Particle-Size-Distribution

October 16, 2022

1 Particle Size Distribution

Notebook by Lukas Grünewald, https://github.com/lukmuk/particle-size-distribution.

1.1 Purpose:

Evaluate (nano)particle (or other) size distribution by fitting a distribution function and extracting statistical parameters in Python.
Requires `numpy`, `scipy`, and `pandas`. Additionally, the uncertainties package is used to handle error propagation.

1.2 Usage:

Segmentation and size measurements (e.g. areas, Feret diameters, …) were extracted using *Fiji*.
The `Results.csv` of the `Analyze particles...` function in *Fiji* is loaded here for analysis.
Multiple `.csv` files can be loaded and stacked using `pandas`.
To start, put the `.csv` files into the same folder with a copy of this notebook.

In the following example, particle/grain sizes of an SEM image were measured in *Fiji* using ParticleSizer.
The projected areas and the mininmum Feret diameters are taken as the size metric and a log-normal distribution is fitted to the histograms.

[1]:
```
%load_ext watermark
```

[2]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
import glob

from scipy.optimize import curve_fit

#For error propagation:
from uncertainties import ufloat, unumpy
from uncertainties.umath import *
```

[3]:
```
#Print package versions
%watermark -i -v -u -m --iversions
```

```
Last updated: 2022-10-16T12:08:22.915201+02:00

Python implementation: CPython
Python version       : 3.9.13
IPython version      : 8.5.0

Compiler    : MSC v.1916 64 bit (AMD64)
OS          : Windows
Release     : 10
Machine     : AMD64
Processor   : Intel64 Family 6 Model 165 Stepping 5, GenuineIntel
CPU cores   : 16
Architecture: 64bit

pandas       : 1.4.3
uncertainties: 3.1.7
matplotlib   : 3.5.2
numpy        : 1.21.5
```

1.2.1 Define a particle size distribution

Here, we use a log-normal distribution (or probability density function, PDF) as an example.
I tested other variants such as using scipy.stats.lognorm but the following approach gave me best results and easy access to the statistical fitting errors.

[4]:
```
def pdf(x, mu, sigma):
    """Probability density function of a log-normal distribution"""
    return (np.exp(-(np.log(x) - mu)**2 / (2 * sigma**2)) / (x * sigma * np.
↪sqrt(2 * np.pi)))
```

For a nice discussion about the log-normal distribution in this context, see
E. Limpert, W. A. Stahel, and M. Abbt, *BioScience*, **51**, 5,(2001) 341–352, doi: 10.1641/0006-3568(2001)051. The above definition is

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma x} \exp\Big(-\frac{(\ln(x)-\mu)^2}{2\sigma^2}\Big), \quad x > 0$$

with the mean μ and standard deviation σ of $\ln(x)$ as fit parameters.

1.2.2 Properties for the log-normal distribution

We calculate the mode M, median m, arithmetic mean μ_a, and standard deviation σ_a for the measured values x from the fitted μ and σ parameters.
Statistical fitting errors on μ and σ will be propagated by the `uncertainties` package.

$$M(x) = e^{\mu-\sigma^2}$$

$$m(x) = e^{\mu}$$

$$\mu_{\mathrm{a}}(x) = e^{\mu + \frac{\sigma^2}{2}}$$

$$\sigma_{\mathrm{a}}(x) = e^{\mu + \frac{1}{2}\sigma^2} \sqrt{e^{\sigma^2} - 1}$$

Scatter intervals For a log-normal distribution, with geometric mean and standard deviation $\mu^* = e^\mu$ and $\sigma^* = e^\sigma$,

$$[\mu^*/\sigma^*, \mu^* \cdot \sigma^*]$$

contains 68 %, and

$$[\mu^*/\left(\sigma^*\right)^2, \mu^* \cdot \left(\sigma^*\right)^2]$$

contains 95 % of the probability.

1.3 Load and inspect data

Load the data:

[5]:
```
# Grab and stack all csv files in working directory in a pandas data frame
df = pd.concat([pd.read_csv(filename, header=0, index_col=None) for filename in␣
↪glob.glob('*.csv')], ignore_index=True)
```

[6]:
```
df.shape
```

[6]:
```
(2313, 27)
```

[7]:
```
print(f'Number of measured particles/grains: {df.shape[0]}')
```

```
Number of measured particles/grains: 2313
```

[8]:
```
# Inspect data set
df.head()
```

[8]:
```
      Frame  Label         X       Y        Area  Area Conv. Hull    Peri.  \
0  1      1      1  5212.984  58.421  17268.571        17565.719  484.196
1  2      1      2  2357.451  42.488   3744.071         3803.500  209.429
2  3      1      3  4118.055  62.085   6732.535         6868.374  303.054
3  4      1      4  1474.562  43.515   3226.183         3319.573  199.627
4  5      1      5  2183.952  69.811   7640.960         7802.270  346.958

   Peri. Conv. Hull    Feret  …   Circ.  Elong.  Convexity  Solidity  \
0           492.264  188.315  …  13.576   0.575        1.0     0.983
1           215.342   74.912  …  11.715   0.349        1.0     0.984
2           305.301  118.321  …  13.641   0.631        1.0     0.980
3           203.314   76.483  …  12.352   0.512        1.0     0.972
4           350.991  146.153  …  15.755   0.717        1.0     0.979

   Num. of Holes  Thinnes Rt.  Contour Temp.  Orientation  Fract. Dim.  \
0              0        0.926          0.145        8.018        1.624
1              0        1.000          0.163      167.523        1.485
2              0        0.921          0.124       60.433        1.582
```

```
3                 0        1.000            0.148      132.645          1.432
4                 0        0.798            0.135       64.133          1.623

   Fract. Dim. Goodness
0                  0.992
1                  0.964
2                  0.992
3                  0.951
4                  0.991

[5 rows x 27 columns]
```

1.3.1 Metric: Area-Equivalent Circle Diameter

An often used metric is the area-equivalent circle diameter.
We calculate circles with equal size as the measured projected particle/grain size (`Area` column).

[9]:
```
data = df['Area'].to_numpy()
```

Calculate area-equivalent diameters from areas:

$$d_p = \sqrt{\frac{4A}{\pi}}.$$

[10]:
```
data = np.sqrt(4*data/np.pi)
```

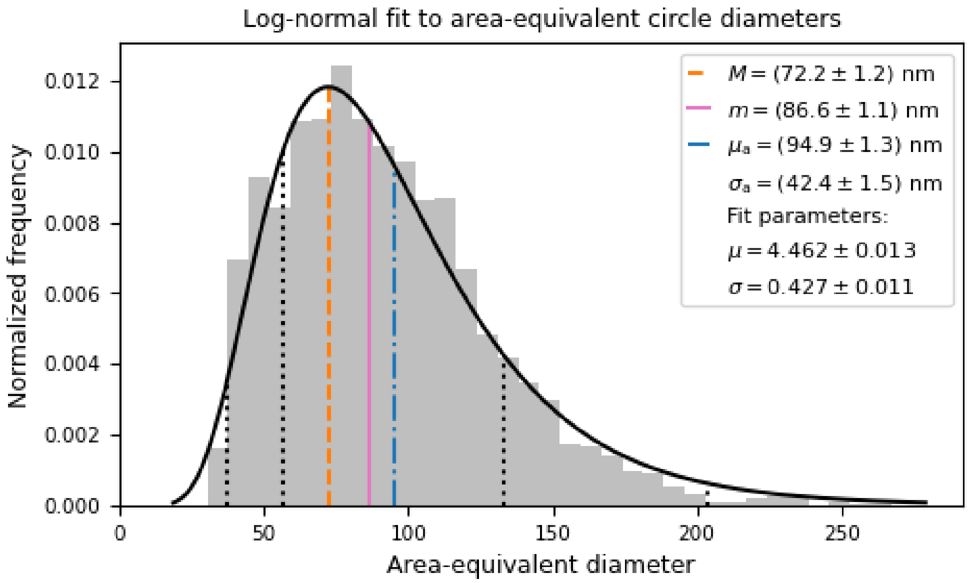
The next cell, plots the histogram, performs a fit of the (log-normal) distribution, and displays/saves the result.

[11]:
```
# Create plot
fig, ax = plt.subplots(figsize=(5, 3))

# Normalized histogram
n, bins, patches = ax.hist(data, bins='auto', density=True, facecolor = 'grey',␣
 ↪alpha = 0.5, label=None)
centers = (0.5*(bins[1:]+bins[:-1]))

# Fit of pdf
pars, cov = curve_fit(pdf, centers, n)

# Draw pdf
pdfcol ='k'
xmin, xmax = ax.get_xlim()
x = np.linspace(xmin, xmax, 1000)
ax.plot(x, pdf(x, *pars), pdfcol , linewidth = 1.5, label=None, zorder=10)

# Add fit parameters (mu, sigma, mode) as labels
# Errors are from diagonal elements of cov (covariance matrix) -->␣
 ↪sqrt(Var)=Std dev
```

```python
mu, sigma = unumpy.uarray(pars, np.sqrt(np.diag(cov)))

muStar = exp(mu)
sigStar = exp(sigma)
confidence68 = (muStar/sigStar, muStar*sigStar)
confidence95 = (muStar/sigStar**2, muStar*sigStar**2)

mode = exp(mu - sigma ** 2)
median = exp(mu)
mean = exp(mu + sigma ** 2 / 2)
std = exp(mu + sigma**2/2) * sqrt(exp(sigma**2)-1)

print(f'Mode:\t\t {mode}')
print(f'Median:\t\t {median}')
print(f'Mean:\t\t {mean}')
print(f'Std. dev.:\t {std}')
print(f'68% conf. intervall: {np.round(confidence68[0].nominal_value)}+/-{np.round(confidence68[0].std_dev)} to {np.round(confidence68[1].nominal_value)}+/-{np.round(confidence68[1].std_dev)}')
print(f'95% conf. intervall: {np.round(confidence95[0].nominal_value)}+/-{np.round(confidence95[0].std_dev)} to {np.round(confidence95[1].nominal_value)}+/-{np.round(confidence95[1].std_dev)}')

# Plot labels
lb_std = rf'$\sigma_\mathregular{{a}} = ({np.round(std.nominal_value,1)} \pm {np.round(std.std_dev,1)})$ nm'
lb_mean = rf'$\mu_\mathregular{{a}} = ({np.round(mean.nominal_value,1)} \pm {np.round(mean.std_dev,1)})$ nm'
lb_mode = rf'$M = ({np.round(mode.nominal_value,1)} \pm {np.round(mode.std_dev,1)})$ nm'
lb_median = rf'$m = ({np.round(median.nominal_value,1)} \pm {np.round(median.std_dev,1)})$ nm'
lb_mu = f'$\mu = {np.round(mu.nominal_value,3)} \pm {np.round(mu.std_dev,3)}$'
lb_sig = f'$\sigma = {np.round(sigma.nominal_value,3)} \pm {np.round(sigma.std_dev,3)}$'

# Add vertical markers for positions of calculated properties
# Mode
ax.plot([mode.nominal_value, mode.nominal_value], [0, pdf(mode.nominal_value, *pars)], c='tab:orange', ls='--', label=lb_mode)

# Median
ax.plot([median.nominal_value, median.nominal_value], [0, pdf(median.nominal_value, *pars)], c='tab:pink', ls='-', label=lb_median)

# Mean
```

```
ax.plot([mean.nominal_value, mean.nominal_value], [0, pdf(mean.nominal_value,␣
↪*pars)], c='tab:blue', ls='-.', label=lb_mean)

# Confidence intervall 68%
ci = confidence68
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')

# Confidence intervall 95%
ci = confidence95
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')

# Gemerate empty plots, so that fit parameters are added in legend
plt.plot([], [], ' ', label=lb_std)
plt.plot([], [], ' ', label='Fit parameters:')
plt.plot([], [], ' ', label=lb_mu)
plt.plot([], [], ' ', label=lb_sig)

# Cosmetics
ax.set_title(f'Log-normal fit to area-equivalent circle diameters', fontsize=9)
ax.set_xlabel('Area-equivalent diameter', fontsize=9)
ax.set_ylabel("Normalized frequency", fontsize=9)
plt.tick_params(axis='both', which='major', labelsize=7.5)

ax.set_xlim(0,)
#ax.set_ylim(0, np.max(pdf(x, *pars))*1.8)

ax.legend(loc='best', handlelength=1, fontsize=8, ncol=1, columnspacing=0.1)
plt.tight_layout(pad=0.1)
fig.savefig('plots/AreaEquivalentCircleDiameter_normalized.pdf', pad_inches=0)
```

```
Mode:              72.2+/-1.2
Median:            86.6+/-1.1
Mean:              94.9+/-1.3
Std. dev.:         42.4+/-1.5
68% conf. intervall: 57.0+/-1.0 to 133.0+/-2.0
95% conf. intervall: 37.0+/-1.0 to 203.0+/-5.0
```



1.3.2 Metric: Minimum Feret Diameter

We can fit to another size metric from the pandas table by adjusting the `data` variable. Here, we switch to the minimum Feret diameter:

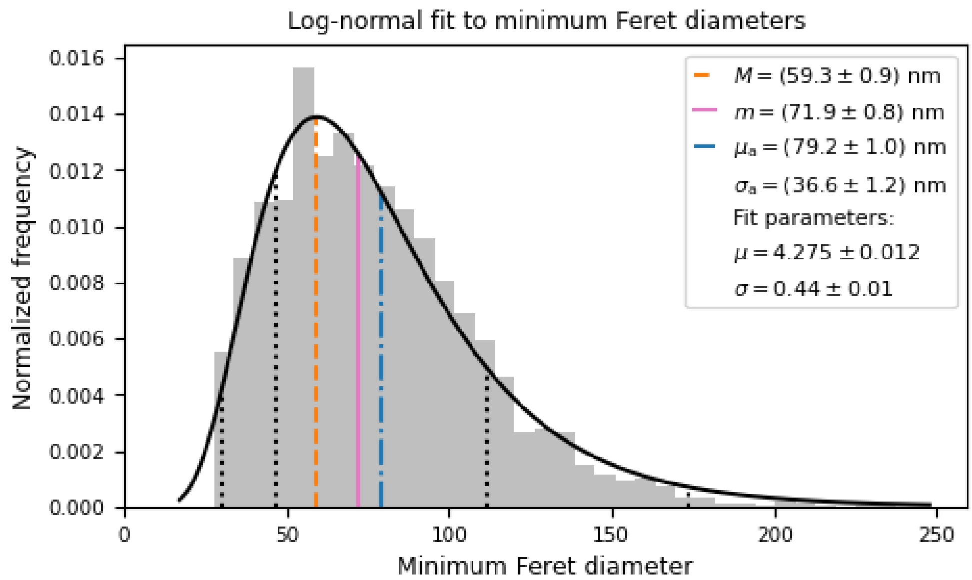
[12]:
```
data = df['Min. Feret'].to_numpy()
```

[13]:
```
# Create plot
fig, ax = plt.subplots(figsize=(5, 3))

# Normalized histogram
n, bins, patches = ax.hist(data, bins='auto', density=True, facecolor = 'grey',␣
 ↪alpha = 0.5, label=None)
centers = (0.5*(bins[1:]+bins[:-1]))

# Fit of pdf
pars, cov = curve_fit(pdf, centers, n)

# Draw pdf
pdfcol ='k'
xmin, xmax = ax.get_xlim()
x = np.linspace(xmin, xmax, 1000)
ax.plot(x, pdf(x, *pars), pdfcol , linewidth = 1.5, label=None, zorder=10)

# Add fit parameters (mu, sigma, mode) as labels
# Errors are from diagonal elements of cov (covariance matrix) -->␣
 ↪sqrt(Var)=Std dev
```

```python
mu, sigma = unumpy.uarray(pars, np.sqrt(np.diag(cov)))

muStar = exp(mu)
sigStar = exp(sigma)
confidence68 = (muStar/sigStar, muStar*sigStar)
confidence95 = (muStar/sigStar**2, muStar*sigStar**2)

mode = exp(mu - sigma ** 2)
median = exp(mu)
mean = exp(mu + sigma ** 2 / 2)
std = exp(mu + sigma**2/2) * sqrt(exp(sigma**2)-1)

print(f'Mode:\t\t {mode}')
print(f'Median:\t\t {median}')
print(f'Mean:\t\t {mean}')
print(f'Std. dev.:\t {std}')
print(f'68% conf. intervall: {np.round(confidence68[0].nominal_value)}+/-{np.round(confidence68[0].std_dev)} to {np.round(confidence68[1].nominal_value)}+/-{np.round(confidence68[1].std_dev)}')
print(f'95% conf. intervall: {np.round(confidence95[0].nominal_value)}+/-{np.round(confidence95[0].std_dev)} to {np.round(confidence95[1].nominal_value)}+/-{np.round(confidence95[1].std_dev)}')

# Plot labels
lb_std = rf'$\sigma_\mathregular{{a}} = ({np.round(std.nominal_value,1)} \pm {np.round(std.std_dev,1)})$ nm'
lb_mean = rf'$\mu_\mathregular{{a}} = ({np.round(mean.nominal_value,1)} \pm {np.round(mean.std_dev,1)})$ nm'
lb_mode = rf'$M = ({np.round(mode.nominal_value,1)} \pm {np.round(mode.std_dev,1)})$ nm'
lb_median = rf'$m = ({np.round(median.nominal_value,1)} \pm {np.round(median.std_dev,1)})$ nm'
lb_mu = f'$\mu = {np.round(mu.nominal_value,3)} \pm {np.round(mu.std_dev,3)}$'
lb_sig = f'$\sigma = {np.round(sigma.nominal_value,3)} \pm {np.round(sigma.std_dev,3)}$'

# Add vertical markers for positions of calculated properties
# Mode
ax.plot([mode.nominal_value, mode.nominal_value], [0, pdf(mode.nominal_value, *pars)], c='tab:orange', ls='--', label=lb_mode)

# Median
ax.plot([median.nominal_value, median.nominal_value], [0, pdf(median.nominal_value, *pars)], c='tab:pink', ls='-', label=lb_median)

# Mean
```

```
ax.plot([mean.nominal_value, mean.nominal_value], [0, pdf(mean.nominal_value,␣
↪*pars)], c='tab:blue', ls='-.', label=lb_mean)

# Confidence intervall 68%
ci = confidence68
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')

# Confidence intervall 95%
ci = confidence95
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)], c=pdfcol, ls='dotted')

# Gemerate empty plots, so that fit parameters are added in legend
plt.plot([], [], ' ', label=lb_std)
plt.plot([], [], ' ', label='Fit parameters:')
plt.plot([], [], ' ', label=lb_mu)
plt.plot([], [], ' ', label=lb_sig)

# Cosmetics
ax.set_title(f'Log-normal fit to minimum Feret diameters', fontsize=9)
ax.set_xlabel('Minimum Feret diameter', fontsize=9)
ax.set_ylabel("Normalized frequency", fontsize=9)
plt.tick_params(axis='both', which='major', labelsize=7.5)

ax.set_xlim(0,)
#ax.set_ylim(0, np.max(pdf(x, *pars))*1.8)

ax.legend(loc='best', handlelength=1, fontsize=8, ncol=1, columnspacing=0.1)
plt.tight_layout(pad=0.1)
fig.savefig('plots/MinFeretDiameter_normalized.pdf', pad_inches=0)
```

```
Mode:             59.3+/-0.9
Median:           71.9+/-0.8
Mean:             79.2+/-1.0
Std. dev.:        36.6+/-1.2
68% conf. intervall: 46.0+/-1.0 to 112.0+/-2.0
95% conf. intervall: 30.0+/-1.0 to 173.0+/-4.0
```



1.3.3 Plot with absolute values on y-axis instead of normalized values

The above distributions show the normalized histograms (`density=True` keyword) and the fraction on the y axis.
Alternatively, the absolute values (the actual number of counted grains/particles in the histogram bins) can also be displayed.
This is done by
- Fitting the distribution to the normalized values (then we do not need to fit a scaling factor as another fit parameter) - Plotting the histogram with absolute frequencies (`density=False`) - Use a scaling factor to scale up the fitted distribution (taken from here)

[14]:
```
# Create plot
fig, ax = plt.subplots(figsize=(5, 3))

# Fit distribution using normalized histogram
n2, bins2, patches2 = ax.hist(data, bins='auto', density=True, facecolor =␣
↪'grey', alpha = 0, label=None)
centers2 = (0.5*(bins[1:]+bins[:-1]))
pars, cov = curve_fit(pdf, centers2, n2)

# Plot histogram with absolute values, i.e. density=False
n, bins, patches = ax.hist(data, bins='auto', density=False, facecolor =␣
↪'grey', alpha = 0.5, label=None)
centers = (0.5*(bins[1:]+bins[:-1]))

# Scaling factor for distribution
```

```
# https://stackoverflow.com/questions/41024455/
 ↪histogram-with-non-normalized-fit-line-matplotlib
scaling_factor = sum(n * np.diff(bins))

# Draw pdf
pdfcol ='k'
xmin, xmax = ax.get_xlim()
x = np.linspace(xmin, xmax, 1000)
ax.plot(x, pdf(x, *pars)*scaling_factor, pdfcol, linewidth = 1.5, label=None,␣
 ↪zorder=100)

# Add fit parameters (mu, sigma, mode) as labels
# Errors are from diagonal elements of cov (covariance matrix) -->␣
 ↪sqrt(Var)=Std dev
mu, sigma = unumpy.uarray(pars, np.sqrt(np.diag(cov)))

muStar = exp(mu)
sigStar = exp(sigma)
confidence68 = (muStar/sigStar, muStar*sigStar)
confidence95 = (muStar/sigStar**2, muStar*sigStar**2)

mode = exp(mu - sigma ** 2)
median = exp(mu)
mean = exp(mu + sigma ** 2 / 2)
std = exp(mu + sigma**2/2) * sqrt(exp(sigma**2)-1)

print(f'Mode:\t\t {mode}')
print(f'Median:\t\t {median}')
print(f'Mean:\t\t {mean}')
print(f'Std. dev.:\t {std}')
print(f'68% conf. intervall: {np.round(confidence68[0].nominal_value)}+/-{np.
 ↪round(confidence68[0].std_dev)} to {np.round(confidence68[1].
 ↪nominal_value)}+/-{np.round(confidence68[1].std_dev)}')
print(f'95% conf. intervall: {np.round(confidence95[0].nominal_value)}+/-{np.
 ↪round(confidence95[0].std_dev)} to {np.round(confidence95[1].
 ↪nominal_value)}+/-{np.round(confidence95[1].std_dev)}')

# Plot labels
lb_std = rf'$\sigma_\mathregular{{a}} = ({np.round(std.nominal_value,1)} \pm␣
 ↪{np.round(std.std_dev,1)})$ nm'
lb_mean = rf'$\mu_\mathregular{{a}} = ({np.round(mean.nominal_value,1)} \pm {np.
 ↪round(mean.std_dev,1)})$ nm'
lb_mode = rf'$M = ({np.round(mode.nominal_value,1)} \pm {np.round(mode.
 ↪std_dev,1)})$ nm'
lb_median = rf'$m = ({np.round(median.nominal_value,1)} \pm {np.round(median.
 ↪std_dev,1)})$ nm'
```

```
lb_mu = f'$\mu = {np.round(mu.nominal_value,3)} \pm {np.round(mu.std_dev,3)}$'
lb_sig = f'$\sigma = {np.round(sigma.nominal_value,3)} \pm {np.round(sigma.
↪std_dev,3)}$'

# Add vertical markers for positions of calculated properties
# Mode
ax.plot([mode.nominal_value, mode.nominal_value], [0, pdf(mode.nominal_value,␣
↪*pars)*scaling_factor], c='tab:orange', ls='--', label=lb_mode)

# Median
ax.plot([median.nominal_value, median.nominal_value], [0, pdf(median.
↪nominal_value, *pars)*scaling_factor], c='tab:pink', ls='-', label=lb_median)

# Mean
ax.plot([mean.nominal_value, mean.nominal_value], [0, pdf(mean.nominal_value,␣
↪*pars)*scaling_factor], c='tab:blue', ls='-.', label=lb_mean)

# Confidence intervall 68%
ci = confidence68
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)*scaling_factor], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)*scaling_factor], c=pdfcol, ls='dotted')

# Confidence intervall 95%
ci = confidence95
ax.plot([ci[0].nominal_value, ci[0].nominal_value], [0, pdf(ci[0].
↪nominal_value, *pars)*scaling_factor], c=pdfcol, ls='dotted')
ax.plot([ci[1].nominal_value, ci[1].nominal_value], [0, pdf(ci[1].
↪nominal_value, *pars)*scaling_factor], c=pdfcol, ls='dotted')

# Gemerate empty plots, so that fit parameters are added in legend
plt.plot([], [], ' ', label=lb_std)
plt.plot([], [], ' ', label='Fit parameters:')
plt.plot([], [], ' ', label=lb_mu)
plt.plot([], [], ' ', label=lb_sig)

# Cosmetics
ax.set_title(f'Log-normal fit to minimum Feret diameters', fontsize=9)
ax.set_xlabel('Minimum Feret diameter', fontsize=9)
ax.set_ylabel("Frequency", fontsize=9)
plt.tick_params(axis='both', which='major', labelsize=7.5)

ax.set_xlim(0,)
#ax.set_ylim(0, np.max(pdf(x, *pars))*1.8)
```

```
ax.legend(loc='best', handlelength=1, fontsize=8, ncol=1, columnspacing=0.1)
plt.tight_layout(pad=0.1)
fig.savefig('plots/MinFeretDiameter_absolute.pdf', pad_inches=0)
fig.savefig('plots/MinFeretDiameter_absolute.png', dpi=600, pad_inches=0)
```

```
Mode:               59.3+/-0.9
Median:             71.9+/-0.8
Mean:               79.2+/-1.0
Std. dev.:          36.6+/-1.2
68% conf. intervall: 46.0+/-1.0 to 112.0+/-2.0
95% conf. intervall: 30.0+/-1.0 to 173.0+/-4.0
```