

Error_analysis_final_EOM

December 2, 2022

0.0.1 EOM

$$\dot{\phi} = p$$

$$\dot{p} = -2\phi(1 + \frac{1}{2+\phi^2})$$

```
[1]: #!/usr/bin/env python
      # coding: utf-8

      import numpy as np
      from math import *
      import matplotlib.pyplot as plt
      import scipy.optimize as so
      import scipy.special as sp
      import mpmath as mp
      import random
```

```
[2]: N_md = 10#Leapfrog integration steps
      N_cfg = 10000
      phi=0
      p_0 = 0
      ar=0

      # This is just defining of variables.
```

```
[3]: def leapfrog_plot():
      global N_md
      p=0.2
      phi=0
      for i in range(100):
          H_0=H(p,phi)
          N_md=i*10+10
          p_new,phi_new=leapfrog(p,phi)
          plt.plot(i*10+10,abs((H(p_new,phi_new)-H_0)/H_0), 'x', color='b')
          #print(p,phi)
      plt.semilogy()
      plt.show()
```

Same idea as last time

```
[4]: def leapfrog(p_l, phi_l):
    # p_0_1, p_0_2, p_0_3,
    global beta
    global f
    global x
    global J
    global N
    global h
    global N_md

    eps=.1/N_md
    phi_l=phi_l+eps/2*p_l

    for i in range(N_md-1):
        p_l=p_l-eps*(2*phi_l)*(1+1/(2+phi_l**2))
        phi_l=phi_l+eps*p_l
        p_l=p_l-eps*(2*phi_l)*(1+1/(2+phi_l**2))
        phi_l=phi_l+eps/2*p_l
    return p_l, phi_l
```

input: p_l, phi_l; output: p_f, phi_f code as explained on the sheet

Last time u commented that the last haft step for phi should be back, but I think forward is correct, because this way we do N_{md} steps forward.

```
[5]: def H(p_h, phi_h):

    return p_h**2/2+phi_h**2+np.log(2+phi_h**2)
```

input p, phi: ; output: H(p, phi)

```
[6]: def HMC(): #Does one iteration of the Markov-Chain and return phi
    global N_md
    global p_0
    global phi
    #global p
    global ar

    p_h=np.random.normal(loc=00.0, scale=1.0)
    p_l, phi_l = leapfrog(p_h, phi)

    P_acc = np.exp(float(H(p_h, phi)-H(p_l, phi_l)))

    if P_acc > np.random.rand():
```

```

phi = phi_1
ar=ar+1

```

HMC copied from last exercise :)

```

[7]: def autocorrelation(o_chain,t,mu_o):
    c_t=0
    for i in range(N_cfg-t):
        c_t+=(o_chain[i]-mu_o)*(o_chain[i+t]-mu_o)
    c_t=c_t/(N_cfg-t)
    return c_t

```

input markov_chain_observables μ_o , t ; output: $C^0(t)$ see sheet

```

[8]: def normalized_autocorrelation(o_chain,t):
    mu_o=np.average(o_chain)
    Gamma_t=autocorrelation(o_chain,t,mu_o)/autocorrelation(o_chain,0,mu_o)
    return Gamma_t

```

input markov_chain_observables, t: ; output: $\Gamma(t)$ see sheet

```

[9]: def int_auto_corr(o_chain):
    tau_int=0
    tau_int=0.5*normalized_autocorrelation(o_chain,0)
    for i in range(N_cfg):
        temp=normalized_autocorrelation(o_chain,i+1)
        if temp>0:
            tau_int+=temp
        else: return tau_int
    return tau_int

```

input: markov_chain_observables output: τ_{int} see sheet

```

[10]: def markov_chain():
    global N_cfg
    global x
    global phi
    global ar

    phi_chain=[]
    for i in range(N_cfg):
        HMC()
        phi_chain.append(phi)
    print(ar/(N_cfg), 'Acceptance rate')
    ar=0
    phi_chain=np.array(phi_chain)
    o_chain=np.cos(np.sqrt(1+phi_chain**2))

```

```
return o_chain
```

creates markov chain as always but convertes the entries in observables. so it “returns” a markov chain of observables

```
[11]: def binning(o_chain,tau_int):
    o_chain_new=[]
    tau_int=int(tau_int)
    o_chain=o_chain[0:N_cfg-N_cfg%tau_int]
    for i in range(int((N_cfg-N_cfg%tau_int)/tau_int)):
        o_chain_new.append(np.average(o_chain[i*tau_int:(i+1)*tau_int]))
    return o_chain_new
```

input: o_chain, τ_{int} output: binned chain, with bin size τ_{int}

```
[12]: def print_nor_auto(o_chain,tau_int):
    N_cfg_temp=len(o_chain)
    normal_auto= []
    exp= []
    for i in range(N_cfg_temp):
        normal_auto.append(normalized_autocorrelation(o_chain,i))
        exp.append(np.exp(-i/tau_int))
    plt.plot(normal_auto,label="data")
    plt.plot(exp,label="theo")
    plt.legend()
    plt.show()
```

This function prints the normalized autocorrelation and $e^{-t/\tau}$. This is very slow and should only be used for short chains. Thats ok, because the autocorrelation can be studied for the first ~ 100 entries of the chain.

```
[13]: def show_auto_dec(o_chain,tau_int):
    global N_cfg
    tau_int_final=[]
    tau_int_final.append(tau_int)
    for i in range(2,int(tau_int)):
        N_cfg=len(o_chain)
        o_chain_new=binning(o_chain,i)
        N_cfg=len(o_chain_new)
        tau_int_new=int_auto_corr(o_chain_new)
        tau_int_final.append(tau_int_new)
    N_cfg=len(o_chain)
    plt.plot(tau_int_final)
    plt.xlabel(r"$N_{bin}$")
    plt.ylabel(r"$\tau_{int}(N_{bin})$")
    plt.show()
```

input: o_chain, τ_{int} output: None this function computes and plots the τ_{int} for different N_{bin}

```
[14]: def show_error_inc(o_chain,tau_int):
    boot_var_final=[]
    for i in range(2,3*int(tau_int)):
        o_chain_new=binning(o_chain,i)
        o_chain_boot=booti(o_chain_new, 200)
        boot_var_final.append(np.sqrt(np.var(o_chain_boot)))
    plt.plot(boot_var_final)
    plt.xlabel(r"$N_{\text{bin}}$")
    plt.ylabel(r"$\sqrt{\text{var}(\text{bootstrap})}$")
    plt.show()
```

input: o_chain , τ_{int} output: None calculates and plots the variance in the bootstrap_o_chain-array for different bin sizes

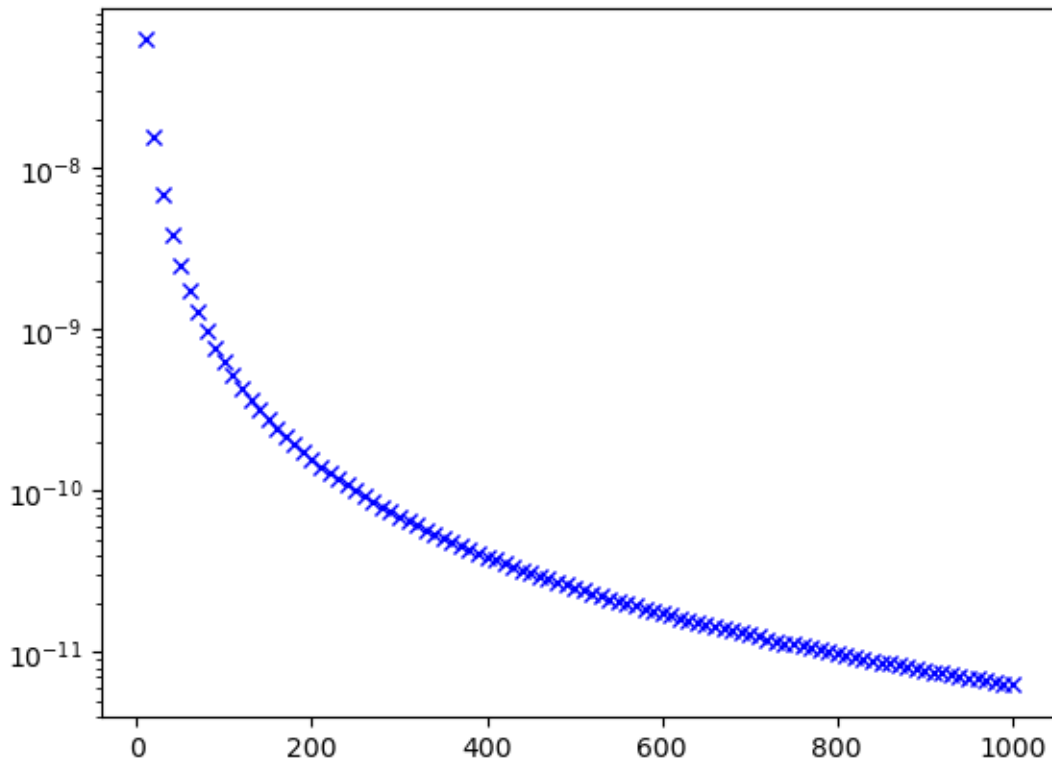
```
[15]: def booti(o_chain,N):
    boot_array=[]
    boot_array_final=[]
    for i in range(N):
        for j in range(len(o_chain)):
            boot_array.append(random.choice(o_chain))
        boot_array_final.append(np.average(boot_array))
        boot_array=[]
    return boot_array_final
```

input: o_chain , N output: bootstrap_o_chain-array picks randomly as many elements from the binned chain as the binned chain has elements in itself and then builds a new o_chain from the averages of N of these randomly arranged arrays.

```
[16]: def booti_ens(N):
    global N_cfg
    booti_error_ens=[]
    for i in range(20):
        N_cfg=(i+1)*50000
        o_chain=markov_chain()
        o_chain_new=binning(o_chain,N)
        o_chain_boot=booti(o_chain_new, 200)
        print(np.average(o_chain_boot),N_cfg)
        booti_error_ens.append(np.sqrt(np.var(o_chain_boot)))
    plt.plot(np.arange(50000,1050000,50000),booti_error_ens,label="data")
    plt.xlabel(r"$N_{\text{ens}}$")
    plt.ylabel(r"$\sqrt{\text{var}(\text{bootstrap})}$")
    plt.plot(np.arange(50000,1050000,50000),1/(6*np.sqrt(np.
    → arange(50000,1050000,50000)/N)),label="theo")
    plt.show()
```

input: N output: calculates the variance in the bootstrap_o_chain-array for different N_{ens} and plots them. The bin-size is always N .

```
[17]: leapfrog_plot()
```



The graph looks like we expected it. It shows that for large N_{md} the energy of the old and new configuration is almost the same. This will later be important to achieve a high acceptance probability.

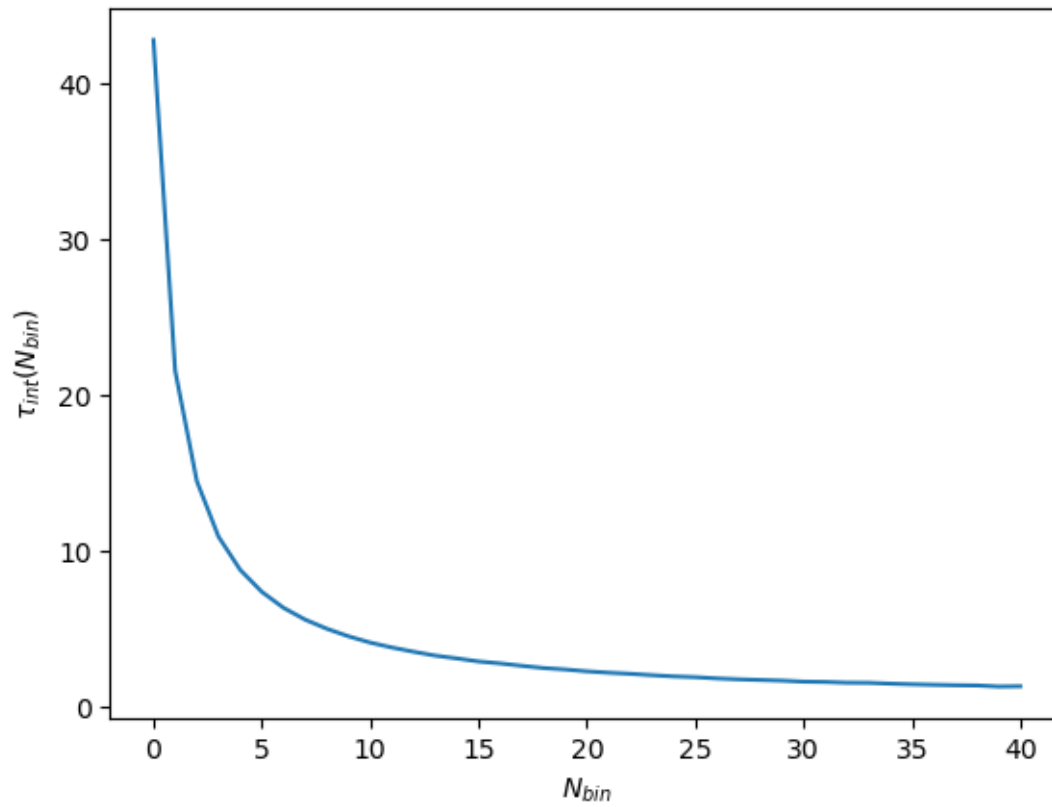
```
[18]: N_md=3
```

```
[19]: o_chain=markov_chain()
```

1.0 Acceptance rate

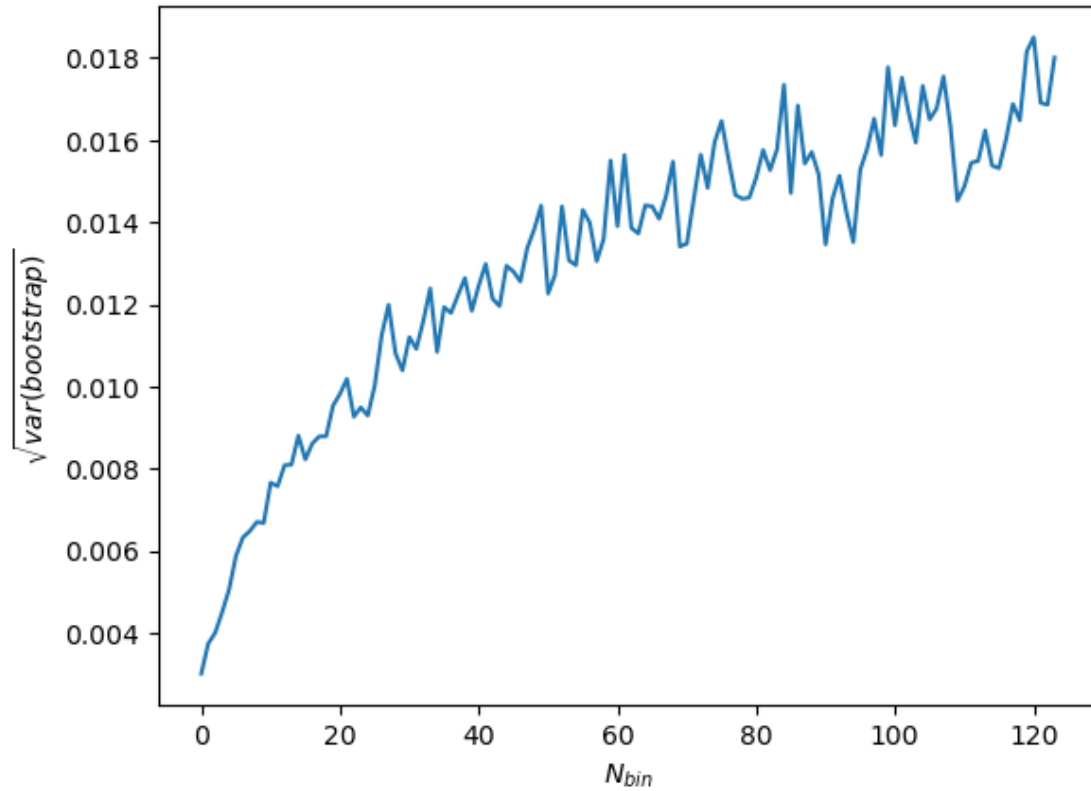
```
[20]: tau_int=int_auto_corr(o_chain)
```

```
[21]: show_auto_dec(o_chain,tau_int)
```



This graph shows the decrease of τ_{int} for increasing bin size. This is to be expected, because elements in the binned chain have less autocorrelation.

```
[22]: show_error_inc(o_chain,tau_int)
```

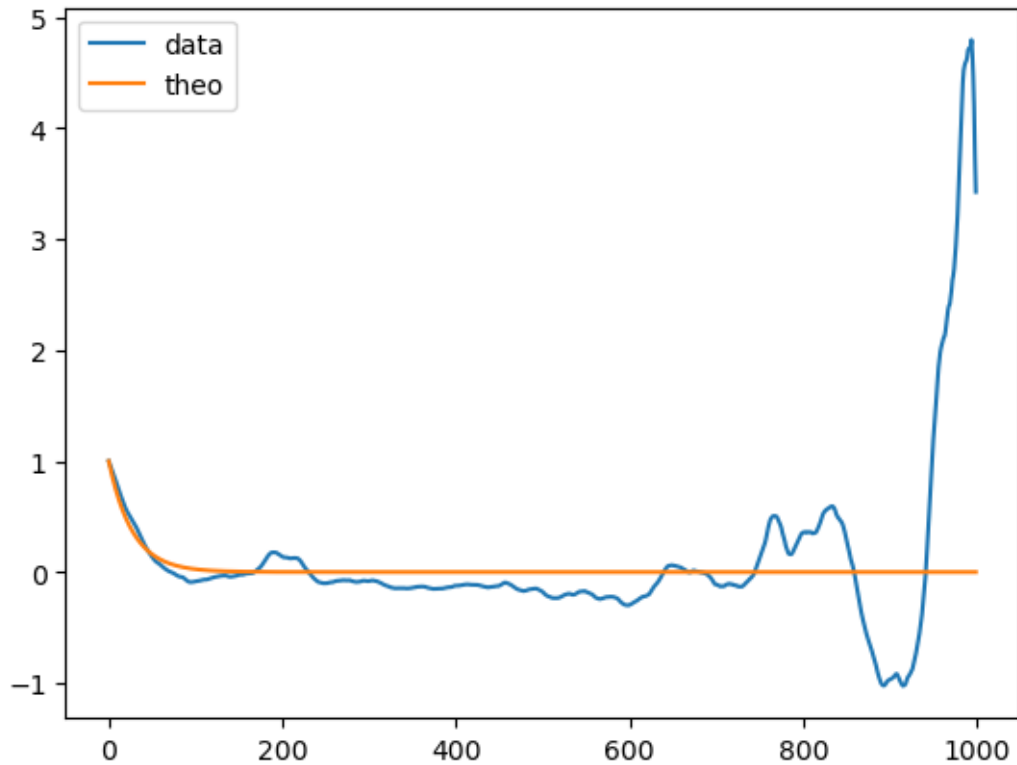


This graph shows the increase in variance for increasing bin size. This is expected because if we increase the bin size we eliminate autocorrelation and values in then bootstrap arrays are more randomly distributed which at the end leads to higher variance. The variance is a lot lower than the expected theoretical value of $\sigma^2 = 0.0349816$. One reason for the low variance can be the autocorrelation and the other reason is that the bootstrap-algo also decreases the variance by a factor of $\frac{1}{\sqrt{n}}$

where n is the number of bins in the binned chain.

```
[23]: N_cfg=1000
      o_chain=markov_chain()
      tau_int=int_auto_corr(o_chain)
      print_nor_auto(o_chain,tau_int) #only use for small N_cfg
```

1.0 Acceptance rate

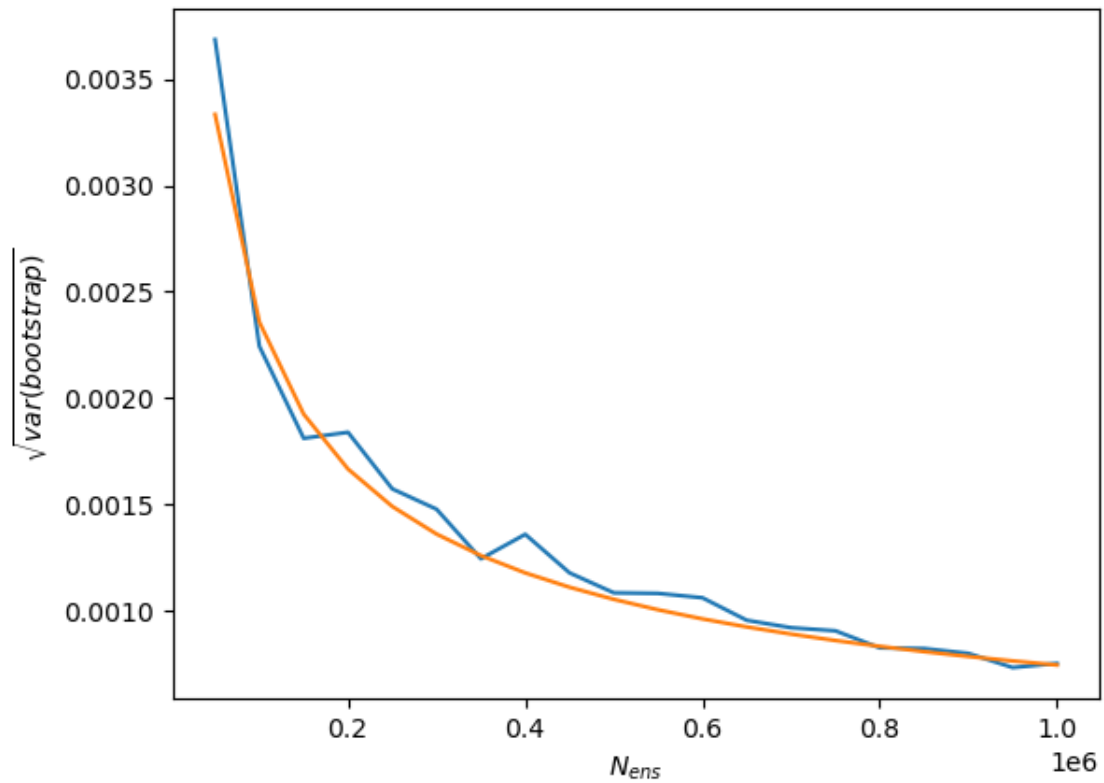


This graph shows the normalized autocorrelation together with $e^{-t/\tau}$. One can see a good fit for the autocorrelation in the beginning of the chain.

[24] : `booti_ens(20)`

```
0.99998 Acceptance rate
0.398873615793857 50000
0.99998 Acceptance rate
0.40748568271085583 100000
0.9999666666666667 Acceptance rate
0.4020710155502145 150000
0.99995 Acceptance rate
0.39927175759064804 200000
0.999972 Acceptance rate
0.3991408551781666 250000
0.9999766666666666 Acceptance rate
0.4011156270148632 300000
0.9999857142857143 Acceptance rate
0.3992090083959357 350000
0.999955 Acceptance rate
0.39836522865075596 400000
0.9999555555555556 Acceptance rate
0.395562923134279 450000
```

0.99996 Acceptance rate
 0.40240694566446406 500000
 0.9999818181818182 Acceptance rate
 0.3967117061284304 550000
 0.99997 Acceptance rate
 0.39857052379608254 600000
 0.9999507692307692 Acceptance rate
 0.3961143512030273 650000
 0.9999571428571429 Acceptance rate
 0.3974218659495058 700000
 0.9999666666666667 Acceptance rate
 0.3993701513958699 750000
 0.99996375 Acceptance rate
 0.39789238454339304 800000
 0.9999564705882353 Acceptance rate
 0.3991121928144202 850000
 0.9999677777777778 Acceptance rate
 0.3971737322645491 900000
 0.9999652631578947 Acceptance rate
 0.4007474146196712 950000
 0.999961 Acceptance rate
 0.4004314105082162 1000000



This graph shows the decrease of variance in the `bootstrap_o_chain` for increasing N_{ens} . This is compared to $\sim \frac{1}{\sqrt{N_{ens}/N_{bin}}}$. The good fit shows that the variance scales with $\frac{1}{\sqrt{N_{ens}/N_{bin}}}$. With increasing N_{ens} the size of the binned chain is increased as well and thereby also the number of elements in the bootstrap arrays is increased. The more values we pick here the better we can apply the Central Limit Theorem and the average values in the `bootstrap_o_chain` array are normal-distributed with mean μ and their standard distribution scales with $\frac{1}{\sqrt{N_{ens}/N_{bin}}}$.

[]: