ps_1_3

April 24, 2023

1 Solution to excercise sheet 1, exercise 3

Solved by Jakub Dokulil

1.1 Theory

We have absservables

$$\underbrace{A_1, A_2, ...A_n}_{A_1^{(n)}}, A_{n+1}, ...A_{2n}, ...$$

The correlation of subsamples - blocks is

$$Var(A^{(n)}) = \frac{1}{n}Var(A)$$

However if tha sample is correlated additional parameter s is needed

$$Var(A^{(n)}) = \frac{1}{n/s}Var(A)$$

Parameter s we can obtain from the equation

$$s = \lim_{n\to\infty} n\frac{Var(A^{(n)})}{Var(A)}$$

1.2 Demonstration of the second equation

The equation will be demonstrated on sets generated by random numbers generator.

Lets have APD monitoring photon counts with poissonian noise.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd
from scipy import constants

plt.style.use('scandic')
```

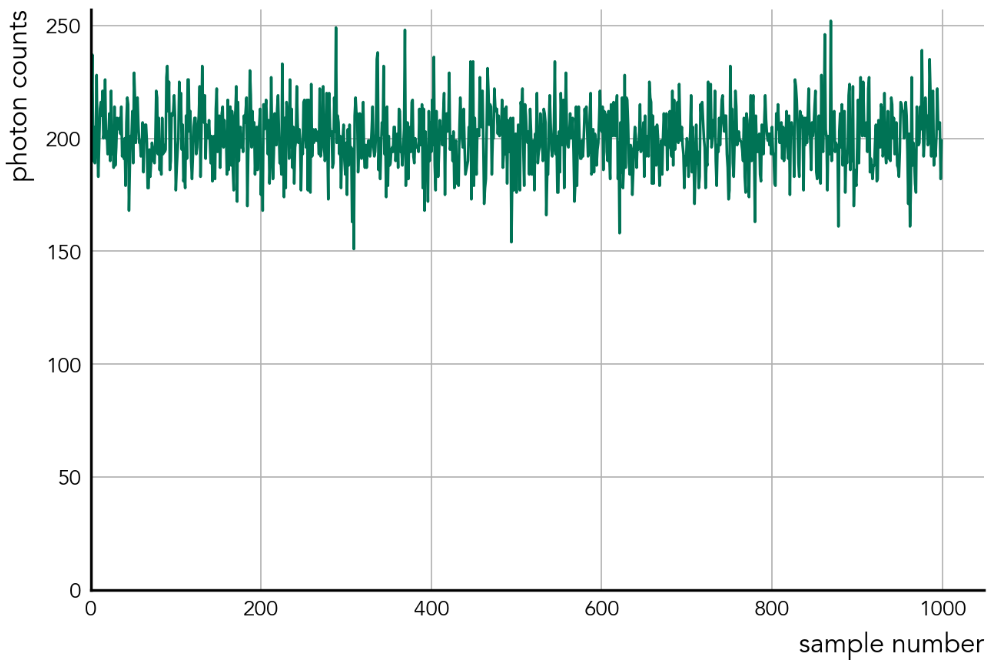
```
Duplicate key in file
PosixPath('/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/matplotlib/mpl-data/stylelib/scandic.mplstyle'), line 28
('xtick.major.size:    0       # major tick size in points')
```

```
Duplicate key in file
PosixPath('/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/matplotlib/mpl-data/stylelib/scandic.mplstyle'), line 31
('ytick.major.size:    0       # major tick size in points')
```

[ ]:
```python
def subsample_data(data, n):
    resample_shape = (sample_size//n, n)
    # print(resample_shape)
    resample_no_of_samples = np.product(resample_shape)
    subsample = data[:resample_no_of_samples]
    # print(subsample.shape)
    subsample = subsample.reshape(resample_shape)
    # print(subsample.shape)
    subsample = subsample.mean(axis=1)
    return subsample
```

[ ]:
```python
mu = 0
sigma = 1
sample_size = 1000

signal_strength = 200

# sample = np.random.default_rng().normal(mu, sigma, sample_size)
sample = np.ones(sample_size)*signal_strength
# add poisson noise
sample = np.random.default_rng().poisson(sample)

# plot the sample
plt.plot(sample)
plt.xlabel('sample number')
plt.ylabel('photon counts')
plt.gca().set_ylim(bottom=0)
plt.gca().set_xlim(left=0)
```

[ ]:
```
(0.0, 1048.95)
```

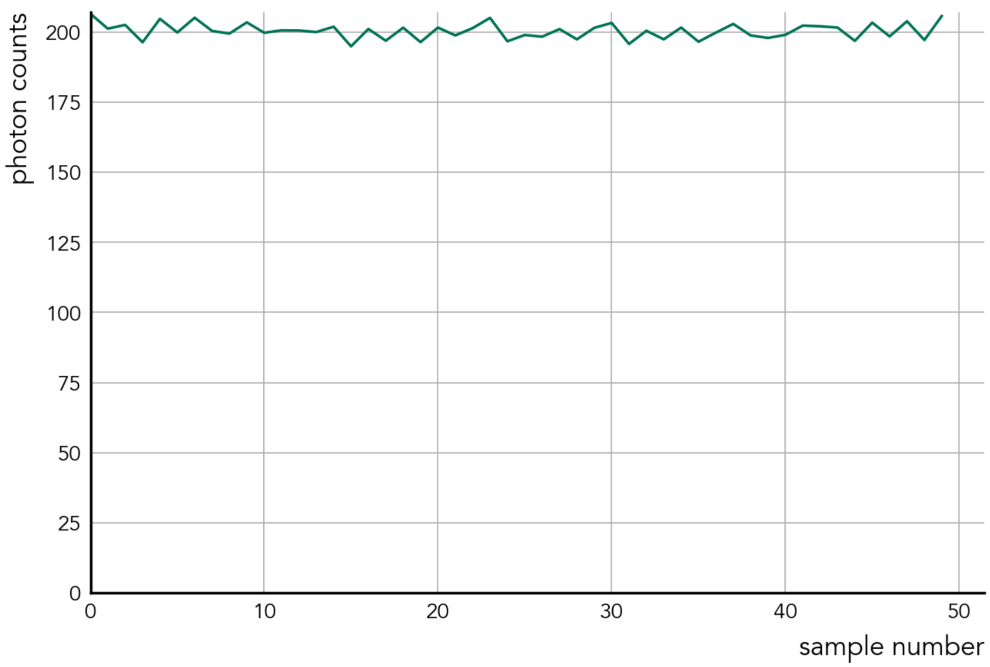



```
[ ]: n_min = 10
     n_max = 100
     step = 5
     n = np.arange(n_min, n_max, step).astype(int) # subsample sizes

     # create list of subsamples
     subsamples = []

     for i in n:
         resample_shape = (sample_size//i, i)
         # print(resample_shape)
         resample_no_of_samples = np.product(resample_shape)
         subsample = sample[:resample_no_of_samples]
         # print(subsample.shape)
         subsample = subsample.reshape(resample_shape)
         # print(subsample.shape)
         subsample = subsample.mean(axis=1)
         # print(subsample.shape)
         subsamples.append(subsample)
```

```
[ ]: # visualize one subsample

     subspl_to_visualise = 2

     # plot the sample
```

```
plt.plot(subsamples[subspl_to_visualise])
plt.xlabel('sample number')
plt.ylabel('photon counts')
plt.gca().set_ylim(bottom=0)
plt.gca().set_xlim(left=0)
```

[ ]: (0.0, 51.45)

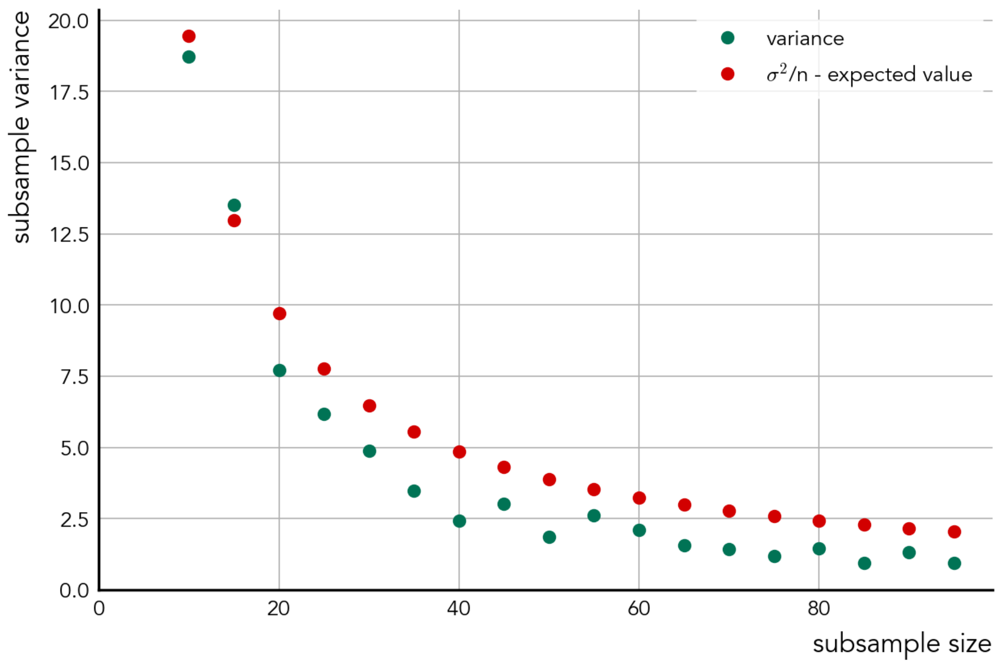


[ ]:
```
print('sample mean: ', sample.mean())
print('sample variance: ', sample.var())

# calculate the mean and variance of the subsamples
subsample_means = []
subsample_vars = []

for subsample in subsamples:
    subsample_means.append(subsample.mean())
    subsample_vars.append(subsample.var())

# plot the mean and variance of the subsamples
plt.plot(n, subsample_vars, 'o', label='variance')
plt.plot(n, sample.var()/n, 'o', label='$\sigma^2$/n - expected value')

# plt.plot(n, n*subsample_vars, '.', label='n $\cdot$ variance')
plt.xlabel('subsample size')
```

```
plt.ylabel('subsample variance')
plt.gca().set_ylim(bottom=0)
plt.gca().set_xlim(left=0)
plt.legend()
```

```
sample mean:  200.374
sample variance:  194.48812399999997
```

[ ]: <matplotlib.legend.Legend at 0x7fe462625fd0>



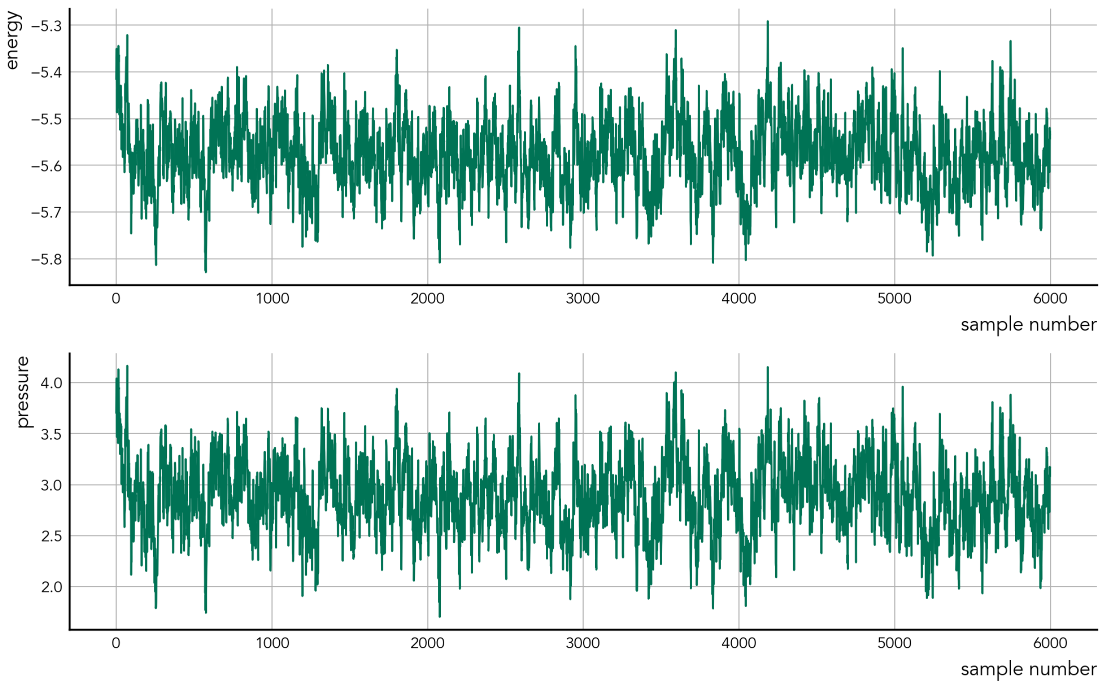
1.2.1 Question for the excercise

Why is it lower?

1.3 Implement procedure for err bar calculation

[ ]:
```
df = pd.read_csv("results/sim_03_run_2.dat", header=None, sep="\s+",␣
↪index_col=0)

energy = df[2].to_numpy()
pressure = df[3].to_numpy()

fig, axs = plt.subplots(2, 1, figsize=(8, 5))

axs[0].plot(energy)
```

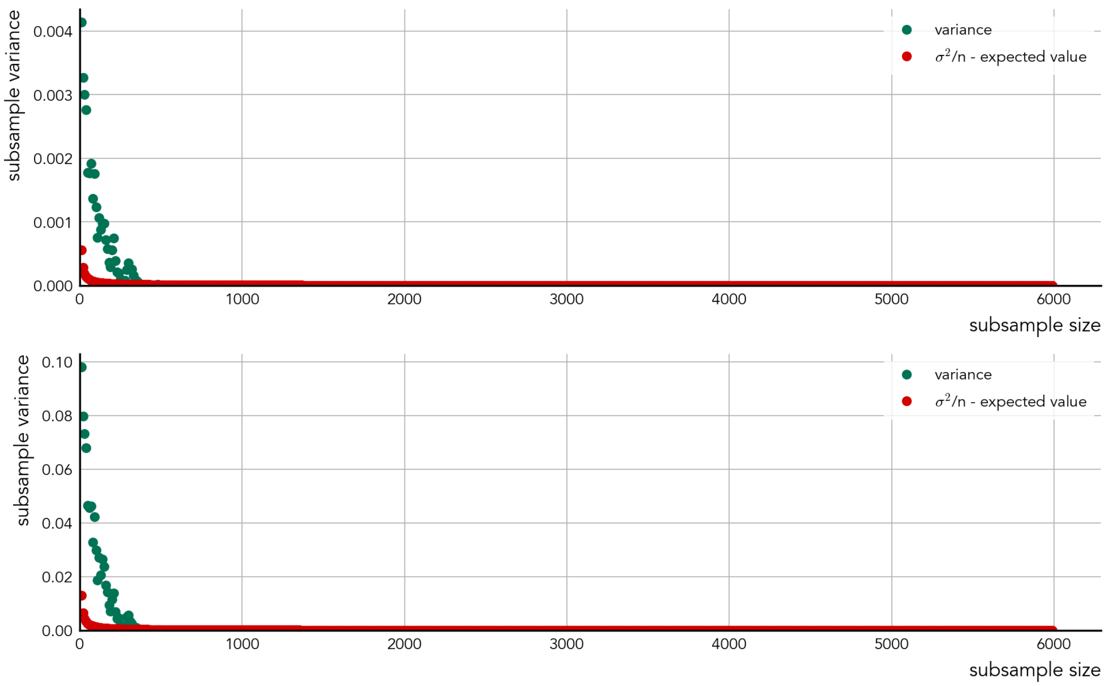
```
axs[0].set_xlabel('sample number')
axs[0].set_ylabel('energy')

axs[1].plot(pressure)
axs[1].set_xlabel('sample number')
axs[1].set_ylabel('pressure')

fig.tight_layout()
```



[ ]:
```
n_min = 10
n_max = 6000
step = 10

n = list(np.arange(n_min, n_max, step).astype(int)) # subsample sizes

energy_subsamples = [subsample_data(energy, i) for i in n]
pressure_subsamples = [subsample_data(pressure, i) for i in n]

energy_variances = np.array([np.var(i) for i in energy_subsamples])
pressure_variances = np.array([np.var(i) for i in pressure_subsamples])

# plot the mean and variance of the subsamples
fig, axs = plt.subplots(2, 1, figsize=(8, 5))
```

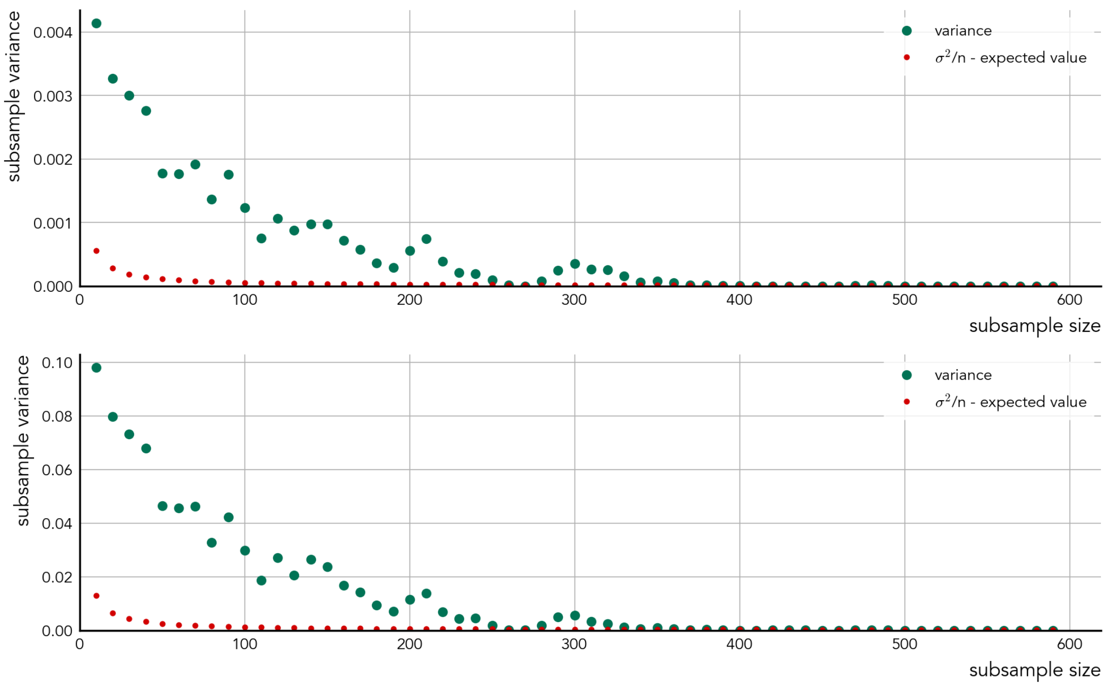
```
axs[0].plot(n, energy_variances, 'o', label='variance')
axs[0].plot(n, np.var(energy)/np.array(n), 'o', label='$\sigma^2$/n - expected␣
 ↪value')

axs[0].set_xlabel('subsample size')
axs[0].set_ylabel('subsample variance')
axs[0].set_ylim(bottom=0)
axs[0].set_xlim(left=0)
axs[0].legend()

axs[1].plot(n, pressure_variances, 'o', label='variance')
axs[1].plot(n, np.var(pressure)/np.array(n), 'o', label='$\sigma^2$/n -␣
 ↪expected value')

axs[1].set_xlabel('subsample size')
axs[1].set_ylabel('subsample variance')
axs[1].set_ylim(bottom=0)
axs[1].set_xlim(left=0)
axs[1].legend()

fig.tight_layout()
```

```
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/fromnumeric.py:3723: RuntimeWarning: Degrees of freedom <= 0
for slice
  return _methods._var(a, axis=axis, dtype=dtype, out=out, ddof=ddof,
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/_methods.py:222: RuntimeWarning: invalid value encountered
in true_divide
  arrmean = um.true_divide(arrmean, div, out=arrmean, casting='unsafe',
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/_methods.py:254: RuntimeWarning: invalid value encountered
in double_scalars
  ret = ret.dtype.type(ret / rcount)
```



[ ]:
```
n_min = 10
n_max = 600
step = 10

n = list(np.arange(n_min, n_max, step).astype(int)) # subsample sizes

energy_subsamples = [subsample_data(energy, i) for i in n]
pressure_subsamples = [subsample_data(pressure, i) for i in n]

energy_variances = np.array([np.var(i) for i in energy_subsamples])
pressure_variances = np.array([np.var(i) for i in pressure_subsamples])

# plot the mean and variance of the subsamples
fig, axs = plt.subplots(2, 1, figsize=(8, 5))

axs[0].plot(n, [np.var(i) for i in energy_subsamples], 'o', label='variance')
axs[0].plot(n, np.var(energy)/np.array(n), '.', label='$\sigma^2$/n - expected␣
↪value')

axs[0].set_xlabel('subsample size')
axs[0].set_ylabel('subsample variance')
axs[0].set_ylim(bottom=0)
axs[0].set_xlim(left=0)
axs[0].legend()
```

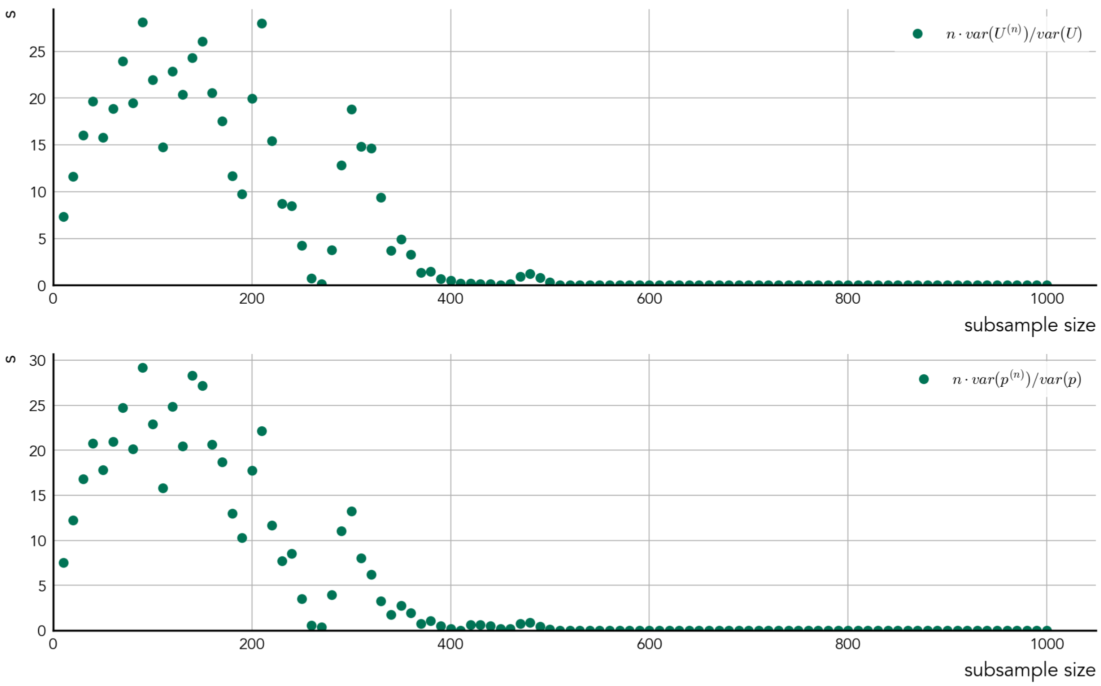
```
axs[1].plot(n, [np.var(i) for i in pressure_subsamples], 'o', label='variance')
axs[1].plot(n, np.var(pressure)/np.array(n), '.', label='$\sigma^2$/n -␣
↪expected value')

axs[1].set_xlabel('subsample size')
axs[1].set_ylabel('subsample variance')
axs[1].set_ylim(bottom=0)
axs[1].set_xlim(left=0)
axs[1].legend()

fig.tight_layout()
```



[ ]:
```
n_min = 10
n_max = 6000
step = 10

n = list(np.arange(n_min, n_max, step).astype(int)) # subsample sizes

energy_subsamples = [subsample_data(energy, i) for i in n]
pressure_subsamples = [subsample_data(pressure, i) for i in n]

energy_variances = np.array([np.var(i) for i in energy_subsamples])
pressure_variances = np.array([np.var(i) for i in pressure_subsamples])
```

```python
s_energy = n*energy_variances/energy.var()
s_pressure = n*pressure_variances/pressure.var()

# plot the s vs n

fig, axs = plt.subplots(2, 1, figsize=(8, 5))

axs[0].plot(n, s_energy, 'o', label='$n \cdot var(U^{(n)})/ var(U)$')
# axs[0].plot(n, n, label='s = 1')
axs[0].set_xlabel('subsample size')
axs[0].set_ylabel('s')
axs[0].set_ylim(bottom=0)
axs[0].set_xlim(left=0)
axs[0].legend()

axs[1].plot(n, s_pressure, 'o', label='$n \cdot var(p^{(n)})/ var(p)$')
# axs[1].plot(n, n, label='s = 1')
axs[1].set_xlabel('subsample size')
axs[1].set_ylabel('s')
axs[1].set_ylim(bottom=0)
axs[1].set_xlim(left=0)
axs[1].legend()

fig.tight_layout()
```

```
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/fromnumeric.py:3723: RuntimeWarning: Degrees of freedom <= 0
for slice
  return _methods._var(a, axis=axis, dtype=dtype, out=out, ddof=ddof,
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/_methods.py:222: RuntimeWarning: invalid value encountered
in true_divide
  arrmean = um.true_divide(arrmean, div, out=arrmean, casting='unsafe',
/Users/jakub.dokulil/opt/anaconda3/lib/python3.9/site-
packages/numpy/core/_methods.py:254: RuntimeWarning: invalid value encountered
in double_scalars
  ret = ret.dtype.type(ret / rcount)
```

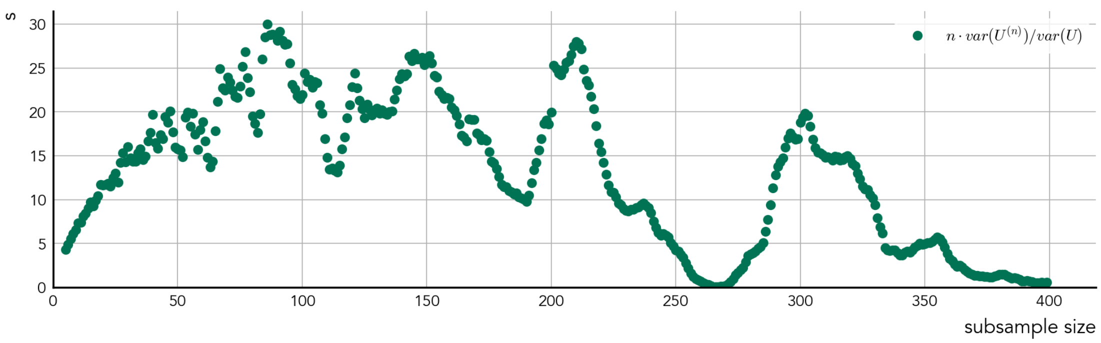


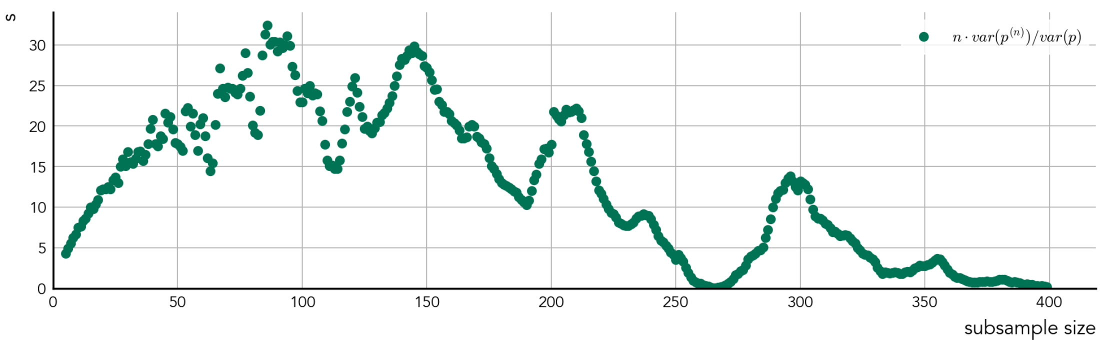
The variance decreases with n. Therefore for 'larger' n we are effectivelly dividing

$$\frac{\text{small number}}{\text{large number}} \to 0$$

[ ]:
```python
n_min = 5
n_max = 400
step = 1

n = list(np.arange(n_min, n_max, step).astype(int)) # subsample sizes

energy_subsamples = [subsample_data(energy, i) for i in n]
pressure_subsamples = [subsample_data(pressure, i) for i in n]

energy_variances = np.array([np.var(i) for i in energy_subsamples])
pressure_variances = np.array([np.var(i) for i in pressure_subsamples])


s_energy = n*energy_variances/energy.var()
s_pressure = n*pressure_variances/pressure.var()

# plot the s vs n

fig, axs = plt.subplots(2, 1, figsize=(8, 5))
```

```
axs[0].plot(n, s_energy, 'o', label='$n \cdot var(U^{(n)})/ var(U)$')
# axs[0].plot(n, n, label='s = 1')
axs[0].set_xlabel('subsample size')
axs[0].set_ylabel('s')
axs[0].set_ylim(bottom=0)
axs[0].set_xlim(left=0)
axs[0].legend()

axs[1].plot(n, s_pressure, 'o', label='$n \cdot var(p^{(n)})/ var(p)$')
# axs[1].plot(n, n, label='s = 1')
axs[1].set_xlabel('subsample size')
axs[1].set_ylabel('s')
axs[1].set_ylim(bottom=0)
axs[1].set_xlim(left=0)
axs[1].legend()

fig.tight_layout()
```





For further calculations lets choose s = 125.

[ ]:
```
s = 125

energy_subsample = subsample_data(energy, s)
pressure_subsample = subsample_data(pressure, s)
```

```
energy_mean = np.mean(energy_subsample)
pressure_mean = np.mean(pressure_subsample)

energy_variance = np.var(energy_subsample)
pressure_variance = np.var(pressure_subsample)

print(f'energy U*: {energy_mean} +- {np.sqrt(energy_variance)}')
print(f'pressure p*: {pressure_mean} +- {np.sqrt(pressure_variance)}')
```

```
energy U*: -5.5679165799999994 +- 0.02948127051421655
pressure p*: 2.9280593 +- 0.14348167591431454
```

1.4 Effect of displacement

originally chosen to 0.4. Lets run the simaltions for values from 0.1 to 0.6.

output for 0.1

```
fname=[mclj_out.dat]

    n=       256
  rho=   0.84186
    t=   1.20000
 disp=   0.10000

   nt=         6000 (*     1)
 accr= 7.15899e-01
<U>/N=-5.56697e+00
 Cv/N= 2.90678e+00
    p= 2.91892e+00

Write g(r) to 'amclj.dat? [y] y
Write PDB format to amclj.pdb? [y] y
```

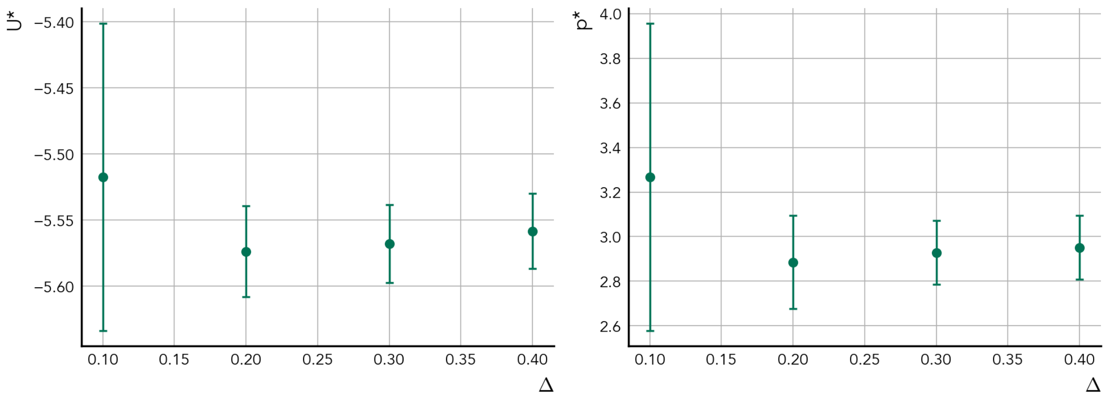
output for r = 0.2

[ ]:
```
s = 125
disp = 1

energies_mean = []
energies_variance = []

pressures_mean = []
pressures_variance = []

for disp in range(1, 5):
    df = pd.read_csv(f"results/sim_0{disp}_run_2.dat", header=None, sep="\s+",␣
↪index_col=0)
```

```python
    energy = df[2].to_numpy()
    pressure = df[3].to_numpy()


    energy_subsample = subsample_data(energy, s)
    pressure_subsample = subsample_data(pressure, s)

    energy_mean = np.mean(energy_subsample)
    pressure_mean = np.mean(pressure_subsample)

    energy_variance = np.var(energy_subsample)
    pressure_variance = np.var(pressure_subsample)

    print(f'energy U*: {energy_mean} +- {np.sqrt(energy_variance)}')
    print(f'pressure p*: {pressure_mean} +- {np.sqrt(pressure_variance)}')
    print()

    energies_mean.append(energy_mean)
    energies_variance.append(energy_variance)

    pressures_mean.append(pressure_mean)
    pressures_variance.append(pressure_variance)


displacement = np.arange(1, 5, 1)/10

fig, axs = plt.subplots(1, 2, figsize=(8, 3))

axs[0].errorbar(displacement, energies_mean, yerr=np.sqrt(energies_variance),␣
 ↪fmt='o')
axs[0].set_xlabel('$\Delta$')
axs[0].set_ylabel('U*')


axs[1].errorbar(displacement, pressures_mean, yerr=np.sqrt(pressures_variance),␣
 ↪fmt='o')
axs[1].set_xlabel('$\Delta$')
axs[1].set_ylabel('p*')

fig.tight_layout()
```

```
energy U*: -5.5173435600000005 +- 0.11615562042799624
pressure p*: 3.2675371900000005 +- 0.6889600524554783

energy U*: -5.573679 +- 0.0344007331277921
pressure p*: 2.88579925 +- 0.20790188196841702
```

```
energy U*: -5.5679165799999994 +- 0.02948127051421655
pressure p*: 2.9280593 +- 0.14348167591431454

energy U*: -5.558228639999999 +- 0.02849613077154221
pressure p*: 2.95132061 +- 0.14376239065420635
```



2 Solution to excercise sheet 1, exercise 4

2.1 (a) background corrections

$$\frac{\Delta U_c}{N} = 2\pi\rho\int_{r_c}^{\infty} dr\, r^2\, 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] = 2\pi\rho\, 4\varepsilon\left(\int_{r_c}^{\infty}\frac{\sigma^{12}}{r^{10}}dr - \int_{r_c}^{\infty}\frac{\sigma^{6}}{r^{4}}\right) =$$

$$= 2\pi\rho\, 4\varepsilon\left(-\left[\frac{\sigma^{12}}{r_c^{9}}\frac{1}{10} - \frac{\sigma^{6}}{r_c^{3}}\frac{1}{3}\right]\right)$$

$$\frac{\Delta W_c}{N} = 2\pi\rho\int_{r_c}^{\infty} dr\, r^2\left[-12\frac{\sigma^{12}}{r^{12}} - 6\frac{\sigma^{6}}{r^{6}}\right] = 2\pi\rho\left(+12\frac{\sigma^{12}}{r^{9}}\frac{1}{10} + 6\cdot\frac{1}{3}\frac{\sigma^{6}}{r^{3}}\right)$$

2.2 (b) background corrections application

From the previous calculations we can see $r_c = 3.345\sigma$.

$$r_c = 3{,}345\,\sigma \quad \Rightarrow \quad \frac{\Delta U_c}{N} = 2\pi\rho 4\varepsilon\left(\frac{\sigma^{\cancel{12}\,3}}{(3{,}345)^9\sigma^{\cancel{9}}}\,\frac{1}{10} + \frac{\sigma^{\cancel{6}\,3}}{(3{,}345)^3\sigma^{\cancel{3}}}\,\frac{1}{3}\right) =$$

$$= 2\pi\rho 4\varepsilon\sigma^3\left(\frac{1}{(3{,}345)^9}\,\frac{1}{10} + \frac{1}{(3{,}345)^3}\,\frac{1}{3}\right)$$

$$\frac{\Delta W_c}{N} = 2\pi\rho 4\varepsilon\left(\frac{\sigma^{\cancel{12}\,3}}{(3{,}345)^9\sigma^{\cancel{9}}}\cdot\frac{6}{5} + 2\,\frac{\sigma^{\cancel{6}\,3}}{(3{,}345)^3\sigma^{\cancel{3}}}\right) =$$

$$= 2\pi\rho 4\varepsilon\sigma^3\left(\frac{6}{5}\,\frac{1}{(3{,}345)^9} + 2\,\frac{1}{(3{,}345)^3}\right)$$

```
[ ]:
```