Dictionary of dictionaries containing the data type of each configuration parameter

5.2.2 features

Features are discussed in more detail in: *Features*.

`dclab.dfn.feature_exists(name, scalar_only=False)`

Return True if *name* is a valid feature name

This function not only checks whether *name* is in *feature_names*, but also validates against the machine learning scores *ml_score_???* (where *?* can be a digit or a lower-case letter in the English alphabet).

`dclab.dfn.get_feature_label(name, rtdc_ds=None)`

Return the label corresponding to a feature name

This function not only checks *feature_name2label*, but also supports registered *ml_score_???* features.

TODO: extract feature label from ancillary information when an *rtdc_ds* is given.

`dclab.dfn.scalar_feature_exists(name)`

Convenience method wrapping *feature_exists(..., scalar_only=True)*

`dclab.dfn.FEATURES_NON_SCALAR`

Non-scalar features

`dclab.dfn.feature_names`

List of valid feature names

`dclab.dfn.feature_labels`

List of human-readable labels for each valid feature

`dclab.dfn.feature_name2label`

Dictionary that maps feature names to feature labels

`dclab.dfn.scalar_feature_names`

List of valid scalar feature names

5.2.3 parse functions

`dclab.parse_funcs.fbool(value)`

boolean

`dclab.parse_funcs.fint(value)`

integer

`dclab.parse_funcs.fintlist` (*alist*)
A list of integers

`dclab.parse_funcs.lcstr` (*astr*)
lower-case string

`dclab.parse_funcs.func_types` = {<function fbool>: <class 'bool'>, <function fint>: <class 'int'>, <function flist>: <class 'list'>}
maps functions to their expected output types

5.3 RT-DC dataset manipulation

5.3.1 Base class

`class dclab.rtdc_dataset.RTDCBase` (*identifier=None*)
RT-DC measurement base class

Notes

Besides the filter arrays for each data feature, there is a manual boolean filter array `RTDCBase.filter_manual` that can be edited by the user - a boolean value of `False` means that the event is excluded from all computations.

`apply_filter` (*force=[]*)
Compute the filters for the dataset

`get_downsampled_scatter` (*xax='area_um', yax='deform', downsample=0, xscale='linear', yscale='linear', remove_invalid=False, ret_mask=False*)
Downsampling by removing points at dense locations

Parameters

- **xax** (*str*) – Identifier for x axis (e.g. “area_um”, “aspect”, “deform”)
- **yax** (*str*) – Identifier for y axis
- **downsample** (*int*) – Number of points to draw in the down-sampled plot. This number is either
 - **>=1: exactly downsample to this number by randomly adding** or removing points
 - **0** : do not perform downsampling
- **xscale** (*str*) – If set to “log”, take the logarithm of the x-values before performing downsampling. This is useful when data are displayed on a log-scale. Defaults to “linear”.
- **yscale** (*str*) – See *xscale*.
- **remove_invalid** (*bool*) – Remove nan and inf values before downsampling; if set to *True*, the actual number of samples returned might be smaller than *downsample* due to infinite or nan values (e.g. due to logarithmic scaling).
- **ret_mask** (*bool*) – If set to *True*, returns a boolean array of length *len(self)* where *True* values identify the filtered data.

Returns

- **xnew, ynew** (1d ndarray of length *N*) – Filtered data; *N* is either identical to *downsample* or smaller (if *remove_invalid==True*)

- **mask** (1d boolean array of length *len(RTDCBase)*) – Array for identifying the down-sampled data points

get_kde_contour (*xax*='area_um', *yax*='deform', *xacc*=None, *yacc*=None, *kde_type*='histogram',
kde_kwargs={}, *xscale*='linear', *yscale*='linear')

Evaluate the kernel density estimate for contour plots

Parameters

- **xax** (*str*) – Identifier for X axis (e.g. “area_um”, “aspect”, “deform”)
- **yax** (*str*) – Identifier for Y axis
- **xacc** (*float*) – Contour accuracy in x direction
- **yacc** (*float*) – Contour accuracy in y direction
- **kde_type** (*str*) – The KDE method to use
- **kde_kwargs** (*dict*) – Additional keyword arguments to the KDE method
- **xscale** (*str*) – If set to “log”, take the logarithm of the x-values before computing the KDE. This is useful when data are displayed on a log-scale. Defaults to “linear”.
- **yscale** (*str*) – See *xscale*.

Returns **X, Y, Z** – The kernel density Z evaluated on a rectangular grid (X,Y).

Return type coordinates

get_kde_scatter (*xax*='area_um', *yax*='deform', *positions*=None, *kde_type*='histogram',
kde_kwargs={}, *xscale*='linear', *yscale*='linear')

Evaluate the kernel density estimate for scatter plots

Parameters

- **xax** (*str*) – Identifier for X axis (e.g. “area_um”, “aspect”, “deform”)
- **yax** (*str*) – Identifier for Y axis
- **positions** (*list of two 1d ndarrays or ndarray of shape (2, N)*) – The positions where the KDE will be computed. Note that the KDE estimate is computed from the the points that are set in *self.filter.all*.
- **kde_type** (*str*) – The KDE method to use
- **kde_kwargs** (*dict*) – Additional keyword arguments to the KDE method
- **xscale** (*str*) – If set to “log”, take the logarithm of the x-values before computing the KDE. This is useful when data are displayed on a log-scale. Defaults to “linear”.
- **yscale** (*str*) – See *xscale*.

Returns **density** – The kernel density evaluated for the filtered data points.

Return type 1d ndarray

static get_kde_spacing (*a*, *scale*='linear', *method*=<function bin_width_doane>,
method_kw={}, *feat*='undefined', *ret_scaled*=False)

Convenience function for computing the contour spacing

Parameters

- **a** (*ndarray*) – feature data
- **scale** (*str*) – how the data should be scaled (“log” or “linear”)

- **method** (*callable*) – KDE method to use (see *kde_methods* submodule)
- **method_kw** (*dict*) – keyword arguments to *method*
- **feat** (*str*) – feature name for debugging
- **ret_scale** (*bool*) – whether or not to return the scaled array of *a*

polygon_filter_add (*filt*)

Associate a Polygon Filter with this instance

Parameters **filt** (int or instance of *PolygonFilter*) – The polygon filter to add

polygon_filter_rm (*filt*)

Remove a polygon filter from this instance

Parameters **filt** (int or instance of *PolygonFilter*) – The polygon filter to remove

reset_filter ()

Reset the current filter

config = **None**

Configuration of the measurement

export = **None**

Export functionalities; instance of *dclab.rtdc_dataset.export.Export*.

features

All available features

features_innate

All features excluding ancillary features

features_loaded

All features including ancillaries that have been computed

Notes

Features that are computationally cheap to compute are always included. They are defined in *dclab.rtdc_dataset.ancillaries.FEATURES_RAPID*.

features_scalar

All scalar features available

filter = **None**

Filtering functionalities; instance of *dclab.rtdc_dataset.filter.Filter*.

format = **None**

Dataset format (derived from class name)

hash

Reproducible dataset hash (defined by derived classes)

identifier

Unique (unreproducible) identifier

logs = **None**

Dictionary of log files. Each log file is a list of strings (one string per line).

title = **None**

Title of the measurement

5.3.2 DCOR (online) format

```
class dclab.rtdc_dataset.RTDC_DCOR (url, use_ssl=None, host='dcor.mpl.mpg.de', api_key="",  
                                     *args, **kwargs)
```

Wrap around the DCOR API

Parameters

- **url** (*str*) – Full URL or resource identifier; valid values are
 - <https://dcor.mpl.mpg.de/api/3/action/dcserv?id=b1404eb5-f661-4920-be79-5ff4e85915d5>
 - dcor.mpl.mpg.de/api/3/action/dcserv?id=b1404eb5-f661-4920-be79-5ff4e85915d5
 - [b1404eb5-f661-4920-be79-5ff4e85915d5](https://dcor.mpl.mpg.de/api/3/action/dcserv?id=b1404eb5-f661-4920-be79-5ff4e85915d5)
- **use_ssl** (*bool*) – Set this to False to disable SSL (should only be used for testing). Defaults to None (does not force SSL if the URL starts with “<http://>”).
- **host** (*str*) – The host machine (used if the host is not given in *url*)
- **api_key** (*str*) – API key to access private resources
- ***args** – Arguments for *RTDCBase*
- ****kwargs** – Keyword arguments for *RTDCBase*

path

Full URL to the DCOR resource

Type *str*

```
static get_full_url (url, use_ssl, host)
```

Return the full URL to a DCOR resource

Parameters

- **url** (*str*) – Full URL or resource identifier; valid values are
 - <https://dcor.mpl.mpg.de/api/3/action/dcserv?id=caab96f6-df12-4299-aa2e-089e390aafd5>
 - dcor.mpl.mpg.de/api/3/action/dcserv?id=caab96f6-df12-4299-aa2e-089e390aafd5
 - [caab96f6-df12-4299-aa2e-089e390aafd5](https://dcor.mpl.mpg.de/api/3/action/dcserv?id=caab96f6-df12-4299-aa2e-089e390aafd5)
- **use_ssl** (*bool*) – Set this to False to disable SSL (should only be used for testing). Defaults to None (does not force SSL if the URL starts with “<http://>”).
- **host** (*str*) – Use this host if it is not specified in *url*

hash

Hash value based on file name and content

```
class dclab.rtdc_dataset.fmt_dcor.APIHandler (url, api_key="")
```

Handles the DCOR api with caching for simple queries

```
classmethod add_api_key (api_key)
```

Add an API Key to the base class

When accessing the DCOR API, all available API Keys are used to access a resource (trial and error).

```
api_keys = []
```

DCOR API Keys in the current session

```
cache_queries = ['metadata', 'size', 'feature_list', 'valid']
```

these are cached to minimize network usage

5.3.3 Dictionary format

class dclab.rtdc_dataset.**RTDC_Dict** (*ddict*, **args*, ***kwargs*)
Dictionary-based RT-DC dataset

Parameters

- **ddict** (*dict*) – Dictionary with features as keys (valid features like “area_cvx”, “deform”, “image” are defined by *dclab.definitions.feature_exists*) with which the class will be instantiated. The configuration is set to the default configuration of dclab.

Changed in version 0.27.0: Scalar features are automatically converted to arrays.

- ***args** – Arguments for *RTDCBase*
- ****kwargs** – Keyword arguments for *RTDCBase*

5.3.4 HDF5 (.rtdc) format

class dclab.rtdc_dataset.**RTDC_HDF5** (*h5path*, **args*, ***kwargs*)
HDF5 file format for RT-DC measurements

Parameters

- **h5path** (*str* or *pathlib.Path*) – Path to a ‘.tdms’ measurement file.
- ***args** – Arguments for *RTDCBase*
- ****kwargs** – Keyword arguments for *RTDCBase*

path

Path to the experimental HDF5 (.rtdc) file

Type *pathlib.Path*

static can_open (*h5path*)

Check whether a given file is in the .rtdc file format

static parse_config (*h5path*)

Parse the RT-DC configuration of an hdf5 file

hash

Hash value based on file name and content

dclab.rtdc_dataset.fmt_hdf5.**MIN_DCLAB_EXPORT_VERSION** = '0.3.3.dev2'
rtdc files exported with dclab prior to this version are not supported

5.3.5 Hierarchy format

class dclab.rtdc_dataset.**RTDC_Hierarchy** (*hparent*, *apply_filter=True*, **args*, ***kwargs*)
Hierarchy dataset (filtered from *RTDCBase*)

A few words on hierarchies: The idea is that a subclass of *RTDCBase* can use the filtered data of another subclass of *RTDCBase* and interpret these data as unfiltered events. This comes in handy e.g. when the percentage of different subpopulations need to be distinguished without the noise in the original data.

Children in hierarchies always update their data according to the filtered event data from their parent when *apply_filter* is called. This makes it easier to save and load hierarchy children with e.g. Shape-Out and it makes the handling of hierarchies more intuitive (when the parent changes, the child changes as well).

Parameters

- **hparent** (*instance of RTDCBase*) – The hierarchy parent
- **apply_filter** (*bool*) – Whether to apply the filter during instantiation; If set to *False*, *apply_filter* must be called manually.
- ***args** – Arguments for *RTDCBase*
- ****kwargs** – Keyword arguments for *RTDCBase*

hparent

Hierarchy parent of this instance

Type *RTDCBase*

5.3.6 TDMS format

class `dclab.rtdc_dataset.RTDC_TDMS` (*tdms_path, *args, **kwargs*)
TDMS file format for RT-DC measurements

Parameters

- **tdms_path** (*str or pathlib.Path*) – Path to a ‘.tdms’ measurement file.
- ***args** – Arguments for *RTDCBase*
- ****kwargs** – Keyword arguments for *RTDCBase*

path

Path to the experimental dataset (main .tdms file)

Type *pathlib.Path*

`dclab.rtdc_dataset.fmt_tdms.get_project_name_from_path` (*path, append_mx=False*)
Get the project name from a path.

For a path “/home/peter/hans/HLC12398/online/M1_13.tdms” or For a path “/home/peter/hans/HLC12398/online/data/M1_13.tdms” or without the “.tdms” file, this will return always “HLC12398”.

Parameters

- **path** (*str*) – path to tdms file
- **append_mx** (*bool*) – append measurement number, e.g. “M1”

`dclab.rtdc_dataset.fmt_tdms.get_tdms_files` (*directory*)
Recursively find projects based on ‘.tdms’ file endings

Searches the *directory* recursively and return a sorted list of all found ‘.tdms’ project files, except fluorescence data trace files which end with *_traces.tdms*.

5.3.7 Ancillaries

Computation of ancillary features

Ancillary features are computed on-the-fly in dclab if the required data are available. The features are registered here and are computed when *RTDCBase.__getitem__* is called with the respective feature name. When *RTDCBase.__contains__* is called with the feature name, then the feature is not yet computed, but the prerequisites are evaluated:

```

In [1]: import dclab

In [2]: ds = dclab.new_dataset("data/example.rtdc")

In [3]: ds.config["calculation"]["emodulus medium"] = "CellCarrier"

In [4]: ds.config["calculation"]["emodulus model"] = "elastic sphere"

In [5]: ds.config["calculation"]["emodulus temperature"] = 23.0

In [6]: "emodulus" in ds # nothing is computed
Out[6]: True

In [7]: ds["emodulus"] # now data is computed and cached
Out[7]:
array([1.23006241, 1.08662317,          nan, ...,          nan,          nan,
       0.75430855])

```

Once the data has been computed, *RTDCBase* caches it in the *_ancillaries* property dict together with a hash that is computed with *AncillaryFeature.hash*. The hash is computed from the feature data *req_features* and the configuration metadata *req_config*.

```

exception dclab.rtdc_dataset.ancillaries.ancillary_feature.BadFeatureSizeWarning

class dclab.rtdc_dataset.ancillaries.ancillary_feature.AncillaryFeature (feature_name,
                                                                           method,
                                                                           req_config=[],
                                                                           req_features=[],
                                                                           req_func=<function
An-
cil-
laryFea-
ture.<lambda>>,
                                                                           pri-
or-
ity=0,
                                                                           data=None)

```

A data feature that is computed from existing data

Parameters

- **feature_name** (*str*) – The name of the ancillary feature, e.g. “emodulus”.
- **method** (*callable*) – The method that computes the feature. This method takes an instance of *RTDCBase* as argument.
- **req_config** (*list*) – Required configuration parameters to compute the feature, e.g. [“calculation”, [“emodulus model”, “emodulus viscosity”]]
- **req_features** (*list*) – Required existing features in the dataset, e.g. [“area_cvx”, “deform”]
- **req_func** (*callable*) – A function that takes an instance of *RTDCBase* as an argument and checks whether any other necessary criteria are met. By default, this is a lambda function that returns True. The function should return False if the necessary criteria are not met. This function may also return a hashable object (via `dclab.util.objstr()`) instead of True, if the criteria are subject to change. In this case, the return value is used for identifying the cached ancillary feature.

Changed in version 0.27.0: Support non-boolean return values for caching purposes.

- **priority** (*int*) – The priority of the feature; if there are multiple *AncillaryFeature* defined for the same *feature_name*, then the priority of the features defines which feature returns *True* in *self.is_available*. A higher value means a higher priority.
- **data** (*object*) – Any other data relevant for the feature (e.g. the ML model for computing ‘ml_score_xxx’ features)

Notes

req_config and *req_features* are used to test whether the feature can be computed in *self.is_available*.

static available_features (*rtdc_ds*)

Determine available features for an RT-DC dataset

Parameters *rtdc_ds* (*instance of RTDCBase*) – The dataset to check availability for

Returns *features* – Dictionary with feature names as keys and instances of *AncillaryFeature* as values.

Return type *dict*

compute (*rtdc_ds*)

Compute the feature with *self.method*

Parameters *rtdc_ds* (*instance of RTDCBase*) – The dataset to compute the feature for

Returns *feature* – The computed data feature (read-only).

Return type *array- or list-like*

static get_instances (*feature_name*)

Return all instances that compute *feature_name*

hash (*rtdc_ds*)

Used for identifying an ancillary computation

The data columns and the used configuration keys/values are hashed.

is_available (*rtdc_ds*, *verbose=False*)

Check whether the feature is available

Parameters *rtdc_ds* (*instance of RTDCBase*) – The dataset to check availability for

Returns *available* – *True*, if feature can be computed with *compute*

Return type *bool*

Notes

This method returns *False* for a feature if there is a feature defined with the same name but with higher priority (even if the feature would be available otherwise).

feature_names = ['time', 'index', 'area_ratio', 'area_um', 'aspect', 'deform', 'emodul']
All feature names registered

features = [<AncillaryFeature 'time' (priority 0)>, <AncillaryFeature 'index' (priority 1)>]
All ancillary features registered

5.3.8 config

class `dclab.rtdc_dataset.config.Configuration` (*files=[]*, *cfg={}*, *disable_checks=False*)
 Configuration class for RT-DC datasets

This class has a dictionary-like interface to access and set configuration values, e.g.

```
cfg = load_from_file("/path/to/config.txt")
# access the channel width
cfg["setup"]["channel width"]
# modify the channel width
cfg["setup"]["channel width"] = 30
```

Parameters

- **files** (*list of files*) – The config files with which to initialize the configuration
- **cfg** (*dict-like*) – The dictionary with which to initialize the configuration
- **disable_checks** (*bool*) – Set this to True if you want to avoid checking against section and key names defined in *dclab.definitions* using *verify_section_key()*. This avoids excess warning messages when loading data from configuration files not generated by dclab.

copy ()

Return copy of current configuration

get (*key*, *other*)

Famous *dict.get* function

New in version 0.29.1.

keys ()

Return the configuration keys (sections)

save (*filename*)

Save the configuration to a file

tostring (*sections=None*)

Convert the configuration to its string representation

The optional argument *sections* allows to export only specific sections of the configuration, i.e. *sections=dclab.dfn.CFG_METADATA* will only export configuration data from the original measurement and no filtering data.

update (*newcfg*)

Update current config with a dictionary

`dclab.rtdc_dataset.config.load_from_file` (*cfg_file*)

Load the configuration from a file

Parameters **cfg_file** (*str*) – Path to configuration file

Returns **cfg** – Dictionary with configuration parameters

Return type ConfigurationDict

5.3.9 export

exception `dclab.rtdc_dataset.export.LimitingExportSizeWarning`

class dclab.rtdc_dataset.export.**Export** (*rtdc_ds*)

Export functionalities for RT-DC datasets

avi (*path*, *filtered=True*, *override=False*)

Exports filtered event images to an avi file

Parameters

- **path** (*str*) – Path to a .avi file. The ending .avi is added automatically.
- **filtered** (*bool*) – If set to *True*, only the filtered data (index in *ds.filter.all*) are used.
- **override** (*bool*) – If set to *True*, an existing file *path* will be overridden. If set to *False*, raises *OSError* if *path* exists.

Notes

Raises *OSError* if current dataset does not contain image data

fcs (*path*, *features*, *meta_data={}*, *filtered=True*, *override=False*)

Export the data of an RT-DC dataset to an .fcs file

Parameters

- **mm** (*instance of dclab.RTDCBase*) – The dataset that will be exported.
- **path** (*str*) – Path to an .fcs file. The ending .fcs is added automatically.
- **features** (*list of str*) – The features in the resulting .fcs file. These are strings that are defined by *dclab.definitions.scalar_feature_exists*, e.g. “area_cvx”, “deform”, “frame”, “fl1_max”, “aspect”.
- **meta_data** (*dict*) – User-defined, optional key-value pairs that are stored in the primary TEXT segment of the FCS file; the version of dclab is stored there by default
- **filtered** (*bool*) – If set to *True*, only the filtered data (index in *ds.filter.all*) are used.
- **override** (*bool*) – If set to *True*, an existing file *path* will be overridden. If set to *False*, raises *OSError* if *path* exists.

Notes

Due to incompatibility with the .fcs file format, all events with NaN-valued features are not exported.

hdf5 (*path*, *features*, *filtered=True*, *override=False*, *compression='gzip'*)

Export the data of the current instance to an HDF5 file

Parameters

- **path** (*str*) – Path to an .rtdc file. The ending .rtdc is added automatically.
- **features** (*list of str*) – The features in the resulting .rtdc file. These are strings that are defined by *dclab.definitions.feature_exists*, e.g. “area_cvx”, “deform”, “frame”, “fl1_max”, “image”.
- **filtered** (*bool*) – If set to *True*, only the filtered data (index in *ds.filter.all*) are used.
- **override** (*bool*) – If set to *True*, an existing file *path* will be overridden. If set to *False*, raises *OSError* if *path* exists.

- **compression** (*str* or *None*) – Compression method for e.g. “contour”, “image”, and “trace” data as well as logs; one of [None, “lzf”, “gzip”, “szip”].

tsv (*path*, *features*, *meta_data*={'dclab version': '0.31.0'}, *filtered*=True, *override*=False)

Export the data of the current instance to a .tsv file

Parameters

- **path** (*str*) – Path to a .tsv file. The ending .tsv is added automatically.
- **features** (*list* of *str*) – The features in the resulting .tsv file. These are strings that are defined by `dclab.definitions.scalar_feature_exists`, e.g. “area_cvx”, “deform”, “frame”, “fl1_max”, “aspect”.
- **meta_data** (*dict*) – User-defined, optional key-value pairs that are stored at the beginning of the tsv file - one key-value pair is stored per line which starts with a hash. The version of dclab is stored there by default.
- **filtered** (*bool*) – If set to *True*, only the filtered data (index in `ds.filter.all`) are used.
- **override** (*bool*) – If set to *True*, an existing file `path` will be overridden. If set to *False*, raises *OSError* if `path` exists.

5.3.10 filter

class `dclab.rtdc_dataset.filter.Filter` (*rtdc_ds*)

Boolean filter arrays for RT-DC measurements

Parameters `rtdc_ds` (*instance of RTDCBase*) – The RT-DC dataset the filter applies to

reset ()

Reset all filters

update (*rtdc_ds*, *force*=[])

Update the filters according to `rtdc_ds.config[“filtering”]`

Parameters

- **rtdc_ds** (`dclab.rtdc_dataset.core.RTDCBase`) – The measurement to which the filter is applied
- **force** (*list*) – A list of feature names that must be refiltered with min/max values.

Notes

This function is called when `ds.apply_filter` is called.

5.4 low-level functionalities

5.4.1 downsampling

Content-based downsampling of ndarrays

`dclab.downsampling.downsample_rand` (*a*, *samples*, *remove_invalid*=False, *ret_idx*=False)

Downsampling by randomly removing points

Parameters

- **a** (*1d ndarray*) – The input array to downsample
- **samples** (*int*) – The desired number of samples
- **remove_invalid** (*bool*) – Remove nan and inf values before downsampling
- **ret_idx** (*bool*) – Also return a boolean array that corresponds to the downsampled indices in *a*.

Returns

- **dsa** (*1d ndarray of size samples*) – The pseudo-randomly downsampled array *a*
- **idx** (*1d boolean array with same shape as a*) – Only returned if *ret_idx* is True. A boolean array such that *a[idx] == dsa*

`dclab.downsampling.norm(a, ref1, ref2)`

Normalize *a* with min/max values of *ref1*, using all elements of *ref1* where the *ref1* and *ref2* are not nan or inf

`dclab.downsampling.valid(a, b)`

Check whether *a* and *b* are not inf or nan

5.4.2 features

image-based

`dclab.features.contour.get_contour(mask)`

Compute the image contour from a mask

The contour is computed in a very inefficient way using scikit-image and a conversion of float coordinates to pixel coordinates.

Parameters **mask** (*binary ndarray of shape (M,N) or (K,M,N)*) – The mask outlining the pixel positions of the event. If a 3d array is given, then *K* indexes the individual contours.

Returns **cont** – A 2D array that holds the contour of an event (in pixels) e.g. obtained using *mm.contour* where *mm* is an instance of *RTDCBase*. The first and second columns of *cont* correspond to the x- and y-coordinates of the contour.

Return type ndarray or list of K ndarrays of shape (J,2)

`dclab.features.bright.get_bright(mask, image, ret_data='avg, sd')`

Compute avg and/or std of the event brightness

The event brightness is defined by the gray-scale values of the image data within the event mask area.

Parameters

- **mask** (*ndarray or list of ndarrays of shape (M,N) and dtype bool*) – The mask values, True where the event is located in *image*.
- **image** (*ndarray or list of ndarrays of shape (M,N)*) – A 2D array that holds the image in form of grayscale values of an event.
- **ret_data** (*str*) – A comma-separated list of metrics to compute - “avg”: compute the average - “sd”: compute the standard deviation Selected metrics are returned in alphabetical order.

Returns

- **bright_avg** (*float or ndarray of size N*) – Average image data within the contour

- **bright_std** (*float or ndarray of size N*) – Standard deviation of image data within the contour

`dclab.features.inert_ratio.get_inert_ratio_cvx(cont)`

Compute the inertia ratio of the convex hull of a contour

The inertia ratio is computed from the central second order of moments along x (μ_{20}) and y (μ_{02}) via $\sqrt{\mu_{20}/\mu_{02}}$.

Parameters `cont` (*ndarray or list of ndarrays of shape $(N, 2)$*) – A 2D array that holds the contour of an event (in pixels) e.g. obtained using `mm.contour` where `mm` is an instance of `RTDCBase`. The first and second columns of `cont` correspond to the x- and y-coordinates of the contour.

Returns `inert_ratio_cvx` – The inertia ratio of the contour's convex hull

Return type `float` or ndarray of size N

Notes

The contour moments μ_{20} and μ_{02} are computed the same way they are computed in OpenCV's `moments.cpp`.

See also:

`get_inert_ratio_raw()` Compute inertia ratio of a raw contour

References

- https://en.wikipedia.org/wiki/Image_moment#Central_moments
- <https://github.com/opencv/opencv/blob/f81370232a651bdac5042efe907bcaa50a66c487/modules/imgproc/src/moments.cpp#L93>

`dclab.features.inert_ratio.get_inert_ratio_raw(cont)`

Compute the inertia ratio of a contour

The inertia ratio is computed from the central second order of moments along x (μ_{20}) and y (μ_{02}) via $\sqrt{\mu_{20}/\mu_{02}}$.

Parameters `cont` (*ndarray or list of ndarrays of shape $(N, 2)$*) – A 2D array that holds the contour of an event (in pixels) e.g. obtained using `mm.contour` where `mm` is an instance of `RTDCBase`. The first and second columns of `cont` correspond to the x- and y-coordinates of the contour.

Returns `inert_ratio_raw` – The inertia ratio of the contour

Return type `float` or ndarray of size N

Notes

The contour moments μ_{20} and μ_{02} are computed the same way they are computed in OpenCV's `moments.cpp`.

See also:

`get_inert_ratio_cvx()` Compute inertia ratio of the convex hull of a contour

References

- https://en.wikipedia.org/wiki/Image_moment#Central_moments
- <https://github.com/opencv/opencv/blob/f81370232a651bdac5042efe907bcaa50a66c487/modules/imgproc/src/moments.cpp#L93>

`dclab.features.volume.get_volume(cont, pos_x, pos_y, pix)`

Calculate the volume of a polygon revolved around an axis

The volume estimation assumes rotational symmetry. Green's theorem and the Gaussian divergence theorem allow to formulate the volume as a line integral.

Parameters

- **cont** (*ndarray or list of ndarrays of shape (N,2)*) – A 2D array that holds the contour of an event [px] e.g. obtained using `mm.contour` where `mm` is an instance of `RTDCBase`. The first and second columns of `cont` correspond to the x- and y-coordinates of the contour.
- **pos_x** (*float or ndarray of length N*) – The x coordinate(s) of the centroid of the event(s) [μm] e.g. obtained using `mm.pos_x`
- **pos_y** (*float or ndarray of length N*) – The y coordinate(s) of the centroid of the event(s) [μm] e.g. obtained using `mm.pos_y`
- **px_um** (*float*) – The detector pixel size in μm . e.g. obtained using: `mm.config["image"] ["pix size"]`

Returns **volume** – volume in um^3

Return type `float` or `ndarray`

Notes

The computation of the volume is based on a full rotation of the upper and the lower halves of the contour from which the average is then used.

The volume is computed radially from the the center position given by `(pos_x, pos_y)`. For sufficiently smooth contours, such as densely sampled ellipses, the center position does not play an important role. For contours that are given on a coarse grid, as is the case for RT-DC, the center position must be given.

References

- Halpern et al. [HWT02], chapter 5, Section 5.4
- This is a translation from a [Matlab script](#) by Geoff Olynyk.

emodulus

Computation of apparent Young's modulus for RT-DC measurements

exception `dclab.features.emodulus.KnowWhatYouAreDoingWarning`

exception `dclab.features.emodulus.YoungsModulusLookupTableExceededWarning`

`dclab.features.emodulus.extrapolate_emodulus` (*lut, datax, deform, emod, deform_norm, deform_thresh=0.05, inplace=True*)

Use spline interpolation to fill in nan-values

When points (*datax, deform*) are outside the convex hull of the *lut*, then `scipy.interpolate.griddata()` returns nan-values.

With this function, some of these nan-values are extrapolated using `scipy.interpolate.SmoothBivariateSpline`. The supported extrapolation values are currently limited to those where the deformation is above 0.05.

A warning will be issued, because this is not really recommended.

Parameters

- **lut** (*ndarray of shape (N, 3)*) – The normalized (!! see `normalize()`) LUT (first axis is points, second axis enumerates *datax*, *deform*, and *emodulus*)
- **datax** (*ndarray of size N*) – The normalized x data (corresponding to *lut[:, 0]*)
- **deform** (*ndarray of size N*) – The normalized deform (corresponding to *lut[:, 1]*)
- **emod** (*ndarray of size N*) – The emodulus (corresponding to *lut[:, 2]*); If *emod* does not contain nan-values, there is nothing to do here.
- **deform_norm** (*float*) – The normalization value used to normalize *lut[:, 1]* and *deform*.
- **deform_thresh** (*float*) – Not the entire LUT is used for bivariate spline interpolation. Only the points where *lut[:, 1] > deform_thresh/deform_norm* are used. This is necessary, because for small deformations, the LUT has an extreme slope that kills any meaningful spline interpolation.

`dclab.features.emodulus.get_emodulus` (*area_um=None, deform=None, volume=None, medium='CellCarrier', channel_width=20.0, flow_rate=0.16, px_um=0.34, temperature=23.0, lut_data='FEM-2Daxis', extrapolate=False, copy=True*)

Compute apparent Young's modulus using a look-up table

Parameters

- **area_um** (*float or ndarray*) – Apparent (2D image) area [μm^2] of the event(s)
- **deform** (*float or ndarray*) – Deformation (1-circularity) of the event(s)
- **volume** (*float or ndarray*) – Apparent volume of the event(s). It is not possible to define *volume* and *area_um* at the same time (makes no sense).

New in version 0.25.0.

- **medium** (*str or float*) – The medium to compute the viscosity for. If a string is given, the viscosity is computed. If a float is given, this value is used as the viscosity in $\text{mPa}\cdot\text{s}$ (Note that *temperature* must be set to *None* in this case).
- **channel_width** (*float*) – The channel width [μm]
- **flow_rate** (*float*) – Flow rate [$\mu\text{L/s}$]
- **px_um** (*float*) – The detector pixel size [μm] used for pixelation correction. Set to zero to disable.
- **temperature** (*float, ndarray, or None*) – Temperature [$^{\circ}\text{C}$] of the event(s)

- **lut_data** (*path, str, or tuple of (np.ndarray of shape (N, 3), dict)*) – The LUT data to use. If it is a key in `INTERNAL_LUTS`, then the respective LUT will be used. Otherwise, a path to a file on disk or a tuple (LUT array, meta data) is possible. The LUT meta data is used to check whether the given features (e.g. `area_um` and `deform`) are valid interpolation choices.

New in version 0.25.0.

- **extrapolate** (*bool*) – Perform extrapolation using `extrapolate_emodulus()`. This is discouraged!
- **copy** (*bool*) – Copy input arrays. If set to false, input arrays are overridden.

Returns `elasticity` – Apparent Young’s modulus in kPa

Return type `float` or `ndarray`

Notes

- The look-up table used was computed with finite elements methods according to [MMM+17] and complemented with analytical isoelastics from [MOG+15]. The original simulation results are available on figshare [WMM+20].
- The computation of the Young’s modulus takes into account a correction for the viscosity (medium, channel width, flow rate, and temperature) [MOG+15] and a correction for pixelation for the deformation which were derived from a (pixelated) image [Her17].
- Note that while deformation is pixelation-corrected, `area_um` and volume are scaled to match the LUT data. This is somewhat fortunate, because we don’t have to worry about the order of applying pixelation correction and scale conversion.
- By using external LUTs, it is possible to interpolate on the volume-deformation plane. This feature was added in version 0.25.0.

See also:

`dclab.features.emodulus.viscosity.get_viscosity()` compute viscosity for known media

`dclab.features.emodulus.load_lut(lut_data='FEM-2Daxis')`

Load LUT data from disk

Parameters **lut_data** (*path, str, or tuple of (np.ndarray of shape (N, 3), dict)*) – The LUT data to use. If it is a key in `INTERNAL_LUTS`, then the respective LUT will be used. Otherwise, a path to a file on disk or a tuple (LUT array, meta data) is possible.

Returns

- **lut** (*np.ndarray of shape (N, 3)*) – The LUT data for interpolation
- **meta** (*dict*) – The LUT metadata

Notes

If `lut_data` is a tuple of (lut, meta), then nothing is actually done (this is implemented for user convenience).

`dclab.features.emodulus.load_mtext(path)`

Load column-based data from text files with metadata

This file format is used for isoelasticity lines and look-up table data in dclab.

The text file is loaded with `numpy.loadtxt`. The metadata are stored as a json task between the “BEGIN METADATA” and the “END METADATA” tags. The last comment (#) line before the actual data defines the features with units in square brackets and tab-separated. For instance:

```
# [...] ## BEGIN METADATA # { # "authors": "A. Mietke, C. Herold, J. Guck", # "channel_width": 20.0, # "channel_width_unit": "um", # "date": "2018-01-30", # "dimensionality": "2Daxis", # "flow_rate": 0.04, # "flow_rate_unit": "uL/s", # "fluid_viscosity": 15.0, # "fluid_viscosity_unit": "mPa s", # "method": "analytical", # "model": "linear elastic", # "publication": "https://doi.org/10.1016/j.bpj.2015.09.006", # "software": "custom Matlab code", # "summary": "2D-axis-symmetric analytical solution" # } # END METADATA ## [...] ## area_um [um^2] deform emodulus [kPa] 3.75331e+00 5.14496e-03 9.30000e-01 4.90368e+00 6.72683e-03 9.30000e-01 6.05279e+00 8.30946e-03 9.30000e-01 7.20064e+00 9.89298e-03 9.30000e-01 [...]
```

```
dclab.features.emodulus.normalize(data, dmax)
```

Perform normalization in-place for interpolation

Note that `scipy.interpolate.griddata()` has a *rescale* option which rescales the data onto the unit cube. For some reason this does not work well with LUT data, so we just normalize it by dividing by the maximum value.

```
dclab.features.emodulus.INACCURATE_SPLINE_EXTRAPOLATION = False
```

Set this to True to globally enable spline extrapolation when the *area_um/deform* data are outside of a LUT. This is discouraged and a *KnowWhatYouAreDoingWarning* warning will be issued.

```
dclab.features.emodulus.INTERNAL_LUTS = {'FEM-2Daxis': 'emodulus_lut.txt'}
```

Dictionary of look-up tables shipped with dclab.

Pixelation correction definitions

```
dclab.features.emodulus.pxcorr.corr_deform_with_area_um(area_um, px_um=0.34)
```

Deformation correction for area_um-deform data

The contour in RT-DC measurements is computed on a pixelated grid. Due to sampling problems, the measured deformation is overestimated and must be corrected.

The correction formula is described in [Her17].

Parameters

- **area_um** (*float* or *ndarray*) – Apparent (2D image) area in μm^2 of the event(s)
- **px_um** (*float*) – The detector pixel size in μm .

Returns **deform_delta** – Error of the deformation of the event(s) that must be subtracted from *deform*. $\text{deform_corr} = \text{deform} - \text{deform_delta}$

Return type *float* or *ndarray*

```
dclab.features.emodulus.pxcorr.corr_deform_with_volume(volume, px_um=0.34)
```

Deformation correction for volume-deform data

The contour in RT-DC measurements is computed on a pixelated grid. Due to sampling problems, the measured deformation is overestimated and must be corrected.

The correction is derived in `scripts/pixelation_correction.py`.

Parameters

- **volume** (*float* or *ndarray*) – The “volume” feature (rotation of raw contour) [μm^3]
- **px_um** (*float*) – The detector pixel size in μm .

Returns **deform_delta** – Error of the deformation of the event(s) that must be subtracted from *deform*. $\text{deform_corr} = \text{deform} - \text{deform_delta}$

Return type `float` or `ndarray`

`dclab.features.emodulus.pxcorr.get_pixelation_delta` (*feat_corr*, *feat_absc*, *data_absc*,
px_um=0.34)

Convenience function for obtaining pixelation correction

Parameters

- **feat_corr** (*str*) – Feature for which to compute the pixelation correction (e.g. “deform”)
- **feat_absc** (*str*) – Feature with which to compute the correction (e.g. “area_um”);
- **data_absc** (*ndarray or float*) – Corresponding data for *feat_absc*
- **px_um** (*float*) – Detector pixel size [μm]

`dclab.features.emodulus.pxcorr.get_pixelation_delta_pair` (*feat1*, *feat2*, *data1*, *data2*,
px_um=0.34)

Convenience function that returns pixelation correction pair

Scale conversion applicable to a linear elastic model

`dclab.features.emodulus.scale_linear.convert` (*area_um*, *deform*, *channel_width_in*,
channel_width_out, *emodulus*=None,
flow_rate_in=None, *flow_rate_out*=None,
viscosity_in=None, *viscosity_out*=None,
inplace=False)

convert area-deformation-emodulus triplet

The conversion formula is described in [MOG+15].

Parameters

- **area_um** (*ndarray*) – Convex cell area [μm^2]
- **deform** (*ndarray*) – Deformation
- **channel_width_in** (*float*) – Original channel width [μm]
- **channel_width_out** (*float*) – Target channel width [μm]
- **emodulus** (*ndarray*) – Young’s Modulus [kPa]
- **flow_rate_in** (*float*) – Original flow rate [$\mu\text{L/s}$]
- **flow_rate_out** (*float*) – Target flow rate [$\mu\text{L/s}$]
- **viscosity_in** (*float*) – Original viscosity [mPa*s]
- **viscosity_out** (*float or ndarray*) – Target viscosity [mPa*s]; This can be an array
- **inplace** (*bool*) – If True, override input arrays with corrected data

Returns

- **area_um_corr** (*ndarray*) – Corrected cell area [μm^2]
- **deform_corr** (*ndarray*) – Deformation (a copy if *inplace* is False)
- **emodulus_corr** (*ndarray*) – Corrected emodulus [kPa]; only returned if *emodulus* is given.

Notes

If only *area_um*, *deform*, *channel_width_in* and *channel_width_out* are given, then only the area is corrected and returned together with the original deform. If all other arguments are not set to None, the emodulus is corrected and returned as well.

```
dclab.features.emodulus.scale_linear.scale_area_um(area_um, channel_width_in, chan-
                                                    nel_width_out,    inplace=False,
                                                    **kwargs)
```

Perform scale conversion for area_um (linear elastic model)

The area scales with the characteristic length “channel radius” L according to $(L'/L)^2$.

The conversion formula is described in [MOG+15].

Parameters

- **area_um** (*ndarray*) – Convex area [μm^2]
- **channel_width_in** (*float*) – Original channel width [μm]
- **channel_width_out** (*float*) – Target channel width [μm]
- **inplace** (*bool*) – If True, override input arrays with corrected data
- **kwargs** – not used

Returns **area_um_corr** – Scaled area [μm^2]

Return type *ndarray*

```
dclab.features.emodulus.scale_linear.scale_emodulus(emodulus,    channel_width_in,
                                                    channel_width_out,
                                                    flow_rate_in,    flow_rate_out,
                                                    viscosity_in,    viscosity_out,
                                                    inplace=False)
```

Perform scale conversion for area_um (linear elastic model)

The conversion formula is described in [MOG+15].

Parameters

- **emodulus** (*ndarray*) – Young’s Modulus [kPa]
- **channel_width_in** (*float*) – Original channel width [μm]
- **channel_width_out** (*float*) – Target channel width [μm]
- **flow_rate_in** (*float*) – Original flow rate [$\mu\text{L/s}$]
- **flow_rate_out** (*float*) – Target flow rate [$\mu\text{L/s}$]
- **viscosity_in** (*float*) – Original viscosity [mPa*s]
- **viscosity_out** (*float or ndarray*) – Target viscosity [mPa*s]; This can be an array
- **inplace** (*bool*) – If True, override input arrays with corrected data

Returns **emodulus_corr** – Scaled emodulus [kPa]

Return type *ndarray*

```
dclab.features.emodulus.scale_linear.scale_feature(feat,    data,    inplace=False,
                                                    **scale_kw)
```

Convenience function for scale conversions (linear elastic model)

This method wraps around all the other `scale_*` methods and also supports `deform/circ`.

Parameters

- **feat** (*str*) – Valid scalar feature name
- **data** (*float* or *ndarray*) – Feature data
- **inplace** (*bool*) – If True, override input arrays with corrected data
- ****scale_kw** – Scale keyword arguments for the wrapped methods

`dclab.features.emodulus.scale_linear.scale_volume` (*volume*, *channel_width_in*, *channel_width_out*, *inplace=False*, ***kwargs*)

Perform scale conversion for volume (linear elastic model)

The volume scales with the characteristic length “channel radius” L according to $(L'/L)^3$.

Parameters

- **volume** (*ndarray*) – Volume [μm^3]
- **channel_width_in** (*float*) – Original channel width [μm]
- **channel_width_out** (*float*) – Target channel width [μm]
- **inplace** (*bool*) – If True, override input arrays with corrected data
- **kwargs** – not used

Returns `volume_corr` – Scaled volume [μm^3]

Return type `ndarray`

Viscosity computation for various media

exception `dclab.features.emodulus.viscosity.TemperatureOutOfRangeWarning`

`dclab.features.emodulus.viscosity.get_viscosity` (*medium='CellCarrier'*, *channel_width=20.0*, *flow_rate=0.16*, *temperature=23.0*)

Returns the viscosity for RT-DC-specific media

Media that are not pure (e.g. ketchup or polymer solutions) often exhibit a non-linear relationship between shear rate (determined by the velocity profile) and shear stress (determined by pressure differences). If the shear stress grows non-linearly with the shear rate resulting in a slope in log-log space that is less than one, then we are talking about shear thinning. The viscosity is not a constant anymore (as it is e.g. for water). At higher flow rates, the viscosity becomes smaller, following a power law. Christoph Herold characterized shear thinning for the CellCarrier media [Her17]. The resulting formulae for computing the viscosities of these media at different channel widths, flow rates, and temperatures, are implemented here.

Parameters

- **medium** (*str*) – The medium to compute the viscosity for; Valid values are defined in `KNOWN_MEDIA`.
- **channel_width** (*float*) – The channel width in μm
- **flow_rate** (*float*) – Flow rate in $\mu\text{L/s}$
- **temperature** (*float* or *ndarray*) – Temperature in $^{\circ}\text{C}$

Returns `viscosity` – Viscosity in $\text{mPa}\cdot\text{s}$

Return type `float` or `ndarray`

Notes

- CellCarrier and CellCarrier B media are optimized for RT-DC measurements.
- Values for the viscosity of water are computed using equation (15) from [KSW78].
- A *TemperatureOutOfRangeWarning* is issued if the input temperature range exceeds the temperature ranges given by [Her17] and [KSW78].

```
dclab.features.emodulus.viscosity.KNOWN_MEDIA = ['CellCarrier', 'CellCarrierB', 'water']
```

Media for which computation of viscosity is defined

fluorescence

```
dclab.features.fl_crosstalk.correct_crosstalk(fl1, fl2, fl3, fl_channel, ct21=0, ct31=0,
                                              ct12=0, ct32=0, ct13=0, ct23=0)
```

Perform crosstalk correction

Parameters

- **fl1** (*int*, *float*, or *np.ndarray*) – Measured fluorescence signals
- **fl_channel** (*int* (1, 2, or 3)) – The channel number for which the crosstalk-corrected signal should be computed
- **cij** (*float*) – Spill (crosstalk or bleed-through) from channel i to channel j This spill is computed from the fluorescence signal of e.g. single-stained positive control cells; It is defined by the ratio of the fluorescence signals of the two channels, i.e $c_{ij} = f_{lj} / f_{li}$.

See also:

get_compensation_matrix() compute the inverse crosstalk matrix

Notes

If there are only two channels (e.g. fl1 and fl2), then the crosstalk to and from the other channel (ct31, ct32, ct13, ct23) should be set to zero.

```
dclab.features.fl_crosstalk.get_compensation_matrix(ct21, ct31, ct12, ct32, ct13, ct23)
```

Compute crosstalk inversion matrix

The spillover matrix is

```
| c11 c12 c13 |
| c21 c22 c23 |
| c31 c32 c33 |
```

The diagonal elements are set to 1, i.e.

$c_{11} = c_{22} = c_{33} = 1$

Parameters **cij** (*float*) – Spill from channel i to channel j

Returns **inv** – Compensation matrix (inverted spillover matrix)

Return type *np.ndarray*

5.4.3 isoelastics

Isoelastics management

exception `dclab.isoelastics.IsoelasticsEmodulusMeaninglessWarning`

class `dclab.isoelastics.Isoelastics` (*paths=[]*)

Isoelasticity line management

Changed in version 0.24.0: The isoelasticity lines of the analytical model [MOG+15] and the linear-elastic numerical model [MMM+17] were recomputed with an equidistant spacing. The metadata section of the text file format was restructured.

add (*isoel, col1, col2, channel_width, flow_rate, viscosity, method*)

Add isoelastics

Parameters

- **isoel** (*list of ndarrays*) – Each list item resembles one isoelastic line stored as an array of shape (N,3). The last column contains the emodulus data.
- **col1** (*str*) – Name of the first feature of all isoelastics (e.g. `isoel[0][:,0]`)
- **col2** (*str*) – Name of the second feature of all isoelastics (e.g. `isoel[0][:,1]`)
- **channel_width** (*float*) – Channel width in μm
- **flow_rate** (*float*) – Flow rate through the channel in $\mu\text{L/s}$
- **viscosity** (*float*) – Viscosity of the medium in $\text{mPa}\cdot\text{s}$
- **method** (*str*) – The method used to compute the isoelastics (must be one of `VALID_METHODS`).

Notes

The following isoelastics are automatically added for user convenience:

- isoelastics with *col1* and *col2* interchanged
- isoelastics for circularity if deformation was given

static add_px_err (*isoel, col1, col2, px_um, inplace=False*)

Undo pixelation correction

Since isoelasticity lines are usually computed directly from the simulation data (e.g. the contour data are not discretized on a grid but are extracted from FEM simulations), they are not affected by pixelation effects as described in [Her17].

If the isoelasticity lines are displayed alongside experimental data (which are affected by pixelation effects), then the lines must be “un”-corrected, i.e. the pixelation error must be added to the lines to match the experimental data.

Parameters

- **isoel** (*list of 2d ndarrays of shape (N, 3)*) – Each item in the list corresponds to one isoelasticity line. The first column is defined by *col1*, the second by *col2*, and the third column is the emodulus.
- **col2** (*col1,*) – Define the first two columns of each isoelasticity line.
- **px_um** (*float*) – Pixel size [μm]

static convert (*isoel*, *col1*, *col2*, *channel_width_in*, *channel_width_out*, *flow_rate_in*, *flow_rate_out*, *viscosity_in*, *viscosity_out*, *inplace=False*)
 Perform isoelastics scale conversion

Parameters

- **isoel** (*list of 2d ndarrays of shape (N, 3)*) – Each item in the list corresponds to one isoelasticity line. The first column is defined by *col1*, the second by *col2*, and the third column is the emodulus.
- **col1** (*col1*,) – Define the first to columns of each isoelasticity line. One of [“area_um”, “circ”, “deform”]
- **channel_width_in** (*float*) – Original channel width [μm]
- **channel_width_out** (*float*) – Target channel width [μm]
- **flow_rate_in** (*float*) – Original flow rate [μL/s]
- **flow_rate_out** (*float*) – Target flow rate [μL/s]
- **viscosity_in** (*float*) – Original viscosity [mPa*s]
- **viscosity_out** (*float*) – Target viscosity [mPa*s]

Returns **isoel_scale** – The scale-converted isoelasticity lines.

Return type list of 2d ndarrays of shape (N, 3)

Notes

If only the positions of the isoelastics are of interest and not the value of the elastic modulus, then it is sufficient to supply values for the channel width and set the values for flow rate and viscosity to a constant (e.g. 1).

See also:

[`dclab.features.emodulus.scale_linear.scale_feature\(\)`](#) scale conversion method used

get (*col1*, *col2*, *method*, *channel_width*, *flow_rate=None*, *viscosity=None*, *add_px_err=False*, *px_um=None*)
 Get isoelastics

Parameters

- **col1** (*str*) – Name of the first feature of all isoelastics (e.g. `isoel[0][:,0]`)
- **col2** (*str*) – Name of the second feature of all isoelastics (e.g. `isoel[0][:,1]`)
- **method** (*str*) – The method used to compute the isoelastics (must be one of `VALID_METHODS`).
- **channel_width** (*float*) – Channel width in μm
- **flow_rate** (float or *None*) – Flow rate through the channel in μL/s. If set to *None*, the flow rate of the imported data will be used (only do this if you do not need the correct values for elastic moduli).
- **viscosity** (float or *None*) – Viscosity of the medium in mPa*s. If set to *None*, the flow rate of the imported data will be used (only do this if you do not need the correct values for elastic moduli).

- **add_px_err** (*bool*) – If True, add pixelation errors according to C. Herold (2017), <https://arxiv.org/abs/1704.00572> and scripts/pixelation_correction.py
- **px_um** (*float*) – Pixel size [μm], used for pixelation error computation

See also:

`dclab.features.emodulus.scale_linear.scale_feature()` scale conversion method used

`dclab.features.emodulus.pxcorr.get_pixelation_delta()` pixelation correction (applied to the feature data)

get_with_rtdcbase (*col1, col2, method, dataset, viscosity=None, add_px_err=False*)
Convenience method that extracts the metadata from RTDCBase

Parameters

- **col1** (*str*) – Name of the first feature of all isoelastics (e.g. `isoel[0][:,0]`)
- **col2** (*str*) – Name of the second feature of all isoelastics (e.g. `isoel[0][:,1]`)
- **method** (*str*) – The method used to compute the isoelastics (must be one of `VALID_METHODS`).
- **dataset** (`dclab.rtdc_dataset.RTDCBase`) – The dataset from which to obtain the metadata.
- **viscosity** (*float, None, or False*) – Viscosity of the medium in $\text{mPa}\cdot\text{s}$. If set to *None*, the viscosity is computed from the meta data (medium, flow rate, channel width, temperature) in the [setup] config section. If this is not possible, the flow rate of the imported data is used and a warning will be issued.
- **add_px_err** (*bool*) – If True, add pixelation errors according to C. Herold (2017), <https://arxiv.org/abs/1704.00572> and scripts/pixelation_correction.py

load_data (*path*)
Load isoelastics from a text file

Parameters *path* (*str*) – Path to an isoelasticity lines text file

class `dclab.isoelastics.IsoelasticsDict`

`dclab.isoelastics.get_default()`
Return default isoelasticity lines

5.4.4 kde_contours

`dclab.kde_contours.find_contours_level` (*density, x, y, level, closed=False*)
Find iso-valued density contours for a given level value

Parameters

- **density** (*2d ndarray of shape (M, N)*) – Kernel density estimate for which to compute the contours
- **x** (*2d ndarray of shape (M, N) or 1d ndarray of size M*) – X-values corresponding to *density*
- **y** (*2d ndarray of shape (M, N) or 1d ndarray of size M*) – Y-values corresponding to *density*

- **level** (*float between 0 and 1*) – Value along which to find contours in *density* relative to its maximum

Returns **contours** – Contours found for the given level value

Return type list of ndarrays of shape (P, 2)

See also:

`skimage.measure.find_contours()` Contour finding algorithm used

`dclab.kde_contours.get_quantile_levels(density, x, y, xp, yp, q, normalize=True)`

Compute density levels for given quantiles by interpolation

For a given 2D density, compute the density levels at which the resulting contours contain the fraction $1-q$ of all data points. E.g. for a measurement of 1000 events, all contours at the level corresponding to a quantile of $q=0.95$ (95th percentile) contain 50 events (5%).

Parameters

- **density** (*2d ndarray of shape (M, N)*) – Kernel density estimate for which to compute the contours
- **x** (*2d ndarray of shape (M, N) or 1d ndarray of size M*) – X-values corresponding to *density*
- **y** (*2d ndarray of shape (M, N) or 1d ndarray of size M*) – Y-values corresponding to *density*
- **xp** (*1d ndarray of size D*) – Event x-data from which to compute the quantile
- **yp** (*1d ndarray of size D*) – Event y-data from which to compute the quantile
- **q** (*array_like or float between 0 and 1*) – Quantile along which to find contours in *density* relative to its maximum
- **normalize** (*bool*) – Whether output levels should be normalized to the maximum of *density*

Returns **level** – Contours level(s) corresponding to the given quantile

Return type np.ndarray or float

Notes

NaN-values events in *xp* and *yp* are ignored.

5.4.5 kde_methods

Kernel Density Estimation methods

`dclab.kde_methods.bin_num_doane(a)`

Compute number of bins based on Doane's formula

Notes

If the bin width cannot be determined, then a bin number of 5 is returned.

See also:

`bin_width_doane()` method used to compute the bin width

`dclab.kde_methods.bin_width_doane(a)`
Compute contour spacing based on Doane's formula

References

- https://en.wikipedia.org/wiki/Histogram#Number_of_bins_and_width
- <https://stats.stackexchange.com/questions/55134/doanes-formula-for-histogram-binning>

Notes

Doane's formula is actually designed for histograms. This function is kept here for backwards-compatibility reasons. It is highly recommended to use `bin_width_percentile()` instead.

`dclab.kde_methods.bin_width_percentile(a)`
Compute contour spacing based on data percentiles

The 10th and the 90th percentile of the input data are taken. The spacing then computes to the difference between those two percentiles divided by 23.

Notes

The Freedman–Diaconis rule uses the interquartile range and normalizes to the third root of `len(a)`. Such things do not work very well for RT-DC data, because `len(a)` is huge. Here we use just the top and bottom 10th percentiles with a fixed normalization.

`dclab.kde_methods.get_bad_vals(x, y)`

`dclab.kde_methods.ignore_nan_inf(kde_method)`
Ignores nans and infs from the input data

Invalid positions in the resulting density are set to nan.

`dclab.kde_methods.kde_gauss(events_x, events_y, xout=None, yout=None, *args, **kwargs)`
Gaussian Kernel Density Estimation

Parameters

- **events_y** (*events_x*,) – The input points for kernel density estimation. Input is flattened automatically.
- **yout** (*xout*,) – The coordinates at which the KDE should be computed. If set to none, input coordinates are used.

Returns **density** – The KDE for the points in (*xout*, *yout*)

Return type ndarray, same shape as *xout*

See also:

`scipy.stats.gaussian_kde`

Notes

This is a wrapped version that ignores nan and inf values.

`dclab.kde_methods.kde_histogram(events_x, events_y, xout=None, yout=None, *args, **kwargs)`
Histogram-based Kernel Density Estimation

Parameters

- **events_y** (*events_x*,) – The input points for kernel density estimation. Input is flattened automatically.
- **yout** (*xout*,) – The coordinates at which the KDE should be computed. If set to none, input coordinates are used.
- **bins** (*tuple* (*binsx*, *binsy*)) – The number of bins to use for the histogram.

Returns **density** – The KDE for the points in (*xout*, *yout*)

Return type ndarray, same shape as *xout*

See also:

numpy.histogram2d *scipy.interpolate.RectBivariateSpline*

Notes

This is a wrapped version that ignores nan and inf values.

`dclab.kde_methods.kde_multivariate(events_x, events_y, xout=None, yout=None, *args, **kwargs)`
Multivariate Kernel Density Estimation

Parameters

- **events_y** (*events_x*,) – The input points for kernel density estimation. Input is flattened automatically.
- **bw** (*tuple* (*bw_x*, *bw_y*) or *None*) – The bandwidth for kernel density estimation.
- **yout** (*xout*,) – The coordinates at which the KDE should be computed. If set to none, input coordinates are used.

Returns **density** – The KDE for the points in (*xout*, *yout*)

Return type ndarray, same shape as *xout*

See also:

statsmodels.nonparametric.kernel_density.KDEMultivariate

Notes

This is a wrapped version that ignores nan and inf values.

`dclab.kde_methods.kde_none(events_x, events_y, xout=None, yout=None)`
No Kernel Density Estimation

Parameters

- **events_y** (*events_x*,) – The input points for kernel density estimation. Input is flattened automatically.

- **yout** (*xout*,) – The coordinates at which the KDE should be computed. If set to none, input coordinates are used.

Returns **density** – The KDE for the points in (*xout*, *yout*)

Return type ndarray, same shape as *xout*

Notes

This method is a convenience method that always returns ones in the shape that the other methods in this module produce.

5.4.6 polygon_filter

exception dclab.polygon_filter.FilterIdExistsWarning

exception dclab.polygon_filter.PolygonFilterError

class dclab.polygon_filter.PolygonFilter (*axes=None, points=None, inverted=False, name=None, filename=None, fileid=0, unique_id=None*)

An object for filtering RTDC data based on a polygonal area

Parameters

- **axes** (*tuple of str*) – The axes/features on which the polygon is defined. The first axis is the x-axis. Example: (“area_um”, “deform”).
- **points** (*array-like object of shape (N, 2)*) – The N coordinates (x,y) of the polygon. The exact order is important.
- **inverted** (*bool*) – Invert the polygon filter. This parameter is overridden if *filename* is given.
- **name** (*str*) – A name for the polygon (optional).
- **filename** (*str*) – A path to a .poly file as create by this classes’ *save* method. If *filename* is given, all other parameters are ignored.
- **fileid** (*int*) – Which filter to import from the file (starting at 0).
- **unique_id** (*int*) – An integer defining the unique id of the new instance.

Notes

The minimal arguments to this class are either *filename* OR (*axes*, *points*). If *filename* is set, all parameters are taken from the given .poly file.

static **clear_all_filters** ()

Remove all filters and reset instance counter

copy (*invert=False*)

Return a copy of the current instance

Parameters **invert** (*bool*) – The copy will be inverted w.r.t. the original

filter (*datax, datay*)

Filter a set of datax and datay according to *self.points*

static `get_instance_from_id(unique_id)`
 Get an instance of the *PolygonFilter* using a unique id

static `import_all(path)`
 Import all polygons from a .poly file.
 Returns a list of the imported polygon filters

static `instace_exists(unique_id)`
 Determine whether an instance with this unique id exists

static `point_in_poly(p, poly)`
 Determine whether a point is within a polygon area
 Uses the ray casting algorithm.

Parameters

- **p** (*tuple of floats*) – Coordinates of the point
- **poly** (*array_like of shape (N, 2)*) – Polygon (*PolygonFilter.points*)

Returns `inside` – *True*, if point is inside.

Return type `bool`

Notes

If *p* lies on a side of the polygon, it is defined as

- “inside” if it is on the lower or left
- “outside” if it is on the top or right

Changed in version 0.24.1: The new version uses the cython implementation from scikit-image. In the old version, the inside/outside definition was the other way around. In favor of not having to modify upstram code, the scikit-image version was adapted.

static `remove(unique_id)`
 Remove a polygon filter from *PolygonFilter.instances*

save (*polyfile, ret_fobj=False*)
 Save all data to a text file (appends data if file exists).

Polyfile can be either a path to a file or a file object that was opened with the write “w” parameter. By using the file object, multiple instances of this class can write their data.

If *ret_fobj* is *True*, then the file object will not be closed and returned.

static `save_all(polyfile)`
 Save all polygon filters

static `unique_id_exists(pid)`
 Whether or not a filter with this unique id exists

hash
 Hash of *axes*, *points*, and *inverted*

instances = [*dclab.polygon_filter.PolygonFilter* object>]

points

`dclab.polygon_filter.get_polygon_filter_names()`
 Get the names of all polygon filters in the order of creation

5.4.7 statistics

Statistics computation for RT-DC dataset instances

exception `dclab.statistics.BadMethodWarning`

class `dclab.statistics.Statistics` (*name, method, req_feature=False*)

A helper class for computing statistics

All statistical methods are registered in the dictionary `Statistics.available_methods`.

get_feature (*ds, feat*)

Return filtered feature data

The features are filtered according to the user-defined filters, using the information in `ds.filter.all`. In addition, all *nan* and *inf* values are purged.

Parameters

- **ds** (`dclab.rtdc_dataset.RTDCBase`) – The dataset containing the feature
- **feat** (*str*) – The name of the feature; must be a scalar feature

`available_methods = {'%-gated': <dclab.statistics.Statistics object>, 'Events': <dcl`

`dclab.statistics.flow_rate` (*ds*)

Return the flow rate of an RT-DC dataset

`dclab.statistics.get_statistics` (*ds, methods=None, features=None*)

Compute statistics for an RT-DC dataset

Parameters

- **ds** (`dclab.rtdc_dataset.RTDCBase`) – The dataset for which to compute the statistics.
- **methods** (*list of str or None*) – The methods with which to compute the statistics. The list of available methods is given with `dclab.statistics.Statistics.available_methods.keys()` If set to *None*, statistics for all methods are computed.
- **features** (*list of str*) – Feature name identifiers are defined by `dclab.definitions.feature_exists`. If set to *None*, statistics for all scalar features available are computed.

Returns

- **header** (*list of str*) – The header (feature + method names) of the computed statistics.
- **values** (*list of float*) – The computed statistics.

`dclab.statistics.mode` (*data*)

Compute an intelligent value for the mode

The most common value in experimental is not very useful if there are a lot of digits after the comma. This method approaches this issue by rounding to bin size that is determined by the Freedman–Diaconis rule.

Parameters **data** (*1d ndarray*) – The data for which the mode should be computed.

Returns **mode** – The mode computed with the Freedman-Diaconis rule.

Return type *float*

5.5 R and lme4

exception dclab.lme4.rlibs.VersionError

class dclab.lme4.rlibs.MockRPackage

dclab.lme4.rlibs.import_r_submodules()

exception dclab.lme4.rsetup.RNotFoundError

class dclab.lme4.rsetup.AutoRConsole

Helper class for catching R console output

By default, this console always returns “yes” when asked a question. If you need something different, you can subclass and override *consoleread* function. The console stream is recorded in *self.stream*.

close()

Remove the rpy2 monkeypatches

consoleread(prompt)

Read user input, returns “yes” by default

consolewrite_print(s)

consolewrite_warnerror(s)

get_prints()

get_warnerrors()

write_to_stream(topic, s)

lock = False

perform_lock = False

dclab.lme4.rsetup.check_r()

Make sure R is installed and R_HOME is set

dclab.lme4.rsetup.get_r_path()

Get the path of the R executable/binary from rpy2

dclab.lme4.rsetup.get_r_version()

dclab.lme4.rsetup.has_lme4()

Return True if the lme4 package is installed

dclab.lme4.rsetup.has_r()

Return True if R is available

dclab.lme4.rsetup.import_lme4()

dclab.lme4.rsetup.install_lme4()

Install the lme4 package (if not already installed)

The packages are installed to the user data directory given in *lib_path*.

dclab.lme4.rsetup.set_r_path(r_path)

Set the path of the R executable/binary for rpy2

R lme4 wrapper

exception dclab.lme4.wrapr.Lme4InstallWarning

class dclab.lme4.wrapr.Rlme4(model='lmer', feature='deform')

Perform an R-lme4 analysis with RT-DC data

Parameters

- **model** (*str*) – One of:
 - "lmer": linear mixed model using lme4's `lmer`
 - "glmer+loglink": generalized linear mixed model using lme4's `glmer` with an additional a log-link function via the `family=Gamma(link='log')` keyword.
- **feature** (*str*) – Dclab feature for which to compute the model

add_dataset (*ds*, *group*, *repetition*)

Add a dataset to the analysis list

Parameters

- **ds** (*RTDCBase*) – Dataset
- **group** (*str*) – The group the measurement belongs to ("control" or "treatment")
- **repetition** (*int*) – Repetition of the measurement

Notes

- For each repetition, there must be a "treatment" and a "control" group.
- If you would like to perform a differential feature analysis, then you need to pass at least a reservoir and a channel dataset (with same parameters for *group* and *repetition*).

check_data ()

Perform sanity checks on `self.data`

fit (*model=None*, *feature=None*)

Perform (generalized) linear mixed-effects model fit

The response variable is modeled using two linear mixed effect models:

- model `Rlme4.r_func_model` (random intercept + random slope model)
- the null model `Rlme4.r_func_nullmodel` (without the fixed effect introduced by the "treatment" group).

Both models are compared in R using "anova" (from the R-package "stats" [Eve92]) which performs a likelihood ratio test to obtain the p-Value for the significance of the fixed effect (treatment).

If the input datasets contain data from the "reservoir" region, then the analysis is performed for the differential feature.

Parameters

- **model** (*str* (*optional*)) – One of:
 - "lmer": linear mixed model using lme4's `lmer`
 - "glmer+loglink": generalized linear mixed model using lme4's `glmer` with an additional log-link function via `family=Gamma(link='log')` [BMBW15]
- **feature** (*str* (*optional*)) – dclab feature for which to compute the model

Returns

results – Dictionary with the results of the fitting process:

- "anova p-value": Anova likelihood ratio test (significance)
- "feature": name of the feature used for the analysis `self.feature`

- "fixed effects intercept": Mean of `self.feature` for all controls; In the case of the "glmer+loglink" model, the intercept is already backtransformed from log space.
- "fixed effects treatment": The fixed effect size between the mean of the controls and the mean of the treatments relative to "fixed effects intercept"; In the case of the "glmer+loglink" model, the fixed effect is already backtransformed from log space.
- "fixed effects repetitions": The effects (intercept and treatment) for each repetition. The first axis defines intercept/treatment; the second axis enumerates the repetitions; thus the shape is (2, number of repetitions) and `np.mean(results["fixed effects repetitions"], axis=1)` is equivalent to the tuple `(results["fixed effects intercept"], results["fixed effects treatment"])` for the "lmer" model. This does not hold for the "glmer+loglink" model, because of the non-linear inverse transform back from log space.
- "is differential": Boolean indicating whether or not the analysis was performed for the differential (bootstrapped and subtracted reservoir from channel data) feature
- "model": model name used for the analysis `self.model`
- "r anova": Anova model (exposed from R)
- "r model summary": Summary of the model (exposed from R)
- "r model coefficients": Model coefficient table (exposed from R)
- "r stderr": errors and warnings from R
- "r stdout": standard output from R

Return type dict

get_differential_dataset()

Return the differential dataset for channel/reservoir data

The most famous use case is differential deformation. The idea is that you cannot tell what the difference in deformation from channel to reservoir is, because you never measure the same object in the reservoir and the channel. You usually just have two distributions. Comparing distributions is possible via bootstrapping. And then, instead of running the lme4 analysis with the channel deformation data, it is run with the differential deformation (subtraction of the bootstrapped deformation distributions for channel and reservoir).

get_feature_data(group, repetition, region='channel')

Return array containing feature data

Parameters

- **group** (*str*) – Measurement group ("control" or "treatment")
- **repetition** (*int*) – Measurement repetition
- **region** (*str*) – Either "channel" or "reservoir"

Returns `fdata` – Feature data (Nans and Infs removed)

Return type 1d ndarray

is_differential()

Return True if the differential feature is computed for analysis

This effectively just checks the regions of the datasets and returns True if any one of the regions is "reservoir".

See also:

`get_differential_features()` for an explanation

set_options (*model=None, feature=None*)

Set analysis options

data = None

list of [RTDCBase, column, repetition, chip_region]

feature = None

dclab feature for which to perform the analysis

model = None

modeling method to use (e.g. “lmer”)

r_func_model = None

model function

r_func_nullmodel = None

null model function

`dclab.lme4.wrapr.bootstrapped_median_distributions(a, b, bs_iter=1000, rs=117)`

Compute the bootstrapped distributions for two arrays.

Parameters

- **b** (*a*,) – Input data
- **bs_iter** (*int*) – Number of bootstrapping iterations to perform (outtput size).
- **rs** (*int*) – Random state seed for random number generator

Returns `median_dist_a`, `median_dist_b` – Bootstrap distribution of medians for a and b.

Return type 1d arrays of length `bs_iter`

See also:

[https://en.wikipedia.org/wiki/Bootstrapping_\(statistics\)](https://en.wikipedia.org/wiki/Bootstrapping_(statistics))

Notes

From a programmatical point of view, it would have been better to implement this method for just one input array (because of redundant code). However, due to historical reasons (testing and comparability to Shape-Out 1), bootstrapping is done interleaved for the two arrays.

5.6 machine learning

Reading and writing trained machine learning models for dclab

exception `dclab.ml.modc.ModelFormatExportFailedWarning`

`dclab.ml.modc.export_model(path, model, enforce_formats=None)`

Export an ML model to all possible formats

The model must be exportable with at least one method listed in `SUPPORTED_FORMATS`.

Parameters

- **path** (*str* or *pathlib.Path*) – Directory where the model is stored to. For each supported model, a new subdirectory or file is created.

- **model** (An instance of an ML model, NOT `dclab.ml.models.BaseModel`) – Trained model instance
- **enforce_formats** (list of str) – Enforced file formats for export. If the export for one of these file formats fails, a `ValueError` is raised.

`dclab.ml.modc.hash_path(path)`

Create a SHA256 hash of a file or all files in a directory

The files are sorted before hashing for reproducibility.

`dclab.ml.modc.load_modc(path, from_format=None)`

Load models from a `.modc` file for inference

Parameters

- **path** (str or path-like) – Path to a `.modc` file
- **from_format** (str) – If set to `None`, the first available format in `SUPPORTED_FORMATS` is used. If set to a key in `SUPPORTED_FORMATS`, then this format will take precedence and an error will be raised if loading with this format fails.

Returns **model** – Model that can be used for inference via `model.predict`

Return type `dclab.ml.models.BaseModel`

`dclab.ml.modc.save_modc(path, dc_models)`

Save ML models to a `.modc` file

Parameters

- **path** (str, `pathlib.Path`) – Output `.modc` path
- **dc_models** (list of `dclab.ml.models.BaseModel` or `dclab.ml.models.BaseModel`) – Models to save

Returns **meta** – Dictionary written to `index.json` in the `.modc` file

Return type `dict`

`dclab.ml.modc.SUPPORTED_FORMATS = {'tensorflow-SavedModel': {'class': <class 'dclab.ml.m...>}}`
Supported file formats (including respective model classes).

class `dclab.ml.models.BaseModel(bare_model, inputs, outputs, model_name=None, output_labels=None)`

Parameters

- **bare_model** – Underlying ML model
- **inputs** (list of str) – List of model input features, e.g. `["deform", "area_um"]`
- **outputs** (list of str) – List of output features the model provides in that order, e.g. `["ml_score_rbc", "ml_score_rtl", "ml_score_tfe"]`
- **model_name** (str or None) – The name of the models
- **output_labels** (list of str) – List of more descriptive labels for the features, e.g. `["red blood cell", "type 1 cell", "troll cell"]`.

get_dataset_features(ds, dtype=<class 'numpy.float32'>)

Return the dataset features used for inference

Parameters

- **ds** (`dclab.rtdc_dataset.RTDCBase`) – Dataset from which to retrieve the feature data
- **dtype** (`dtype`) – All features are cast to this dtype

Returns **fdata** – 2D array of shape `(len(ds), len(self.inputs))`; i.e. to access the array containing the first feature, for all events, you would do `fdata[:, 0]`.

Return type 2d ndarray

static load_bare_model (*path*)

Load an implementation-specific model from a file

This will set the `self.model` attribute. Make sure that the other attributes are set properly as well.

predict (*ds*)

Return the probabilities of `self.outputs` for *ds*

Parameters **ds** (`dclab.rtdc_dataset.RTDCBase`) – Dataset to apply the model to

Returns **ofdict** – Output feature dictionary with features as keys and 1d ndarrays as values.

Return type dict

Notes

This function calls `BaseModel.get_dataset_features()` to obtain the input feature matrix.

register ()

Register this model to the dclab ancillary features

static save_bare_model (*path*, *bare_model*, *save_format=None*)

Save an implementation-specific model to a file

Parameters

- **path** (*str or path-like*) – Path to store model to
- **bare_model** (*object*) – The implementation-specific bare model
- **save_format** (*str*) – Must be in `supported_formats`

static supported_formats ()

List of dictionaries containing model formats

Returns **fmts** – Each item contains the keys “name” (format name), “suffix” (saved file suffix), “requires” (Python dependencies).

Return type list

unregister ()

Unregister from dclab ancillary features

class `dclab.ml.models.TensorflowModel` (*bare_model*, *inputs*, *outputs*, *model_name=None*, *output_labels=None*)

Handle tensorflow models

Parameters

- **bare_model** – Underlying ML model
- **inputs** (*list of str*) – List of model input features, e.g. `["deform", "area_um"]`

- **outputs** (*list of str*) – List of output features the model provides in that order, e.g. ["ml_score_rbc", "ml_score_rtl", "ml_score_tfe"]
- **model_name** (*str or None*) – The name of the models
- **output_labels** (*list of str*) – List of more descriptive labels for the features, e.g. ["red blood cell", "type 1 cell", "troll cell"].

has_sigmoid_activation (*layer_config=None*)

Return True if final layer has “sigmoid” activation function

has_softmax_layer (*layer_config=None*)

Return True if final layer is a Softmax layer

static load_bare_model (*path*)

Load a tensorflow model

predict (*ds, batch_size=32*)

Return the probabilities of *self.outputs* for *ds*

Parameters

- **ds** (`dclab.rtdc_dataset.RTDCBase`) – Dataset to apply the model to
- **batch_size** (*int*) – Batch size for inference with tensorflow

Returns **ofdict** – Output feature dictionary with features as keys and 1d ndarrays as values.

Return type `dict`

Notes

Before prediction, this method asserts that the outputs of the model are converted to probabilities. If the final layer is one-dimensional and does not have a sigmoid activation, then a sigmoid activation layer is added (binary classification) `tf.keras.layers.Activation("sigmoid")`. If the final layer has more dimensions and is not a `tf.keras.layers.Softmax()` layer, then a softmax layer is added.

static save_bare_model (*path, bare_model, save_format='tensorflow-SavedModel'*)

Save a tensorflow model

static supported_formats ()

List of dictionaries containing model formats

Returns **fmts** – Each item contains the keys “name” (format name), “suffix” (saved file suffix), “requires” (Python dependencies).

Return type `list`

tensorflow helper functions for RT-DC data

```
dclab.ml.tf_dataset.assemble_tf_dataset_scalars(dc_data, feature_inputs, labels=None, split=0.0, shuffle=True, batch_size=32, dtype=<class 'numpy.float32'>)
```

Assemble a *tensorflow.data.Dataset* for scalar features

Scalar feature data are loaded directly into memory.

Parameters

- **dc_data** (*list of pathlib.Path, str, or dclab.rtdc_dataset.RTDCBase*) – List of source datasets (can be anything *dclab.new_dataset()* accepts).

- **feature_inputs** (*list of str*) – List of scalar feature names to extract from *paths*.
- **labels** (*list*) – Labels (e.g. an integer that classifies each element of *path*) used for training. Defaults to None (no labels).
- **split** (*float*) – If set to zero, only one dataset is returned; If set to a float between 0 and 1, a train and test dataset is returned. Please set *shuffle=True*.
- **shuffle** (*bool*) – If True (default), shuffle the dataset (A hard-coded seed is used for reproducibility).
- **batch_size** (*int*) – Batch size for training. The function *tf.data.Dataset.batch* is called with *batch_size* as its argument.
- **dtype** (*numpy.dtype*) – Desired dtype of the output data

Returns *train* [,*test*] – Dataset that can be used for training with tensorflow

Return type tensorflow.data.Dataset

```
dclab.ml.tf_dataset.get_dataset_event_feature(dc_data, feature,  
                                              tf_dataset_indices=None,  
                                              dc_data_indices=None, split_index=0,  
                                              split=0.0, shuffle=True)
```

Return RT-DC features for tensorflow Dataset indices

The functions *assemble_tf_dataset_** return a tensorflow.data.Dataset instance with all input data shuffled (or split). This function retrieves features using the *Dataset* indices, given the same parameters (*paths*, *split*, *shuffle*).

Parameters

- **dc_data** (*list of pathlib.Path, str, or dclab.rtdc_dataset.RTDCBase*) – List of source datasets (Must match the path list used to create the *tf.data.Dataset*).
- **feature** (*str*) – Name of the feature to retrieve
- **tf_dataset_indices** (*list-like*) – *tf.data.Dataset* indices corresponding to the events of interest. If None, all indices are used.
- **dc_data_indices** (*list of int*) – List with indices that correspond to the only items in *dc_data* for which the features should be returned.
- **split_index** (*int*) – The split index; 0 for the first part, 1 for the second part.
- **split** (*float*) – Splitting fraction (Must match the path list used to create the *tf.data.Dataset*)
- **shuffle** (*bool*) – Shuffling (Must match the path list used to create the *tf.data.Dataset*)

Returns *data* – Feature list with elements corresponding to the events given by *dataset_indices*.

Return type *list*

```
dclab.ml.tf_dataset.shuffle_array(arr, seed=42)
```

Shuffle a numpy array in-place reproducibly with a fixed seed

The shuffled array is also returned.

List of changes in-between dclab releases.

6.1 version 0.31

- feat: implement (generalized) linear mixed-effects models via a wrapper around R/lme4 using rpy2 (install with extra “lme4”)

6.2 version 0.30.1

- fix: *new_dataset* attempts to load DCOR dataset when given a non-existent path as a string (#81)

6.3 version 0.30.0

- BREAKING CHANGE: drop support for Python 2 (#34)
- feat: new machine learning (ML) submodule *dclab.ml*
- feat: implement ML model file format *.modc* (#78)
- feat: add tensorflow helper functions for RT-DC data
- setup: bump numpy>=1.17.0
- ref: minor improvements of code readability
- tests: set global temp dir and remove it after testing

6.4 version 0.29.1

- enh: lift restrictions on valid options for [setup]:medium (can now be any arbitrary string)

6.5 version 0.29.0

- feat: support the “image_bg” feature which contains the rolling mean background image computed by Shape-In

6.6 version 0.28.0

- feat: new CLI command dclab-split to split a large dataset into multiple smaller datasets

6.7 version 0.27.11

- fix: do not cache hierarchy child feature values; this might lead to intransparent situations where a child has different features than its parent (you cannot always rely on the user to call *apply_filter*)
- fix: hierarchy child configuration section “calculation” was not updated with the hierarchy parent values
- docs: add example for loading data from DCOR and computing the Young’s modulus

6.8 version 0.27.10

- fix: support unicode characters when writing HDF5 in Python2

6.9 version 0.27.9

- docs: add artwork
- fix: support unicode characters in sample names in Python2

6.10 version 0.27.8

- docs: add more information on emodulus computation
- docs: add script for visualizing emodulus LUTs

6.11 version 0.27.7

- ref: replace deprecated `.tostring()` with `.tobytes()`

6.12 version 0.27.6

- fix: video seek issue workaround also for the first 100 frames
- cli: also skip the final event in `tdms2rtdc` if the image is empty
- cli: renamed kwarg `-include-initial-empty-image` to `include-empty-boundary-images`
- enh: improve detection and recovery of missing images for `fmt_tdms`

6.13 version 0.27.5

- maintenance build

6.14 version 0.27.4

- maintenance build

6.15 version 0.27.3

- fix: ignore `ResourceWarning` due to unknown `_io.BufferedReader` in third-party software when converting `.tdms` to `.rtdc`

6.16 version 0.27.2

- maintenance build

6.17 version 0.27.1

- setup: bump `imageio` to 2.8.0 for `Python>=3.4`
- ref: removed `NoImageWarning` during export (warning is already issued by `fmt_tdms.event_image`)

6.18 version 0.27.0

- feat: introduce new feature names `ml_score_???` where `?` can be a digit or a lower-case letter of the alphabet ([#77](#))
- feat: introduce new functions `dclab.definitions.feature_exists` and `dclab.definitions.scalar_feature_exists` for checking the existence of features (including the `ml_score_???` features which are not in `dclab.definitions.feature_names`)
- feat: introduce ancillary feature `ml_class` which is defined by the `ml_score_???` features
- enh: `fmt_dict` automatically converts scalar features to arrays
- ref: replace check for `dclab.definitions.feature_names` by `dclab.definitions.feature_exists` where applicable

- ref: replace access of *dclab.definitions.feature_name2label* by *dclab.definitions.get_feature_label* where applicable
- ref: do not automatically fill up all the box filtering ranges in *RTDCBase.config["filtering"]* with zeros; raise *ValueError* if user forgets to set both ranges
- docs: major revision (promote Shape-Out 2 and DCOR)

6.19 version 0.26.2

- fix: *kde_methods.bin_num_doane* now uses 5 as default if it encounters nan or zero-division
- docs: updates related to Young's modulus computation

6.20 version 0.26.1

- enh: cache more online data in *fmt_dcor*
- enh: add *dclab.warn.PipelineWarning* which is used as a parent class for warnings that a user might be interested in
- fix: temperature warnings during emodulus computation revealed only the lower temperature limit of the data

6.21 version 0.26.0

- feat: implement volume-deformation isoelasticity lines (#70)
- fix: specifying an external LUT as ndarray did not work
- scripts: finish 'fem2iso_volume.py' for extracting volume- deformation isoelasticity lines
- scripts: add 'pixelation_correction.py' for visualizing pixelation effects on area_um, volume, and emodulus
- ref: renamed isoelasticity line text files

6.22 version 0.25.0

- fix: appending data to an hdf5 file results in a broken "index" feature (re-enumeration from 0), if the given dataset contains the "index_online" feature
- enh: allow to set external LUT files or LUT data when computing the Young's modulus with the *lut_data* keyword argument in *dclab.features.emodulus.get_emodulus*.
- ref: refactored *features.emodulus*: New submodules *pxcorr* and *scale_linear*; *convert* is deprecated in favor of *scale_feature*

6.23 version 0.24.8

- setup: include Python 3.8 builds and remove Python<=3.5 builds
- scripts: renamed 'extract_lut_and_iso.py' to 'fem2lutiso_std.py'

6.24 version 0.24.7

- fix: *ConfigurationDict.update* did not take into account invalid keys (everything is now done with (`__setitem__`'))

6.25 version 0.24.6

- maintenance release

6.26 version 0.24.5

- maintenance release

6.27 version 0.24.4

- maintenance release

6.28 version 0.24.3

- fix: *ConfigurationDict.update* did not actually perform the requested update (does not affect *Configuration.update*)
- enh: also use `points_in_polygon` from `scikit-image` to determine contour levels

6.29 version 0.24.2

- build: import new `skimage` submodules so that `PyInstaller` will find and use them

6.30 version 0.24.1

- enh: improve polygon filter speed by roughly two orders of magnitude with a cython version taken from `scikit-image`; there are only minor differences to the old implementation (top right point included vs. lower left point included), so this is not a breaking change (#23)

6.31 version 0.24.0

- data: refurbished LUT for linear elastic spheres provided by Dominic Mokbel and Lucas Wittwer (based on the FEM simulation results from <https://doi.org/10.6084/m9.figshare.12155064.v2>); compared to the old LUT, there is a relative error in Young's modulus below 0.1 %, which should not cause any breaking changes
- data: updated isoelasticity lines (better spacing): analytical data was made available by Christoph Herold, numerical data was interpolated from the new LUT

- scripts: added 'scripts/extract_lut_and_iso.py' for extracting Young's modulus LUT and isoelastics from FEM simulation data provided by Lucas Wittwer; this is now the default method for extracting new LUTs and isoelastics
- scripts: added 'scripts/fem2rtdc.py' for generating in-silico .rtdc datasets from FEM simulation data provided by Lucas Wittwer
- fix: dclab-verify-dataset failed when the "logs" group was not present in HDF5 files
- fix: use predefined chunks when writing HDF5 data to avoid exploding file sizes when writing one event at a time
- fix: create a deep copy of the metadata dictionary when writing HDF5 data because it leaked to subsequent calls
- ref: changed the way isoelasticity lines and emodulus LUTs are stored and loaded (e.g. json metadata and a few more sanity checks)

6.32 version 0.23.0

- feat: enable emodulus extrapolation for *area_um/deform* values outside of the given LUT.

6.33 version 0.22.7

- enh: dclab-verify-dataset now also checks whether the sheath and sample flow rates add up to the channel flow rate
- ref: Configuration does not anymore load unknown meta data keyword arguments, but ignores them. This implies that dclab-verify-dataset will not anymore check them actively. Instead, any warning issued when opening a file is added to the list of cues.
- setup: bump nptdms to 0.23.0

6.34 version 0.22.6

- fix: data export to HDF5 did not work when the "frame rate" is not given in the configuration

6.35 version 0.22.5

- enh: add checks for valid keys in the Configuration dictionary of a dataset *RTDCBase().config*; unknown keys will issue an *UnknownConfigurationKeyWarning* (#58)
- ref: moved *rtdc_dataset.fmt_hdf5.UnknownKeyWarning* to *rtdc_dataset.config.UnknownConfigurationKeyWarning*
- ref: renamed *rtdc_dataset.config.CaseInsensitiveDict* to *rtdc_dataset.config.ConfigurationDict* and added option to check new keys

6.36 version 0.22.4

- fix: disable computation of Young's modulus for reservoir measurements (#75)

- enh: new keyword argument *req_func* for *AncillaryFeature* to define additional logic for checking whether a feature is available for a given instance of *RTDCBase*.

6.37 version 0.22.3

- enh: add *data* property to ICues (and use it when checking for compression)

6.38 version 0.22.2

- fix: when computing the contour from the mask image, always use the longest contour - critical when the mask image contains artefacts
- fix: minor issue with dclab-verify-dataset when nptdms was not installed and an exception occurred
- enh: dclab-verify-dataset shows some info on data compression

6.39 version 0.22.1

- enh: remember working API Key
- docs: document DCOR format

6.40 version 0.22.0

- feat: implement DCOR client
- enh: improved .rtdc file format detection (with wrong extension)

6.41 version 0.21.2

- enh: dclab-verify-dataset now also checks HDF5 “mask” feature attributes
- setup: bump h5py to 2.10.0 (need *<object>.attrs.get_id*)

6.42 version 0.21.1

- fix: correct type of HDF5 image attributes for “mask” feature

6.43 version 0.21.0

- feat: implement new CLI dclab-repack
- fix: don’t write “logs” group to HDF5 files if there aren’t any
- fix: support HDF5 files that have no “logs” group

- docs: fix docstring of dclab-join

6.44 version 0.20.8

- fix: regression where old .tmds data could not be opened if they did not contain the “area_msd” feature
- fix: convert bytes logs to string in fmt_hdf5
- enh: support len(ds.logs) for fmt_hdf5
- enh: replace “info” by “build” in CLI job info

6.45 version 0.20.7

- fix: ensure file extension is .rtdc in dclab-join
- fix: correct “frame” and “index_online” features when exporting to hdf5
- enh: allow to set metadata dictionary in dclab.cli.join

6.46 version 0.20.6

- fix: typo in contour check resulted in small tolerance

6.47 version 0.20.5

- fix: be more trustful when it comes to contour data in the tdms file format; instead of raising errors, issue warnings (#72)

6.48 version 0.20.4

- ref: move integrity checks to new class check.IntegrityChecker
- docs: document remaining dictionaries in dclab.dfn

6.49 version 0.20.3

- docs: fix bad anchors

6.50 version 0.20.2

- ref: using temperature values outside the range for viscosity computation now issues a warning instead of raising an error; warnings were added for the CellCarrier buffers
- fix: handle number detection correctly in get_emodulus

6.51 version 0.20.1

- fix: always return an array when computing the KDE
- ref: make accessible static function `RTDCBase.get_kde_spacing`

6.52 version 0.20.0

- feat: compute elastic modulus from “temp” feature (#51)
- enh: computing isoelastics from datasets can use [setup]: “temperature” to compute the viscosity/emodulus (#51)
- enh: define new meta data key [setup]: “temperature”
- docs: add an advanced section on Young’s modulus computation (#51)

6.53 version 0.19.1

- fix: hierarchy children did not pass *force* argument to hierarchy parent when *apply_filter* is called
- fix: revert histogram2d “density” argument to “normed” to support numpy 1.10 (Shape-Out 1)
- fix: implement unambiguous `RTDCBase.__repr__`

6.54 version 0.19.0

- feat: added better contour spacing computation based on percentiles (`dclab.kde_methods.bin_width_percentile`)
- feat: add feature “index_online” which may be missing values (#71)
- feat: implement `__getstate__` and `__setstate__` for polygon filters
- fix: write UTF-8 BOM when exporting to .tsv
- enh: add check whether `unique_id` exists in `PolygonFilter`

6.55 version 0.18.0

- fix: correctly handle filtering when features are removed from a dataset
- ref: move `dclab.rtdc_dataset.util` to `dclab.util`
- ref: minor cleanup in computation of viscosity (support lower-case *medium* values, add `dclab.features.emodulus_viscosity.KNOWN_MEDIA`)
- ref: cleanup `dclab.rtdc_dataset.filter` (use logical operators, correctly display nan-warning messages, keep track of polygon filters, add consistency checks, improve readability)

6.56 version 0.17.1

- maintenance release

6.57 version 0.17.0

- feat: add command line script for compressing HDF5 (.rtdc) data “dclab-compress”
- enh: record warnings under “/log” for all command line scripts
- enh: set gzip data compression for all command line scripts

6.58 version 0.16.1

- fix: circumvent UnicodeDecodeErrors which occurred in frozen macOS binaries that use dclab
- enh: support subsecond accuracy in the the configuration key [experiment] time (e.g. “HH:MM:SS.SSS” instead of “HH:MM:SS”)
- enh: store the correct, relative measurement time in dclab-join (#63)

6.59 version 0.16.0

- fix: RTDCBase.downsample_scatter with ret_mask=True did not return boolean array of len(RTDCBase) as indicated in the docs
- ref: remove RTDCBase._plot_filter, which was confusing anyway
- ref: deprecate usage of RTDCBase._filter

6.60 version 0.15.0

- feat: add method RTDCBase.reset_filter
- feat: implement RTDCBase.features_loaded
- feat: allow to instantiate RTDC_Hierarchy without initially applying the filter
- fix: non-scalar columns of RTDC_Hierarchy did not implement len()
- docs: add an example script dedicated to data plotting
- ref: remove circular references between Filter and RTDCBase

6.61 version 0.14.8

- fix: Ignore feature “trace” when the trace folder exists but is empty (HDF5 format)
- fix: If no contour can be found, raise an error before other ancillary features produce cryptic errors

6.62 version 0.14.7

- enh: allow to add meta data when exporting to .fcs or .tsv (dclab version is saved by default)
- setup: bump fcswrite from 0.4.1 to 0.5.0

6.63 version 0.14.6

- fix: improved handling of tdms trace data (split trace with fixed samples per event to avoid ValueError when exporting to hdf5)
- fix: transposed roi size x/y config value when exporting to hdf5

6.64 version 0.14.5

- cli: write warning messages to logs in tdms2rtdc
- ref: increase verbosity of warning messages

6.65 version 0.14.4

- fix: discard trace data when “samples per event” has multiple values for tdms data
- fix: prefer image shape over config keywords when determining the shape of the event mask and check the shape in dclab-verify-dataset
- fix: avoid ContourIndexingError by also searching the neighboring (+2/-2) events when the contour frame number does not match (#67)

6.66 version 0.14.3

- enh: explicitly check contour data when testing whether to include the first event in tdms2rtdc

6.67 version 0.14.2

- ref: convert said ValueError to ContourIndexingError

6.68 version 0.14.1

- fix: ValueError when verifying contour frame index due to comparison of float with int

6.69 version 0.14.0

- feat: new command line script for creating a scalar-feature-only dataset with all available ancillary features “dclab-condense”
- enh: enable scalar feature compression for hdf5 export
- docs: fix doc string for dclab-tdms2rtdc (*–include-initial-empty-image* falsely shown as “enabled by default”)

6.70 version 0.13.0

- feat: allow to obtain a mask representing the filtered data with the *ret_mask* kwarg in *RTDCBase.get_downsampled_scatter*
- feat: allow to force-exclude invalid (inf/nan) events when downsampling using the *remove_invalid* keyword argument
- feat: exclude empty initial images in dclab-tdms2rtdc; they may optionally be included with “--include-initial-empty-image”
- feat: new property *RTDCBase.features_innate* (measured feature)
- enh: log which ancillary features were computed in dclab-tdms2rtdc (#65)
- enh: improved tdms meta data import (also affects dclab-tdms2rtdc)
- enh: update channel count and samples per event when writing hdf5 data
- enh: dclab-verify-dataset now recognizes invalid tdms data
- enh: several other improvements when reading tdms data
- enh: group meta data in log files (dclab-tdms2rtdc and dclab-join)
- fix: correctly handle hdf5 export when the image or contour columns have incorrect sizes (affects dclab-tdms2rtdc)
- fix: ignore empty configuration values when loading tdms data
- fix: image/contour files were searched recursively instead of only in the directory of the tdms file
- fix: check for presence of “time” feature before using it to correct measurement date and time
- fix: ancillary feature computation for brightness had wrong dependency coded (contour instead of mask)
- fix: ancillary feature computation when contour data is involved lead to error, because *LazyContourList* did not implement *identifier* (see #61)
- ref: remove NoContourDataWarning for tdms file format
- tests: improve dataset checks (#64)

6.71 version 0.12.0

- feat: add command line script for joining measurements “dclab-join” (#57)
- feat: make log files available as *RTDCBase.logs*
- feat: include log data in “dclab-join” and “dclab-tdms2rtdc”
- fix: *features* property for tdms file format falsely contains the keys “contour”, “image”, “mask”, and “trace” when they are actually not available.
- enh: support loading TDMS data using the ‘with’ statement
- docs: add example for joining measurements
- docs: other minor improvements
- setup: add Python 3.7 wheels for Windows (#62)
- setup: remove Python 2 wheels for macOS

6.72 version 0.11.1

- docs: add example for fluorescence trace visualization
- docs: restructure advanced usage section
- ref: make dclab in principle compatible with imageio \geq 2.5.0; Dependencies are pinned due to segfaults during testing
- setup: make tdms format support and data export dependency optional; To get the previous behavior, use *pip install dclab[all]*

6.73 version 0.11.0

- feat: compute contours lazily (#61)

6.74 version 0.10.5

- setup: migrate to PEP 517 (pyproject.toml)

6.75 version 0.10.4

- enh: ignore defective feature “aspect” from Shape-In 2.0.6 and 2.0.7
- enh: support loading HDF5 data using the ‘with’ statement (e.g. *with dclab.new_dataset(rtdc_path) as ds:*)

6.76 version 0.10.3

- fix: add numpy build dependency (setup_requires)

6.77 version 0.10.2

- fix: HDF5-export did not re-enumerate “index” feature

6.78 version 0.10.1

- fix: support nan-valued events when computing quantile levels in submodule *kde_contours*

6.79 version 0.10.0

- BREAKING CHANGE: Change np.meshgrid indexing in *RTDCBase.get_kde_contour* from “xy” to “ij”
- feat: new submodule *kde_contours* for computing kernel density contour lines at specific data percentiles (#60)
- fix: range for contour KDE computation did not always contain end value (*RTDCBase.get_kde_contour*)

- fix: *positions* keyword argument in *RTDCBase.get_kde_scatter* was not correctly scaled in the logarithmic case
- ref: cleanup and document *PolygonFilter.point_in_poly*
- ref: move skimage code to separate submodule “external”
- ref: drop dependency on statsmodels and move relevant code to submodule “external”

6.80 version 0.9.1

- fix: all-zero features were treated as non-existent due to relic from pre-0.3.3 era
- fix: correct extraction of start time from tdms format (1h offset from local time and measurement duration offset)
- fix: correct extraction of module composition from tdms format (replace “+” with “,”)
- enh: add configuration key mapping for tdms format to simplify conversion to hdf5 format (see *fmt_tdms.naming*)
- enh: do not add laser info for unused lasers for tdms format
- enh: dclab-verify-dataset checks for image attribute dtype
- enh: include original software version when exporting to rtcd format

6.81 version 0.9.0

- feat: add new feature: gravitational force, temperature, and ambient temperature
- ref: remove unused *has_key* function in *rtcd_dataset.config.CaseInsensitiveDict*
- setup: require numpy>=1.10.0 because of *equal_nan* argument in *allclose*

6.82 version 0.8.0

- fix: usage of “xor” (^) instead of “or” (|) in statistics
- feat: support *remove_invalid=False* in *downsampling.downsample_rand* (#27)
- feat: add keyword arguments *xscale* and *yscale* to improve data visualization in *RTDCBase.get_downsampled_scatter*, *RTDCBase.get_kde_contour*, and *RTDCBase.get_kde_scatter* (#55)
- enh: make downsampling code more transparent
- BREAKING CHANGE: low-level downsampling methods refactored
 - *downsampling.downsample_grid*: removed keyword argument *remove_invalid*, because setting it to *False* makes no sense in this context
 - *downsampling.downsample_rand*: changed default value of *remove_invalid* to *False*, because this is more objective
 - rename keyword argument *retidx* to *ret_idx*
 - these changes do not affect any other higher level functionalities in *dclab.rtdc_dataset* or in Shape-Out

6.83 version 0.7.0

- feat: add new ancillary feature: principal inertia ratio (#46)
- feat: add new ancillary feature: absolute tilt (#53)
- feat: add computation of viscosity for water (#52)

6.84 version 0.6.3

- fix: channel width not correctly identified for old tdms files

6.85 version 0.6.2

- ci: automate release to PyPI with appveyor and travis-ci

6.86 version 0.6.0

- fix: image export as .avi did not have option to use unfiltered data
- fix: avoid a few unicode gotchas
- feat: use Doane’s formula for kernel density estimator defaults (#42)
- docs: usage examples, advanced scripting, and code reference update (#49)

6.87 version 0.5.2

- Migrate from os.path to pathlib (#50)
- fmt_hdf5: Add run index to title

6.88 version 0.5.1

- Setup: add dependencies for statsmodels
- Tests: filter known warnings
- fmt_hdf5: import unknown keys such that “dclab-verify-dataset” can complain about them

6.89 version 0.5.0

- BREAKING CHANGES:
 - definitions.feature_names now contains non-scalar features (including “image”, “contour”, “mask”, and “trace”). To test for scalar features, use definitions.scalar_feature_names.
 - features.bright_* are computed from mask instead of from contour

- Bugfixes:
 - write correct event count in exported hdf5 data files
 - improve implementation of video file handling in fmt_tdms
- add new non-scalar feature “mask” (#48)
- removed configuration key [online_contour]: “bin margin” (#47)
- minor improvements for the tdms file format

6.90 version 0.4.0

- Bugfix: CLI “dclab-tdms2rtdc” did not work for single tdms files (#45)
- update configuration keys:
 - added new keys for [fluorescence]
 - added [setup]: “identifier”
 - removed [imaging]: “exposure time”, “flash current”
 - removed [setup]: “temperature”, “viscosity”
- renamed feature “ncells” to “nevents”

6.91 version 0.3.3

- ref: do not import missing features as zeros in fmt_tdms
- CLI:
 - add tdms-to-rtdc converter “dclab-tdms2rtdc” (#36)
 - improve “dclab-verify-dataset” user experience
- Bugfixes:
 - “limit events” filtering must be integer not boolean (#41)
 - Support opening tdms files with capitalized “userDef” column names
 - OSError when trying to open files from repository root

6.92 version 0.3.2

- CLI: add rudimentary dataset checker “dclab-verify-dataset” (#37)
- Add logic to compute parent/root/child event indices of RTDC_Hierarchy
 - Hierarchy children now support contour, image, and traces
 - Hierarchy children now support and remember manual filters (#22)
- Update emodulus look-up table with larger values for deformation
- Implement pixel size correction for emodulus computation
- Allow to add pixelation error to isoelastics (*add_px_err=True*) (#28)

- Bugfixes:
 - Pixel size not read from tdms-based measurements
 - Young’s modulus computation wrong due to faulty FEM simulations (#39)

6.93 version 0.3.1

- Remove all-zero dummy columns from dict format
- Implement hdf5-based RT-DC data reader (#32)
- Implement hdf5-based RT-DC data writer (#33)
- Bugfixes:
 - Automatically fix inverted box filters
 - RTDC_TDMS trace data contained empty arrays when no trace data was present (trace key should not have been accessible)
 - Not possible to get isoelastics for circularity

6.94 version 0.3.0

- New fluorescence crosstalk correction feature recipe (#35)
- New ancillary features “fl1_max_ctc”, “fl2_max_ctc”, “fl3_max_ctc” (#35)
- Add priority for multiple ancillary features with same name
- Bugfixes:
 - Configuration key values were not hashed for ancillary features
- Code cleanup:
 - Refactoring: Put ancillary columns into a new folder module
 - Refactoring: Use the term “feature” consistently
 - Unify trace handling in dclab (#30)
 - Add functions to convert input config data

6.95 version 0.2.9

- Bugfixes:
 - Regression when loading configuration strings containing quotes
 - Parameters missing when loading ShapeIn 2.0.1 tdms data

6.96 version 0.2.8

- Refactor configuration class to support new format (#26)

6.97 version 0.2.7

- New submodule and classes for managing isoelastics
- New ancillary columns “inert_ratio_raw” and “inert_ratio_cvx”
- Bugfixes:
 - Typo when finding contour data files (tdms file format)
- Refactoring:
 - “features” submodule with basic methods for ancillary columns

6.98 version 0.2.6

- Return event images as gray scale (#17)
- Bugfixes:
 - Shrink ancillary column size if it exceeds dataset size
 - Generate random RTDCBase.identifier (do not use RTDCBase.hash) to fix problem with identical identifiers for hierarchy children
 - Correctly determine contour data files (tdms file format)
 - Allow contour data indices larger than uint8

6.99 version 0.2.5

- Add ancillary columns “bright_avg” and “bright_sd” (#18, #19)
- Standardize attributes of RTDCBase subclasses (#12)
- Refactoring:
 - New column names and removal of redundant column identifiers (#16)
 - Minor improvements towards PEP8 (e.g. #15)
 - New class for handling filters (#13)
- Bugfixes:
 - Hierarchy child computed all ancillary columns of parent upon checking availability of a column

6.100 version 0.2.4

- Replace OpenCV with imageio
- Add (ancillary) computation of volume (#11)
- Add convenience methods for *Configuration*
- Refactoring (#8):
 - Separate classes for .tdms, dict-based, and hierarchy datasets

- Introduce “_events” attribute for stored data
- Data columns (including image, trace, contour) are accessed via keys instead of attributes.
- Make space for new hdf5-based file format
- Introduce ancillary columns that are computed on-the-fly (new “_ancillaries” attribute and “ancillary_columns.py”)

6.101 version 0.2.3

- Add look-up table for elastic modulus (#7)
- Add filtering option “remove invalid events” to remove nan/inf
- Support nan and inf in data analysis
- Improve downsampling performance
- Refactor downsampling methods (#6)

6.102 version 0.2.2

- Add new histogram-based kernel density estimator (#2)
- Refactoring:
 - Configuration fully handled by RTDC_DataSet module (#5)
 - Simplify video export function (#4)
 - Removed “Plotting” configuration key
 - Removed .cfg configuration files

6.103 version 0.2.1

- Support npTDMS 0.9.0
- Add AVI-Export function
- Add lazy submodule for event trace data and rename *RTDC_DataSet.traces* to *RTDC_DataSet.trace*
- Add “Event index” column

6.104 version 0.2.0

- Compute sensible default configuration parameters for KDE estimation and contour plotting
- Speed-up handling of contour text files
- Add support for “User Defined” column in tdms files

6.105 version 0.1.9

- Implement hierarchical instantiation of `RTDC_DataSet`
- Bugfix: Prevent instances of `PolygonFilter` that have same id
- Load `InertiaRatio` and `InertiaRatioRaw` from tdms files

6.106 version 0.1.8

- Allow to instantiate `RTDC_DataSet` without a tdms file
- Add statistics submodule
- Bugfixes:
 - Faulty hashing strategy in `RTDC_DataSet.GetDownSampledScatter`
- Code cleanup (renamed methods, cleaned structure)
- Corrections/additions in definitions (fRT-DC)

6.107 version 0.1.7

- Added channel: distance between to first fl. peaks
- Added fluorescence channels: peak position, peak area, number of peaks
- Allow to disable KDE computation
- Add filter array for manual (user-defined) filtering
- Add config parameters for log axis scaling
- Add channels: bounding box x- and y-size
- Bugfixes:
 - `cached.py` did not handle *None*
 - Limiting number of events caused integer/bool error

6.108 version 0.1.6

- Added `RTDC_DataSet.ExportTSV` for data export
- Bugfixes:
 - Correct determination of video file in `RTDCDataSet`
 - Fix multivariate KDE computation
 - Contour accuracy for `Defo` overridden by that of `Circ`

6.109 version 0.1.5

- Fix regressions with filtering. <https://github.com/ZELLMECHANIK-DRESDEN/ShapeOut/issues/43>
- Ignore empty columns in .tdms files (#1)
- Moved RTDC_DataSet and PolygonFilter classes to separate files
- Introduce more transparent caching - improves speed in some cases

6.110 version 0.1.4

- Added support for 3-channel fluorescence data (FL-1..3 max/width)

6.111 version 0.1.3

- Fixed minor polygon filter problems.
- Fix a couple of Shape-Out-related issues:
 - <https://github.com/ZELLMECHANIK-DRESDEN/ShapeOut/issues/17>
 - <https://github.com/ZELLMECHANIK-DRESDEN/ShapeOut/issues/20>
 - <https://github.com/ZELLMECHANIK-DRESDEN/ShapeOut/issues/37>
 - <https://github.com/ZELLMECHANIK-DRESDEN/ShapeOut/issues/38>

6.112 version 0.1.2

- Add support for limiting amount of data points analyzed with the configuration keyword “Limit Events”
- Comments refer to “events” instead of “points” from now on

CHAPTER 7

Bibliography

8.1 Imprint and disclaimer

For more information, please refer to the imprint and disclaimer (Impressum und Haftungsausschluss) at <https://www.zellmechanik.com/Imprint.html>.

8.2 Privacy policy

This documentation is hosted on <https://readthedocs.org/> whose [privacy policy](#) applies.

CHAPTER 9

Indices and tables

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

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