6th Numerical Lattice Field Theory Training Camp

Lattice QCD Data Analysis

Lattice Parton Collabration

Outline

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- Theory on two-point function

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- Data analysis
    - Programing language/packages
    - `` `iog` `` data format
    - Resampling
    - least χ^2 fit

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- *Introduction to HDF5*

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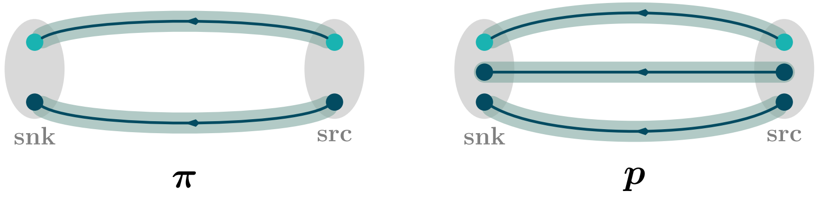

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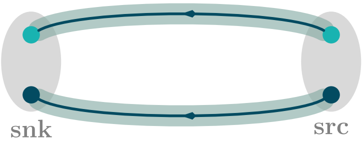

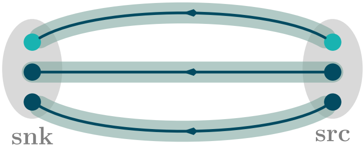

- **For large enough $\tau_f - \tau_i$,** higher excited states decay faster

  $$\langle \mathcal{O}(t_{\mathrm{snk}})\mathcal{O}(t_{\mathrm{src}})^\dagger \rangle \approx$$

  - $c_0 e^{-E_0 t}$ ⇨ one state analysis
  - $c_0 e^{-E_0 t} + c_1 e^{-E_1 t}$ ⇨ two state analysis

- Determine the hadron mass spectrum from lagrangian (first-principle or ab initio calculation)

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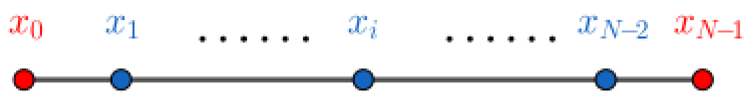
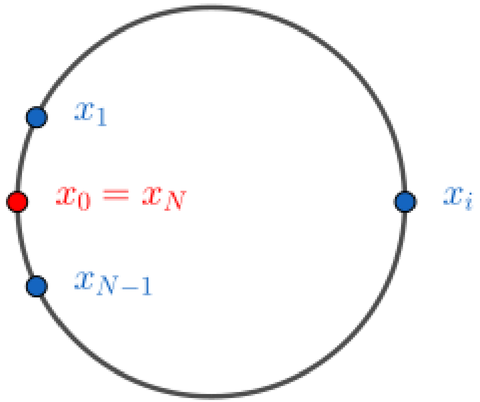
  - $\phi_i = 0$ if $i \geq N$ or $i < N_0$
- Periodic/AntiPeriodic boundary condition
  - $\phi_N = \pm\phi_0, \phi_{N+i} = \pm\phi_i \Rightarrow \phi_{i+N} = \pm\phi_{(i+N) \bmod N}$





- Considering periodic boundary condition
  - propagate in both $\pm t$ direction

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cosh

log

- Determine hadron effective energy E_0 (m_{eff})
  - A glance
    - For $0 < t \ll T/2$ ⇨ $e^{-E_0 t} \gg e^{-E_0(T/2-t)}$ ⇨ $\ln \dfrac{C_2(t)}{C_2(t+a)} \approx aE_0$
    - $\dfrac{C_2(t)}{C_2(t+a)} = \dfrac{\cosh[E_0(T/2-t)]}{\cosh[E_0(T/2-(t+a))]}$ or $\dfrac{C_2(t+a)+C_2(t-a)}{2C_2(t)} = \cosh aE_0$
  - More systematically way ⇨ Fit (see sec. **Least χ^2 fit** for detail)

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  - Regular expression (python package `re`)
- Advanced
  - HDF5, `h5py`
  - MPI

- Documentation

Library/Package	Documentation
pandas	**https://pandas.pydata.org/docs/**
numpy	**https://numpy.org/doc/stable/**
gvar	**https://gvar.readthedocs.io/en/latest/overview.html**
lsqfit	**https://lsqfit.readthedocs.io/en/latest/lsqfit.html**
Scipy	https://scipy.org/
HDF5	https://portal.hdfgroup.org/display/support/documentation
h5py	https://docs.h5py.org/en/stable/

- Installation
  - `pip3`: package installer for python
  - `pip3 install package_name --user`
  - `--user` install under current user enviorment, does not need root permission
- Python devel package (required by `iog.so`)
  - header `/usr/include/python3.6m/`

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# encoding: utf-8
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iog_file = "./2pt_5350.dat.iog"
intrptr = ["cnfg","hdrn","t"]

iog = iog_read(iog_file,intrptr)
print(iog,'\n--------\n')

iog_pi=iog.loc[(iog['hdrn']=='0')]
print(iog_pi['Re'].to_numpy(),'\n--------\n')
print(iog_pi['Re'].to_list(),'\n--------\n')
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- Detailed usage of `pandas.DataFrame.loc`: see documentation

- `iog_reader.py` : `iog` ⇨ pandas.dataframe

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from ctypes import *
import os
import numpy as np
import pandas as pd

lib = cdll.LoadLibrary(os.getcwd()+ '/iog.so')

def iog_read(iog_fl, intrprtrs):
    iog_file = c_char_p(iog_fl.encode('utf-8'))
    size = lib.getsize(iog_file)

    class iog_type(Structure):
        _fields_ = [('info_shape', POINTER(c_int)), ('info', POINTER(c_int)),
                    ('Re', POINTER(c_double)),  ('Im', POINTER(c_double))]

    lib.getdat.restype = POINTER(iog_type)
    iog = lib.getdat(iog_file)

    info_shape = np.ctypeslib.as_array(iog.contents.info_shape, shape=[2])
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- Set the value of `` `INCL` `` pointing to the path containing python develop tools header in `` `Makefile` ``

  `` `INCL = -I/dssg/opt/icelake/linux-centos8-icelake/gcc-8.3.1/python-3.9.12-omx7ttx5qbayml44yyhwifxuooiebvh7/include` ``

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- Execute `` `make iog.so` ``

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...      ...  ...  ..             ...            ...
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[1152 rows x 5 columns]
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[591279.95948887 522915.50556183 482360.00523376 ...
```

string

- Filter by value: `iog.loc[18<=iog['t'].astype(int)]`
- Use logical operator: `iog_pi=iog.loc[(iog['hdrn']=='0') & (iog['t'].astype(int)<18)]`

What is intrptr ? - iog convention

```
       cnfg hdrn   t               Re           Im
0      5350    0   0   591279.959489     0.000005
1      5350    0   1   522915.505562    -0.000003
2      5350    0   2   482360.005234    -0.000012
3      5350    0   3   440684.923986    -0.000002
4      5350    0   4   387859.756810     0.000004
...     ...  ...  ..             ...          ...
```

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- `cnfg`: configuration number

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- `cnfg` : configuration number
- `hdrn` (hadron) : ["PION", "KAON", "PROTON", "RHO", "D", "ETAS", "ETAC", "JPSI", "LAMBDA", "LAMBDAC", "SIGMA", "XI", "XIC", "OMEGA", "DELTA"]

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- `t`: time slice
- `Re`, `Im`: real and imaginary part of two-point function

> theoretically, 2pt should be real valued, but due to numberical errors, it may have a neglectable smallimaginary part

more complicated iog convention (not in this traning camp)

```
        cnfg tsrc lnk snksmr      hdrn    mntm   t   Re   Im
0       2125   18   0      0    200505  505050   0  0.0  0.0
1       2125   18   0      0    200505  505050   1  0.0  0.0
...      ...  ...  ..    ...       ...     ... ...  ...  ...
4606    2125   18   0      1 100001515  505045 126  0.0  0.0
4607    2125   18   0      1 100001515  505045 127  0.0  0.0
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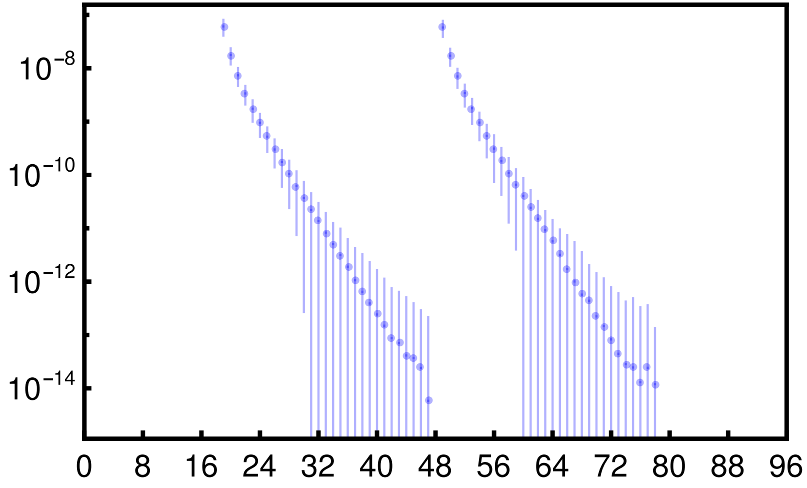

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0       2125   18   0      0    200505  505050    0  0.0  0.0
1       2125   18   0      0    200505  505050    1  0.0  0.0
...      ...  ...  ..    ...       ...     ...  ...  ...  ...
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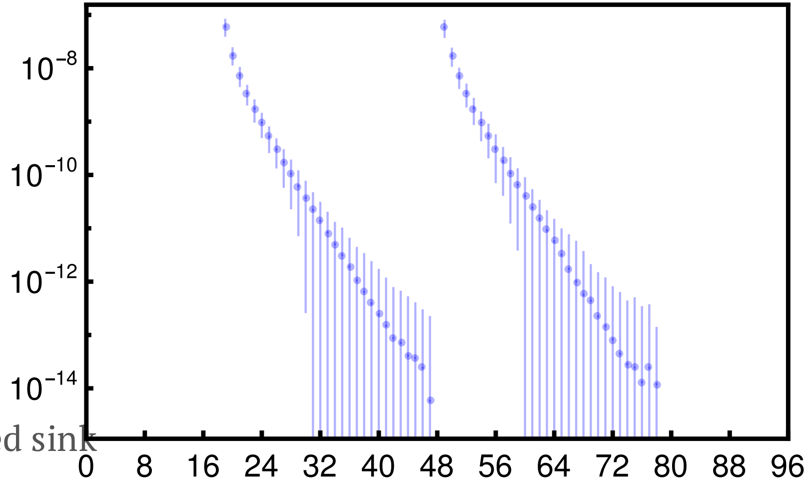

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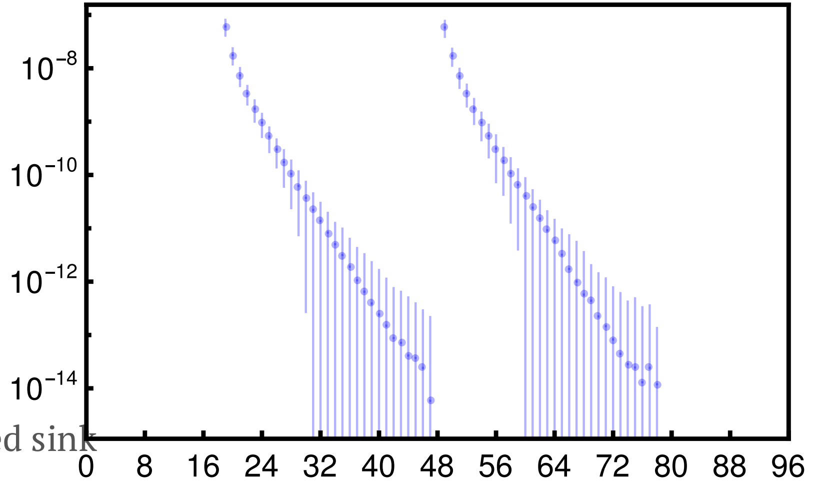

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- `lnk`: dummy label in two-point data file

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0       2125   18   0      0    200505 505050   0 0.0 0.0
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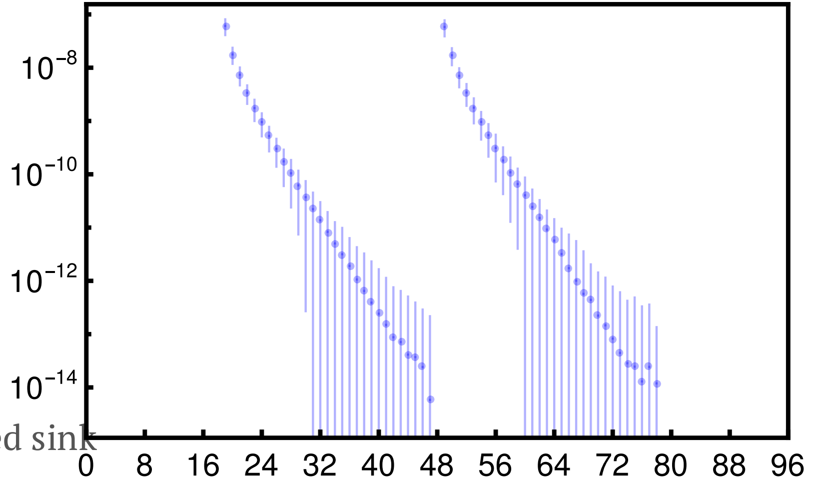

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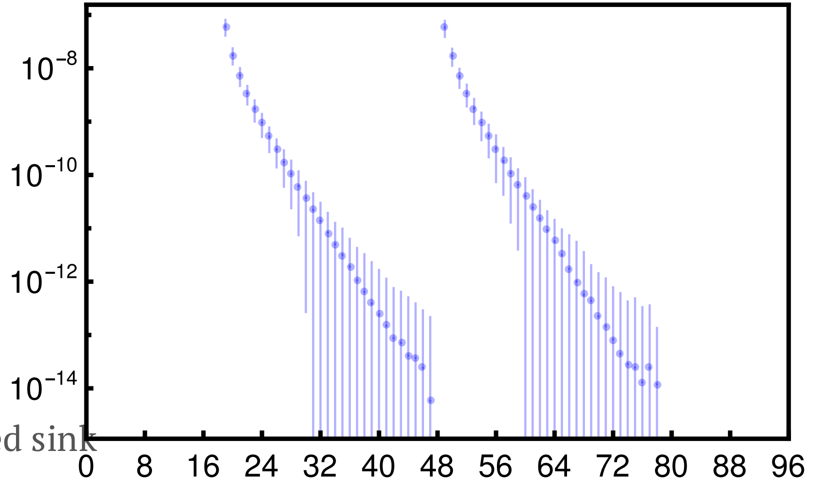

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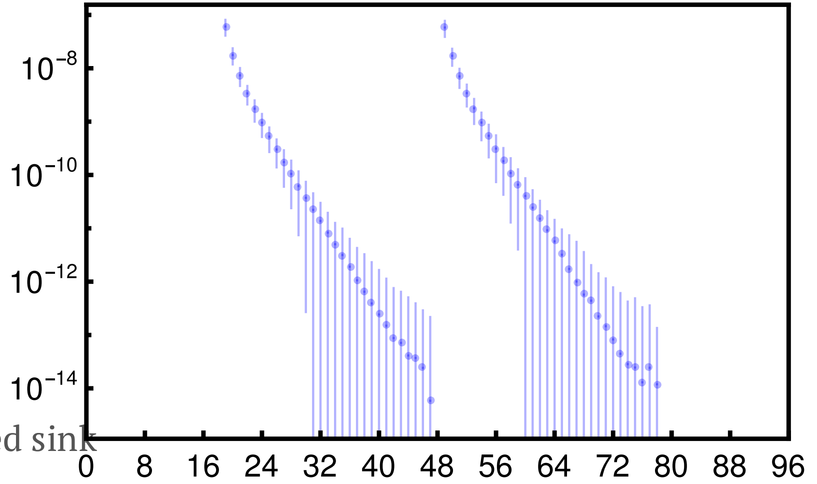

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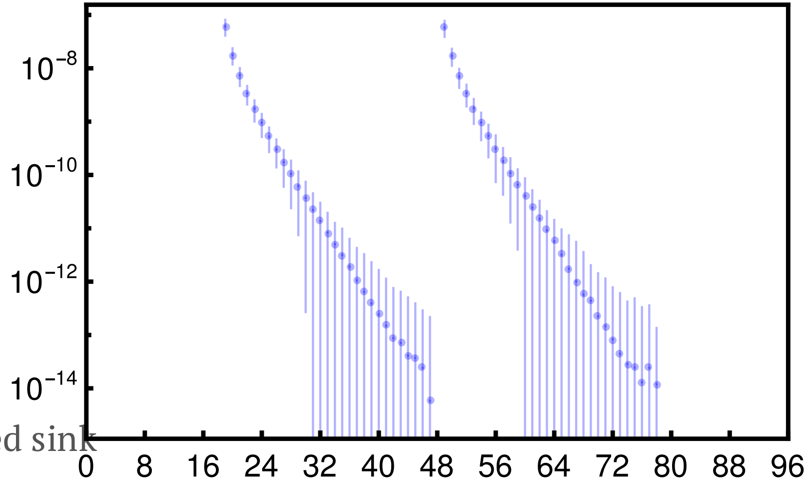

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- momentum : `` `505050` `` ⇨ 50 50 50 ⇨ $0, 0, 0$ ⇨ $\vec{P} = (0, 0, 0)$
  - lattice momentum unit: $\dfrac{2\pi}{L}, L = na$

    > Discertized Fourier transformation

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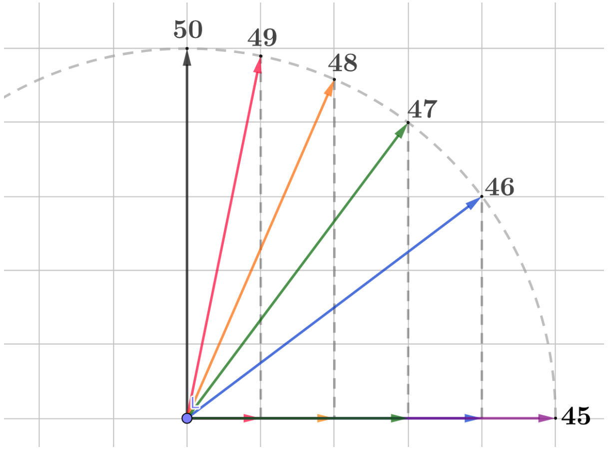
  > Discertized Fourier transformation

- $\tilde{p}_x, \tilde{p}_y, \tilde{p}_z$, eg. 50 50 48
  - $\vec{P} = [(50,50,50) - (\tilde{p}_x, \tilde{p}_y, \tilde{p}_z)] \times \dfrac{2\pi}{L} = (0,0,2) \times \dfrac{2\pi}{L}$ ⇨ 2 unit momentum in z-direction



Resampling

- Conventional resampling method
  - Jack-knife
  - Bootstrap

Why Resampling

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- Suppose C is directly calculate on the lattice, $\mathcal{O} = F(\langle C\rangle)$ is what we are intrested in

> F usually is a nonlinear function

- Usually, $\mathcal{O} = F(\langle C\rangle) \neq \langle F(C)\rangle$
- Error estimation of $\mathcal{O}$
  - usually, the target $\mathcal{O}$ has a complicate dependence (usually nonlinear) on lattice calculable $\mathcal{C}$
  - Error propagation $\sigma_{\mathcal{O}} \approx F'(\langle C\rangle)\sigma_{\mathcal{C}}$?
    - 😭 F is nonlinear
    - 😭 $\sigma_{\mathcal{C}}$ is not small enough to neglect $\mathcal{O}(\sigma_{\mathcal{C}}^2)$ term

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Solution: Resampling

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- Original Datasets:
  - cnfg 1 $\Rightarrow \vec{C}^{(1)} = (C_0^{(1)}, \cdots, C_t^{(1)})$
  - $\cdots\cdots\cdots$
  - cnfg $N \Rightarrow \vec{C}^{(N)} = (C_0^{(N)}, \cdots, C_t^{(N)})$

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- ith Jack-knife sample
  - $\tilde{C}^{(i)} = \frac{N}{N-1}\bar{C} - \frac{1}{N-1}\vec{C}^{(i)} \Rightarrow$ drop cnfg i, calculate mean value of the rest

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- ith Jack-knife sample
  - $\tilde{C}^{(i)} = \frac{N}{N-1}\bar{C} - \frac{1}{N-1}\vec{C}^{(i)}$ ⇨ drop cnfg i, calculate mean value of the rest
- Estimator
  - $\bar{C} = \frac{1}{N}\sum_i \vec{C}^{(i)} = \frac{1}{N}\sum_i \tilde{C}^{(i)}$
  - $\mathrm{cov} = (N-1) \times \tilde{\mathrm{cov}}, \tilde{\mathrm{cov}}$: covaiance matrix of Jack-knife samples
  - $\sigma = \sqrt{N-1} \times \tilde{\sigma}$

- Jacknife samples are highly correlated
  - Mean of almost identical data
  - $\left(\tilde{C}^{(i)} - \bar{C}\right)^2 = \left(\frac{N}{N-1}\bar{C} - \frac{1}{N-1}\vec{C}^{(i)} - \bar{C}\right)^2 = \frac{1}{(N-1)^2}\left(\vec{C}^{(i)} - \bar{C}\right)^2$

Coding tips

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- Vectroize your code instead of using loop

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```python
#!/usr/bin/env python3
# encoding: utf-8

import numpy as np
from os import listdir
from iog_reader import iog_read
from re import match
import cProfile
from functools import reduce

iog_path = "./Data/"
T = 72

files = listdir(iog_path)
iogs = [file for file in files if match(r".*2pt.*.dat.iog",file)!=None]
Ncnfg = len(iogs)

c2pt = np.zeros((Ncnfg,T))
for indx in range(0,Ncnfg):
    dat=iog_read(iog_path+iogs[indx],["cnfg","hdrn","t"])
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c2pt_jcknf_1 = np.zeros((Ncnfg,T))
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```
         115780 function calls in 0.082 seconds
   Ordered by: standard name
   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
     4824    0.003    0.000    0.039    0.000 <__array_function__ internals>:177(delete)
     4824    0.002    0.000    0.036    0.000 <__array_function__ internals>:177(mean)
     ......
 ------
         1612 function calls in 0.001 seconds
   Ordered by: standard name
   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
       67    0.000    0.000    0.001    0.000 <__array_function__ internals>:177(delete)
       67    0.000    0.000    0.001    0.000 <__array_function__ internals>:177(mean)
    ......
------
         13 function calls in 0.000 seconds
   Ordered by: standard name
   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
        1    0.000    0.000    0.000    0.000 <__array_function__ internals>:177(sum)
        1    0.000    0.000    0.000    0.000 <string>:1(<module>)
    ......
------
   [ True  True  True  True  True  True  True  True  True  True  True  True ......
```

```
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- Repeat resampling M times, $M > N$, usually $M \sim \mathcal{O}(10^3)$
  - resampled dataset ⇨ $\left(\tilde{C}^{(1)}, \cdots, \tilde{C}^{(M)}\right)$

- Estimator
  - $\bar{C} = \frac{1}{N} \sum_i \vec{C}^{(i)} = \frac{1}{N} \sum_i \tilde{C}^{(i)}$
  - $\mathrm{cov} = \tilde{\mathrm{cov}}, \tilde{\mathrm{cov}}$: covaiance matrix of bootstrap samples
  - $\sigma = \tilde{\sigma}$

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- Parallel your code to do $F(\tilde{C}^{(i)})$
  - e.g. MPI: each process calculate one $F(\tilde{C}^{(i)})$

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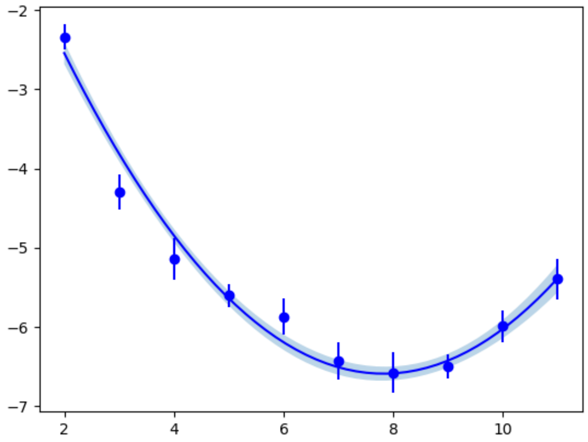
- Model: $f(t, \{p_i\})$
  - t: time slices (w.r.t source)
  - $\{p_i\}$: fit parameters ⇨ $c_0, c_1, E_0, \Delta E$
  - e.g. For two-point function (two-state fit)

$$f(t, \{p_i\}) \implies c_0 e^{-E_0 t}(1 + c_1 e^{-\Delta E t})$$

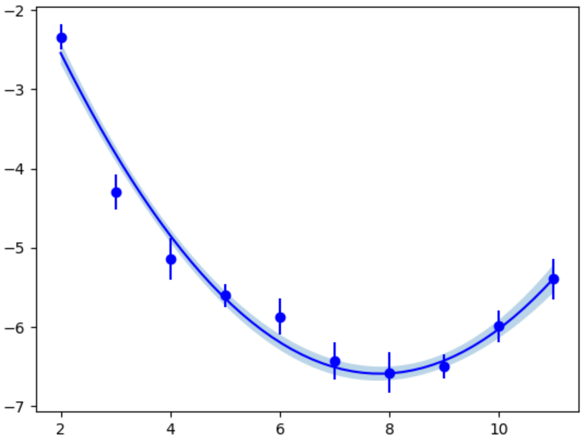
χ^2 definition



χ^2 definition

- Uncorrelated case

$$\chi^2 = \sum_t \frac{\left[\bar{C}_t - f(t, \{p_i\})\right]^2}{\sigma_t^2}$$



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> - σ_t ⇨ standard deviation of the t-th timeslices

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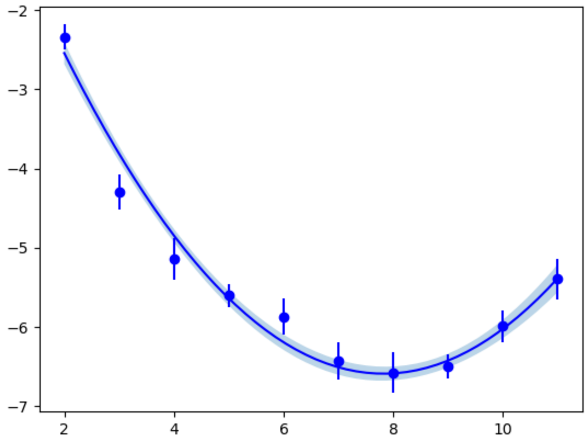

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- Correlated case

$$\chi^2 = \sum_{t,t'} \left[\bar{C}_t - f(t, \{p_i\})\right] \left(\mathrm{cov}^{-1}\right)_{t,t'} \left[\bar{C}_{t'} - f(t', \{p_i\})\right]$$

  - cov : covariance matrix

$$(\mathrm{cov})_{t,t'} = \frac{1}{N-1} \sum_i (C_t^{(i)} - \bar{C}_t)(C_{t'}^{(i)} - \bar{C}_{t'})$$

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- `numpy`: `numpy.mean`, `numpy.std`, `numpy.cov` support high rank tensors
  - Set `axis` parameter in numpy function
  - e.g. $\mathrm{R} = R_{i,j,k,l}, i = 1, \ldots, n_0, j = 1, \ldots, n_1, k = 1, \ldots, n_2, l = 1, \ldots, n_3$
    - Assuming `R, R'` are `numpy` arrays
    - `S=np.mean(R,axis=1)` ⇦⇨ $\mathrm{S}_{i,k,l} = \frac{1}{n_1} \sum_j R_{i,j,k,l}$
    - `R*R'` ⇨ $(\mathrm{R} * \mathrm{R}')_{i,j,k,l} = \mathrm{R}_{i,j,k,l} \times \mathrm{R}'_{i,j,k,l}$

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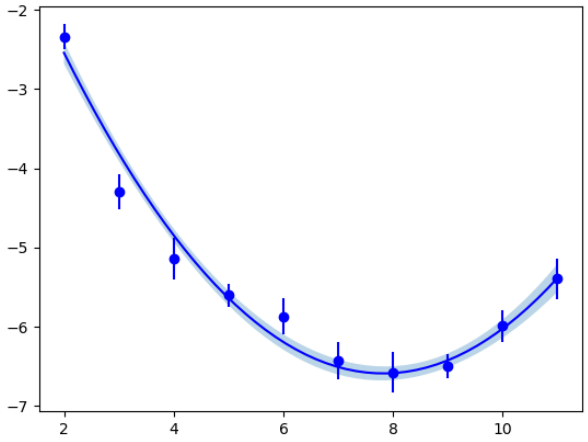
- Not sure about which axis? Print out the shape of R, S: `` `R.shape` ``, `` `S.shape` ``

- $\chi^2 \Rightarrow$ measure the deviation between data and model



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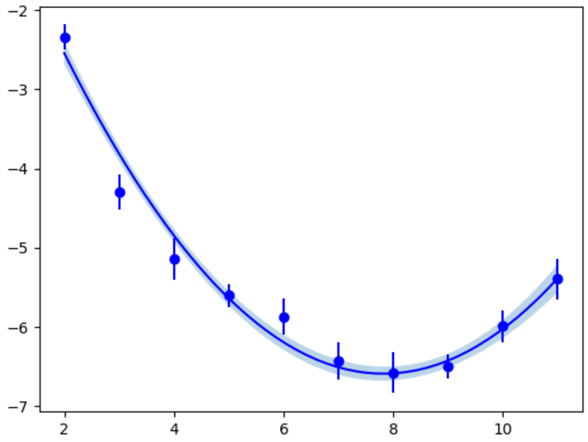

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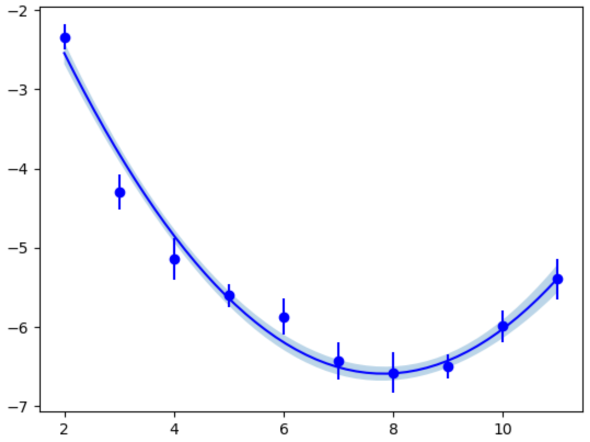
- `lsqfit` ⇨ a python package perform ***l**east* χ-***sq**uare **fit***

```
fit = lsqfit.nonlinear_fit(data=(var_val, dat_val),
                           fcn=model, prior=ini_val, debug=False)
```

  - `var_val` : value of variables ⇨ x-axis
  - `dat_val` : value of datas (with erros) ⇨ y-axis (with err/co
  - `model` : fit model function
  - `ini_val` : initial values of (also constrains on) fit parameters in `model`



`lsqfit` - an example

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import gvar as gv
import lsqfit
import numpy as np
import matplotlib.pyplot as plt

c2pt_raw = np.load("./data_2pt.npy")
c2pt = c2pt_raw[:, 0, :, -2]
Ncnfg = c2pt.shape[0]
T = c2pt.shape[1]
T_hlf = T//2

#? jack-knife resample
#! only used in plot , compare original data with fit
c2pt_sum = np.sum(c2pt,axis=0)
c2pt_jcknf = ((c2pt_sum) - c2pt)/(Ncnfg-1) # jack-knife resample
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T = c2pt.shape[1]
T_hlf = T//2

#? jack-knife resample
#! only used in plot , compare original data with fit
c2pt_sum = np.sum(c2pt,axis=0)
c2pt_jcknf = ((c2pt_sum) - c2pt)/(Ncnfg-1) # jack-knife resample
c2pt_cntrl = np.mean(c2pt_jcknf,axis=0) # jack-knife mean
c2pt_err = np.sqrt(Ncnfg-1)*np.std(c2pt_jcknf,axis=0) # jack-knife std

#? drop the first data point, normalized to c2[1] ~ 1
t_ary = np.array(range(1,T))
c2pt_jcknf = c2pt_jcknf/c2pt_cntrl[1]
```

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value

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key

- dictionary `{index_1: value_1, index_2: value_2, ... }`

value

- Example

```python
dct = {"a":1.0, "b":2.0}
dct["a"]
```

- Why wrap data in dictionaries?
  - Consider the case of
    - fit 2 datasets with 2 models
    - 2 models may have shared parameters

Combined fit

- Combined fit: e.g. 2 data sets, 2 models (with shared parameters)

label	label1	label2
data	$(\vec{x}^{(1)}, \vec{y}^{(1)})$	$(\vec{x}^{(2)}, \vec{y}^{(2)})$
model	$f(x, \{\vec{p}, \vec{q}\})$	$g(x, \{\vec{p}, \vec{r}\})$
ini_val	$\vec{p}_0, \vec{q}_0$	$\vec{p}_0, \vec{r}_0$

- $\vec{p}$ denotes the shared parameters

- Wraping data for combined fit

```
var_val = {'label1': [x1_1,x1_2,...], 'label2': [x2_1,x2_2,...

dat_val = {'label1': [y1_1,y1_2,...], 'label2': [y2_1,y2_2,...

prior = {'p_1': p_1,'p_2': p_2, ..., 'q_1': q_1, 'q_2': q_2, ... ,'r_1': r_1, 'r_2': r_2}
```

  - `y_1,2`: gvar class ⇨ `y_1 = gvar(y_1_cntrl, y_1_cov)` ...
  - `p_1,2`: gvar class ⇨ `p_1 = gvar(p_1_cntrl, p_1_err)` ...
  - Feed the `var_val`, `dat_val` and `prior` to `lsqfit.nonlinear_fit`

Wrapping model for combined fit

```
def fit_mdls(t_dctnry, p):
  mdls = {}
  mdls['label1'] = ...
  mdls['label2'] = ...
  return mdls
```

Multiple/Single source, Open/Periodic boundary condition

Multiple/Single source, Open/Periodic boundary condition

- Put multiple source in time direction to increase the statistics

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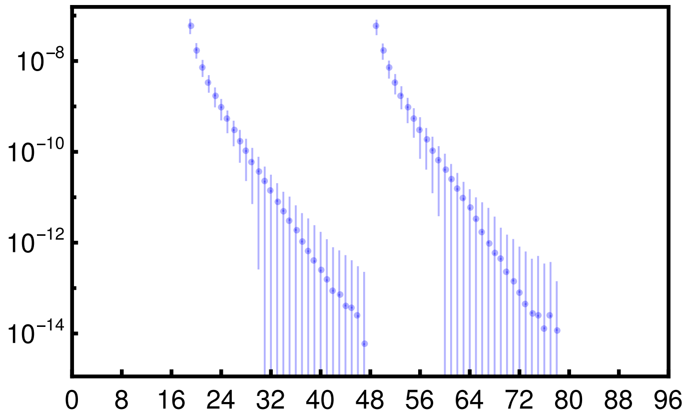

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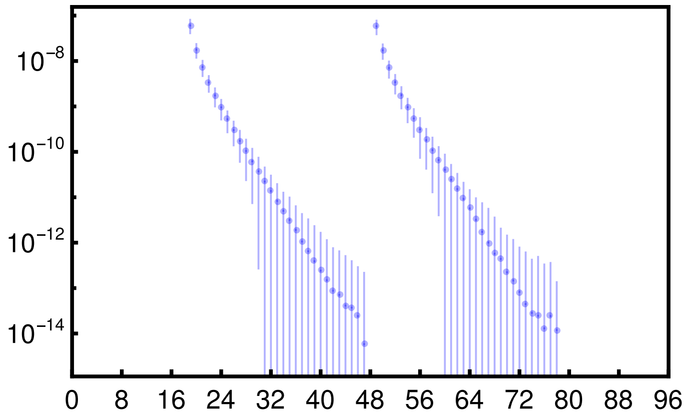

- Single source, periodic boundary condition
- Example
  - $C_(T+a) = C(0)$
  - $C(t) \approx C_0 e^{-E_0 \frac{T}{2}} \cosh\left[E_0\left(\frac{T}{2} - t\right)\right]$

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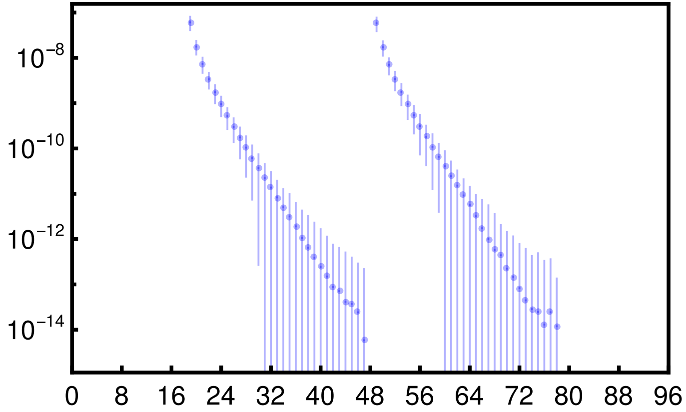

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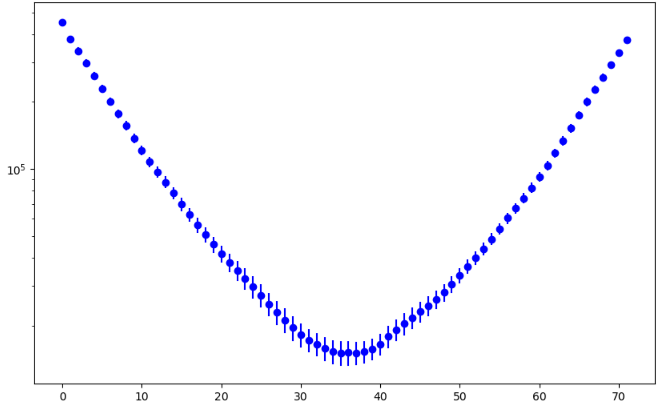

Fit Results - A glance

```
Least Square Fit:
 chi2/dof [dof] = 0.96 [20]    Q = 0.5    logGBF = 116.43

Parameters:
            c0     0.252 (10)     [  0.0 (5.0) ]
            E0    0.1090 (27)     [  0.20 (50) ]
```

- Fences: two-point function data
- Bands: fitted model

> Error has been magnified with factor of 5 in figure

- Fited effective mass: $E_0 =$
  - The fitted E_0 is in lattice unit.
  - $E_0 t$ in $e^{-E_0 t}$ must be dimensionless ⇨ $E_0 = \dfrac{E_{0,\text{latt.}} \times 0.1973}{a}$ [GeV]

Output log

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Parameters:
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Fit:
       key          y[key]       f(p)[key]
----------------------------------------
    c2pt 0       0.277 (12)     0.2712 (79)
         1       0.248 (11)     0.2435 (74)
         2       0.223 (11)     0.2186 (69)
         3       0.199 (10)     0.1964 (66)
         4      0.1790 (94)     0.1765 (62)
         5      0.1610 (87)     0.1586 (59)
         6      0.1446 (79)     0.1427 (56)
         7      0.1304 (75)     0.1284 (54)
         8      0.1180 (71)     0.1157 (51)
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        10      0.0981 (68)     0.0943 (47)
        11      0.0900 (69)     0.0853 (44)
        12      0.0825 (68)     0.0773 (42)
        13      0.0758 (66)     0.0703 (41)
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Print this detailed log by setting `print(fit.format(True))`

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```

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Access the fitted model function

```
fit = lsqfit.nonlinear_fit(data=(tsep_dctnry, c2pt_dctnry),
fcn=ft_mdls, prior=ini_prr, debug=True)

c2pt_fit_gvar = fit.fcn({'c2pt':t_lst}, fit.p)['c2pt']
```

- `` `tsep_dctnry = {'c2pt':np.array(range(T_strt,T_end))}` ``
- `` `fit.p` `` ⇨ fitting parameter, dictionry
  - `` `fit.p['E0']` ``

What is a resonable fit?

Case 1

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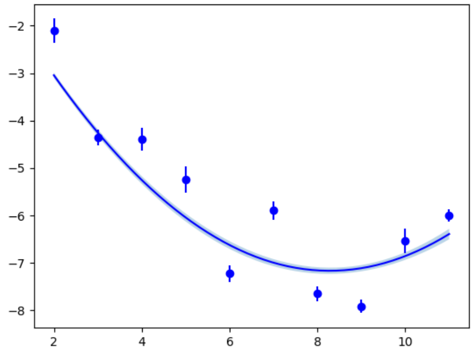

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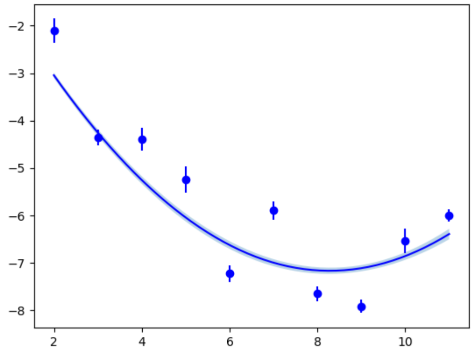


```
Least Square Fit:
  chi2/dof [dof] = 13 [10]
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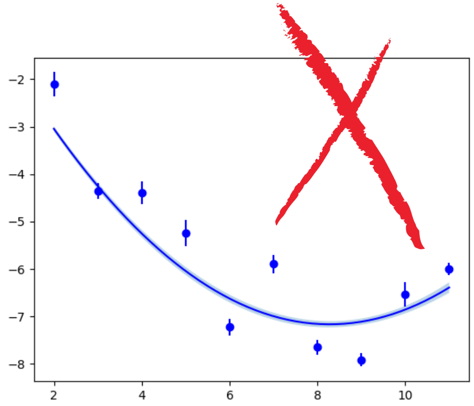


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- Underfit
  - Model failed to discribe data

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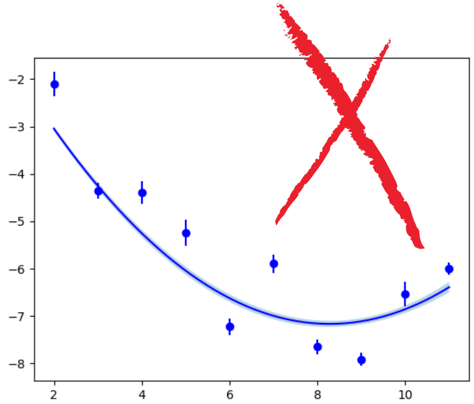


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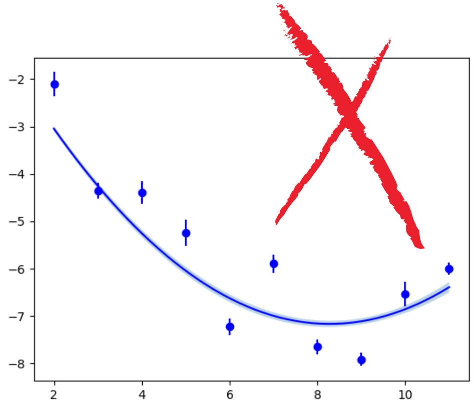


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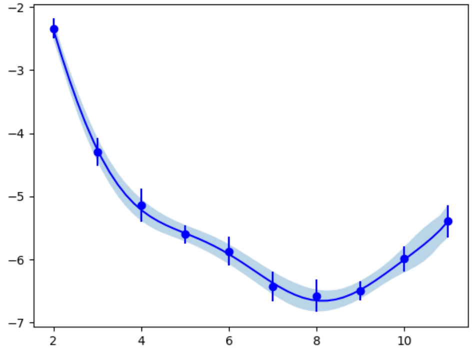

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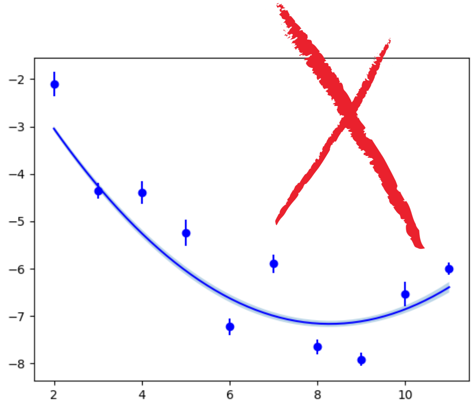

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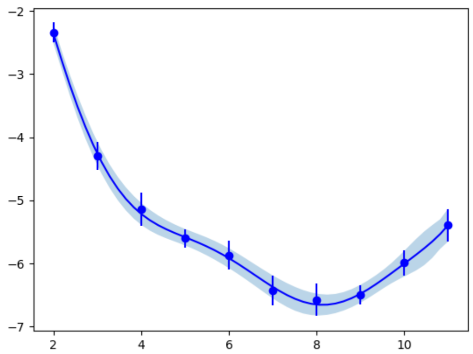

```
Least Square Fit:
  chi2/dof [dof] = 0.07 [10]
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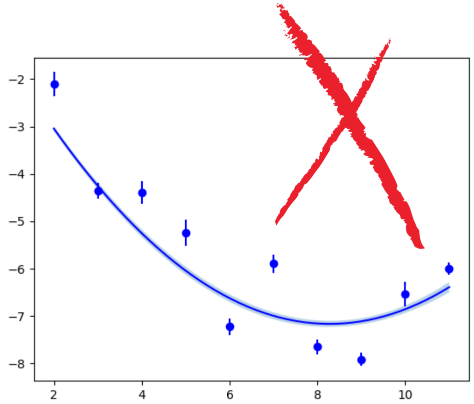


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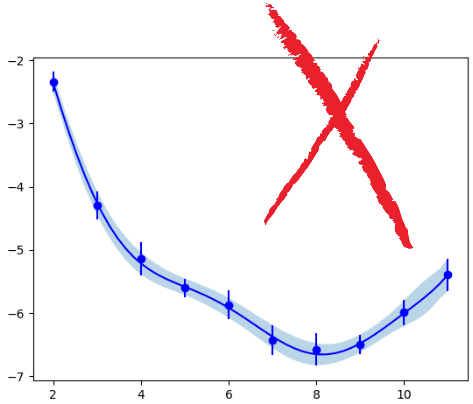


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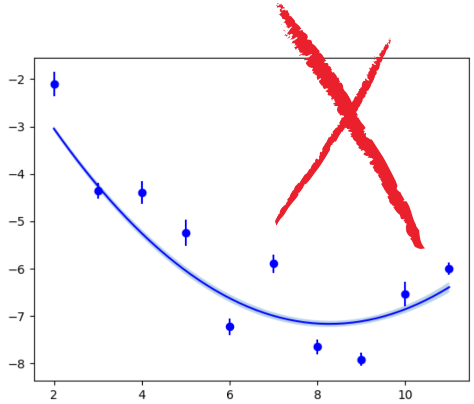


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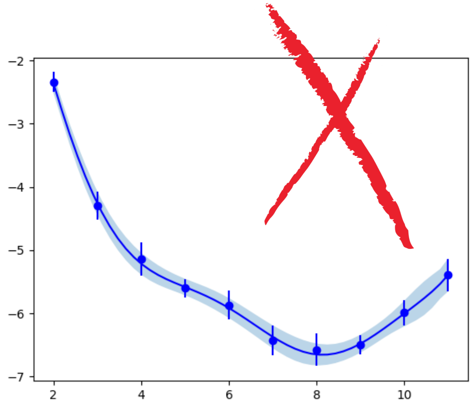


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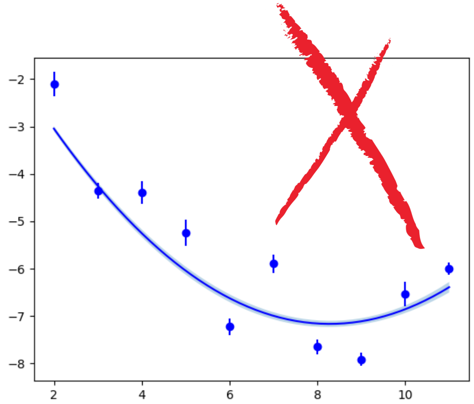


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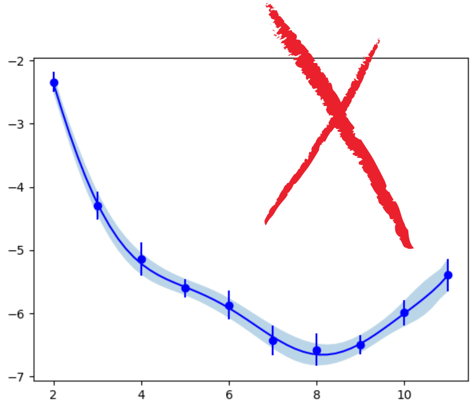


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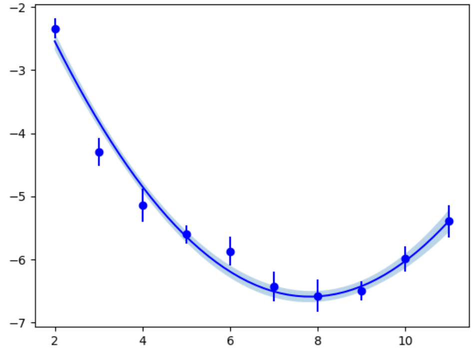

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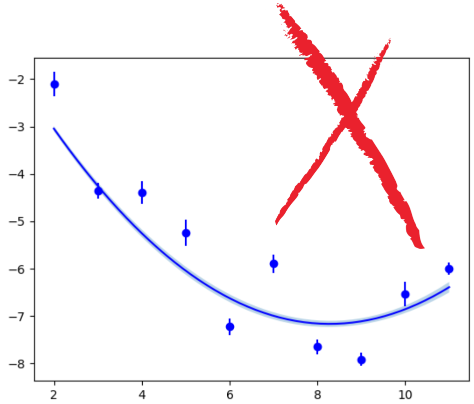


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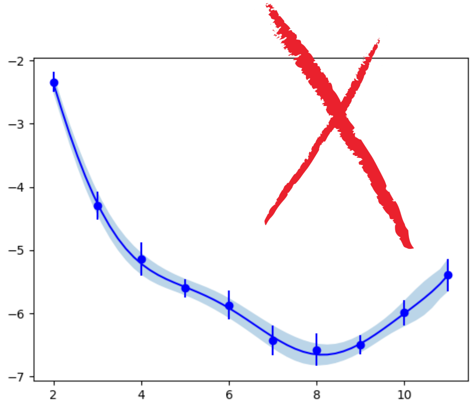


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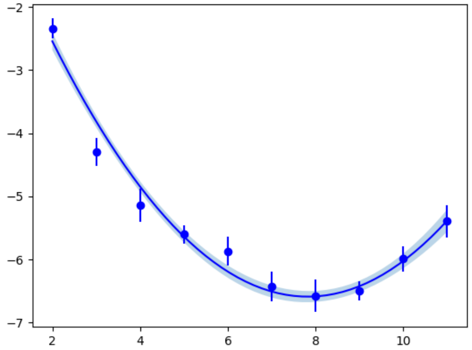


```
Least Square Fit:
  chi2/dof [dof] = 1 [10]
  Q = 0.41
  logGBF = -15.05
```

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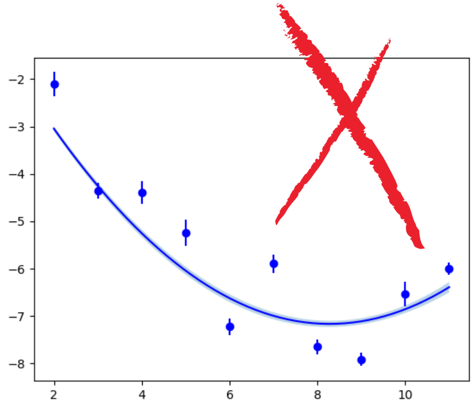


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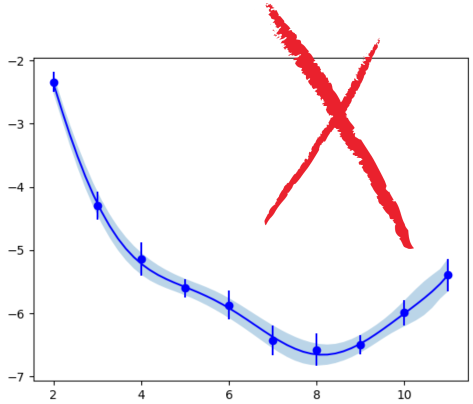


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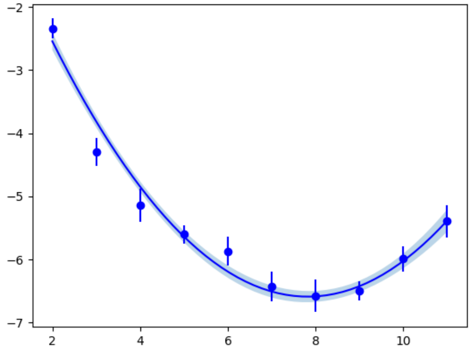
Case 3

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Least Square Fit:
  chi2/dof [dof] = 1 [10]
  Q = 0.41
  logGBF = -15.05
```

- ***Resonable fit***

How good is a fit?

Interpretation of `lsqfit` log

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- `logGBF`: $\ln P(\text{data}|\text{fit})$ ⇨ Probability of obtaining the data by randomly sampling the fitted model
  - Useful for comparing fits of the same data to different models, with different priors and/or fit functions.
  - The model with the largest value of `logGBF` is the one preferred by the data.
  - Differences in fit.logGBF smaller than 1 are not very significant.

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Exercises

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1. **Read the pion two-point function data**

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- Create a directory named by your name under the `home` directory
- copy `/dssg/home/acct-phyww/phyww/qazhang/training_camp_2023/class1_xiong/Ex1_Latt6th.tar.gz/` to the created directory and unzip it

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> For this exercise: lattice spacing: 0.108 fm, $m_\pi \approx 200\mathrm{MeV}$

Hint:

Hint:

- `iog_reader`, `pandas.DataFrame.loc`, `pandas.DataFrame.to_numpy`, `numpy.mean`, `numpy.cov`, `numpy.std`, `lsqfit.nonlinear_fit`
- `Data` containing the 50 two-point function iog data files, from 50 configuration
- 72 lattice spacings in time direction
- `iog_reader` is provided in `iog_read_demo.py`
- `x=gv.gvar('2(0.5)')` : `x.mean` ⇨ `2.00`, `x.sdev` ⇨ `0.50`
- Construct gvar from tuple `x=gv.gvar((2.0.5))`

Notes

- `` `Python` `` indices starts from 0, *Mathmatica*, Julia starts from 1
- `` `numpy.ndarray` `` slice, range doe not include the last index e.g.
  - `` `a[2:5]` `` ⇨ [a_2,a_3,a_4]
  - `` `range(2,5)` `` ⇨ [2,3,4]
- `` `iog_read.py` `` returns `` `pandas.Dataframe` ``, columns in this data frame are strings (not integers)

III. Linux Basics

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  - try WSL

    > https://docs.microsoft.com/zh-cn/windows/wsl/install

  - Powershell

Search for help and tips

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- Online forum
    - https://unix.stackexchange.com/
    - https://stackoverflow.com/
    - Search online ...

Path

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- Autocomplete/suggestions
    - Press `Tab`

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- Similar for copy `cp` and move(rename) `mv`

cat, grep, >

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- compress `tar`
  - try `tar --help`

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    - e.g. `` `ssh stu1947@sylogin.hpc.sjtu.edu.cn` ``
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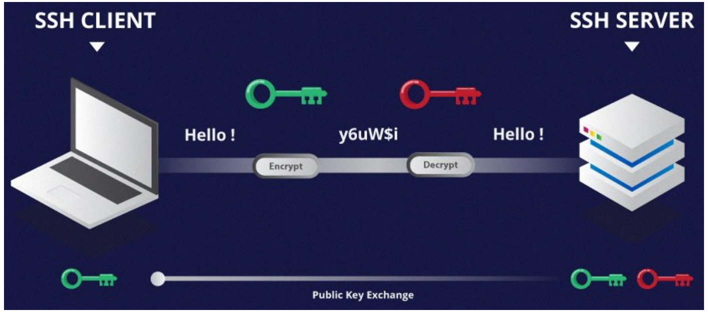
  - `usr`: username, `host`: remote machine
- Use `key` instead of password
  - `ssh-keygen`: generate RSA key (public and private)
  - distribute pubkey `id_rsa.pub` to others
  - keep your private key `id_rsa` private
  - `ssh-copyid usr@host`: install your pubkey to host



SSH login

- SSH config file
  - `~/.ssh/config`

```
Host sjtu
 HostName sylogin.hpc.sjtu.edu.cn
 User stu1947
 IdentityFile /home/chimaoshu/.ssh/id_rsa
 AddKeysToAgent yes
```

- After setting ssh config file ⇨ `ssh sjtu`

SSH via Windows powershell (But recommend using vscode)

- `` `powershell` `` has built-in `` `ssh.exe` ``, `` `ssh-keygen.exe` ``, `` `scp.exe` ``

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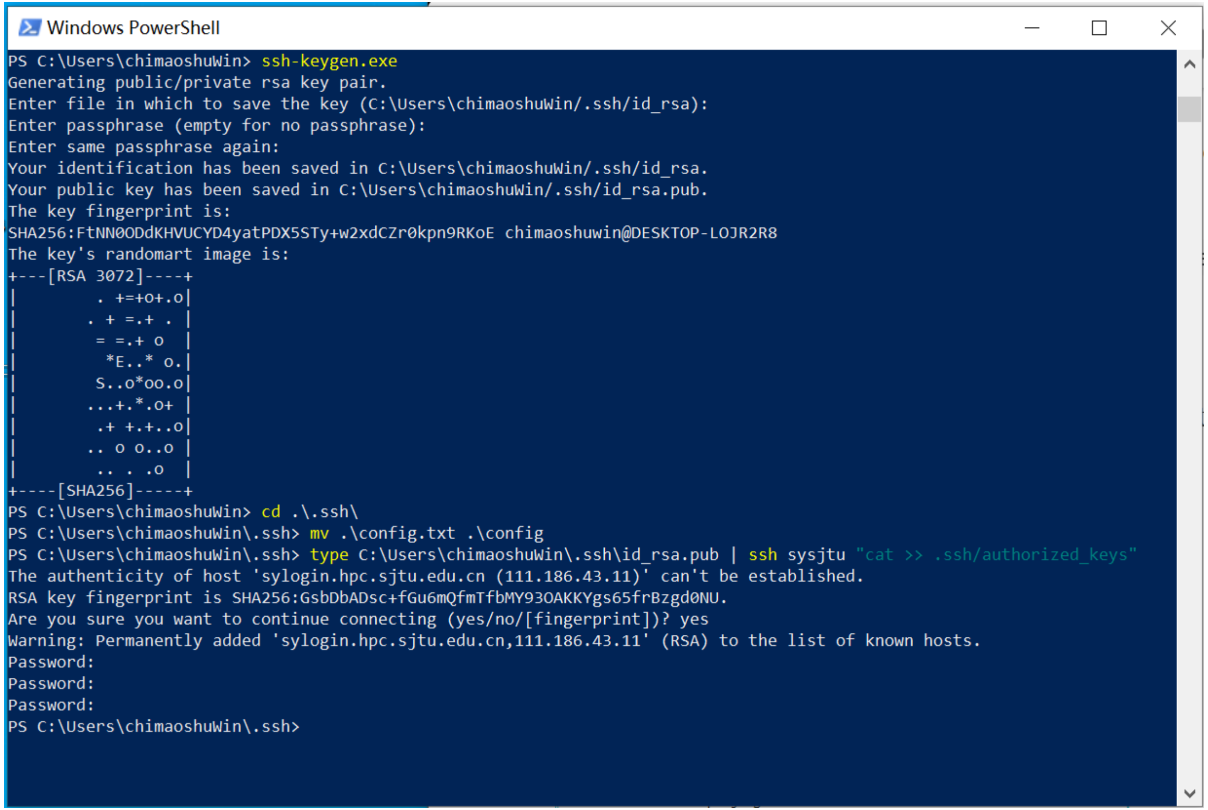

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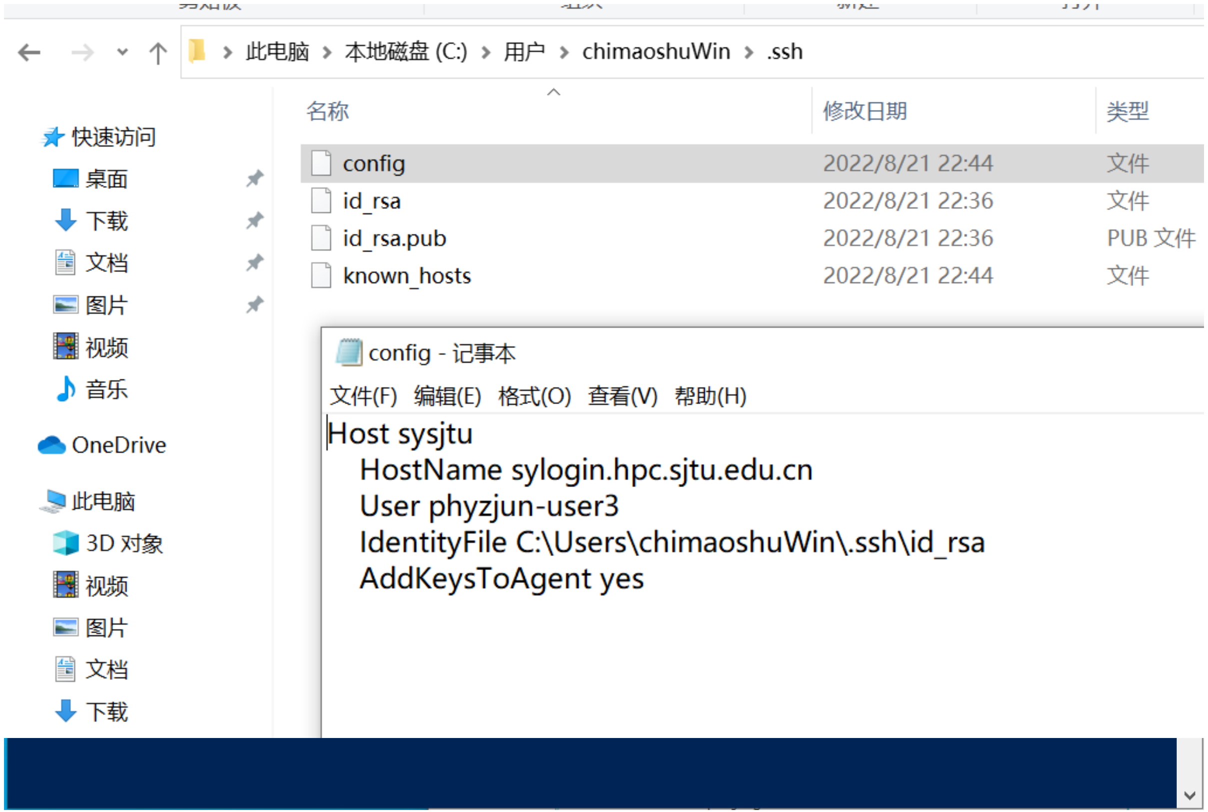

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OpenSSH SSH client

```
PS C:\Users\chimaoshuWin> ssh sysjtu
Password:
Last login: Sun Aug 21 23:12:52 2022 from 42.48.113.177
slurm常用指令：
    sinfo 查看队列状态和信息
    sacct 显示用户作业历史
    squeue 显示当前作业状态
    sbatch 提交作业
    scancel 取消指定作业

集群设置以下队列，使用限制与说明如下：
            允许单作业CPU核数为1~60000，每核配比8G内存；单节点配置为64核，512G内存
         允许单作业GPU卡数为1~92，每卡配比CPU上限为16，每核配比8G内存；单节点配置为64核，512G内存，4块40G显存的A100 GPU
卡
                 仅用于短时间测试，请勿批量投递作业进行完整计算。作业最多申请2节点，运行60分钟，每核配比8G内存；单节点配
置为64核，512G内存
              仅用于短时间测试，请勿批量投递作业进行完整计算。作业最多申请1节点，运行20分钟；单节点配置64核，512G内存，2
8块5G显存的虚拟GPU卡

用户帮助文档：https://docs.hpc.sjtu.edu.cn/

登陆节点禁止运行作业和并行编译，如需交互操作，请申请计算资源： $ srun -p 64c512g -n 4 --pty /bin/bash

登录节点不适合进行大批量数据传输，请通过传输节点data.hpc.sjtu.edu.cn进行数据拷贝，参考 https://docs.hpc.sjtu.edu.cn/tran
sport

邮件支持：hpc@sjtu.edu.cn
acct-phyzjun账户存储使用量为：2.5T
phyzjun-user3用户存储使用量为：2.0G

[phyzjun-user3@sylogin1 ~]$
```

SSH via Windows powershell (But recommend using vscode)

- `powershell` has built-in `ssh.exe`, `ssh-keygen.exe`, `scp.exe`

- `ssh-copy-id` equivlent: type path_to_id_rsa.pub | ssh sjtu "cat >> ~/.ssh/authorized_keys"

Copy between local and remote machines

- `scp source target`, (`scp` = `s`(ssh) + `cp`) e.g.
  - `scp ./demo/lsqfit_2pt.py sysjtu:~/demo`
  - `scp -r sjtu:~/demo /home/chimaoshu`

> `sjtu` could be replaced by `usr@host` if `.ssh/config` is not set

Modify files on remote machine

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- Recommanded: vscode + remote development extension

> https://code.visualstudio.com/docs/remote/ssh-tutorial

> better set `.ssh/config`

vscode

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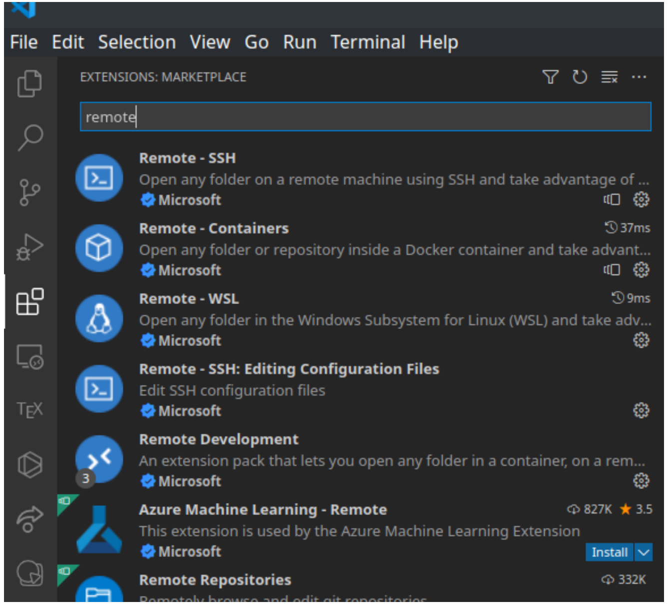

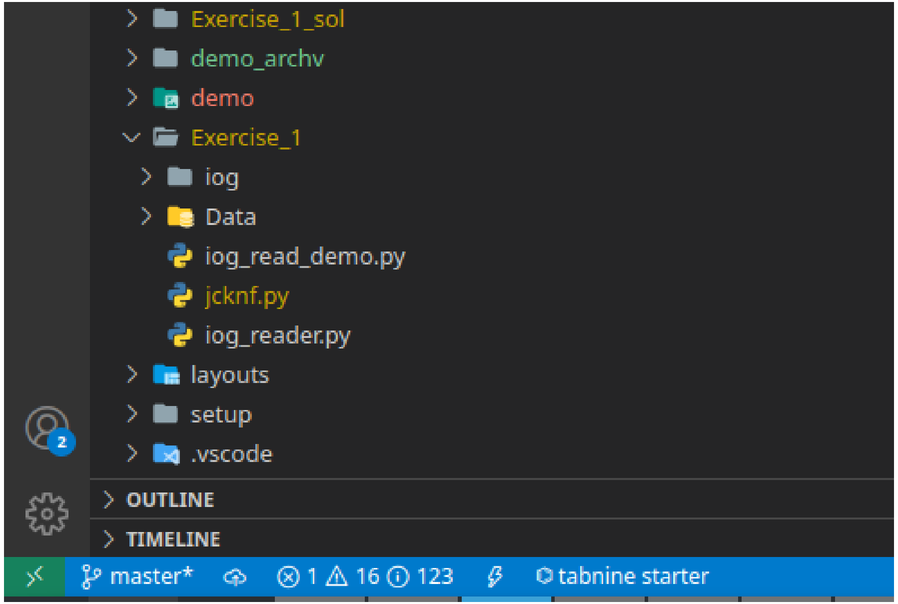

vscode

- https://code.visualstudio.com/Download
- Extensions
  - Python by Microsoft
  - Pylint by Microsoft
  - C/C++ by Microsoft
  - Kite
  - …

Enviormental Modules

- \``module avail`\`: list avaliable modules
- \``module load mod`\`: load mod
- \``module list`\`: list currenly loaded modules
- \``module purge`\`: unload all modules
- …

Setup Python Enviroment

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- Use `export` to set the relavent enviroment variables (`PATH` and `PYTHONPATH`)
  - `export PATH=$PATH:/dssg/home/acct-phyww/phyww/qazhang/packages/anaconda3/bin`
  - `export PYTHONPATH=/dssg/home/acct-phyww/phyww/.local/lib/python3.7/site-packages`
  - Use `python`, do not use `python3`, `python3.x`

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- Or excute them everytime after login/reconnect...

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- Basic usage:
  - `` `h5glance h5_file [path]` ``
  - `` `path` ``: unix like path to data (string)
- Advanced usage:
  - show attributes : `` `h5glance --attrs h5_file [path]` ``
  - peek data: `` `h5glance --attrs h5_file path` ``
  - slice data: `` `h5glance -s slice --attrs h5_file path` ``
    - `` `slice` ``: `` `numpy` `` like slice, e.g: `` `2,10:15` ``

IV. Introduction to HDF5

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- HDF5: Hierarchical Data Format Version 5

> **High-performance data management and storage suite** Utilize the HDF5 high performance data software library and file format to manage, process, and store your heterogeneous data. HDF5 is built for fast I/O processing and storage.

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- HDF5: Hierarchical Data Format Version 5

> **High-performance data management and storage suite** Utilize the HDF5 high performance data software library and file format to manage, process, and store your heterogeneous data. HDF5 is built for fast I/O processing and storage.

  - Sell sheet : https://www.hdfgroup.org/wp-content/uploads/2017/12/HDF512-17.pdf

- Open source library

- Supported by C/C++, Julia, Mathmetaica, Python ...

  - HDF5 does not provide native complex type, different software may have different interpretation of complex type

    - e.g. Interpreted as association (dictironary) in mathmatica

```
 In[1]:= c = 1 + 0.2*I;
 In[2]:= Export["cmplx.h5", "/cmplx" -> c];
 In[3]:= Import["cmplx.h5", {"Datasets", "/cmplx"}]
Out[4] = <|"Re" -> 1., "Im" -> 0.2|>
```

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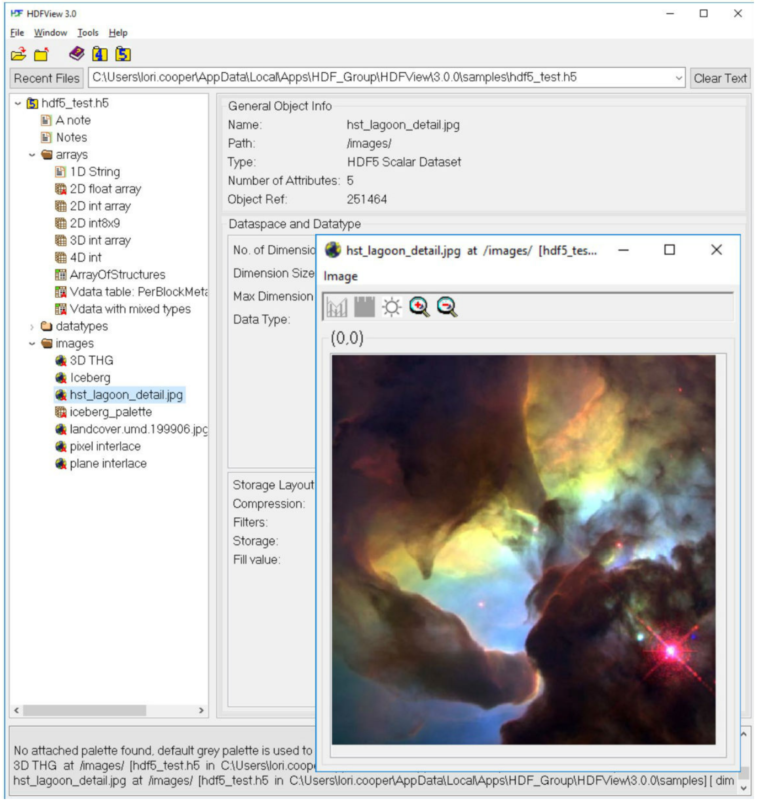

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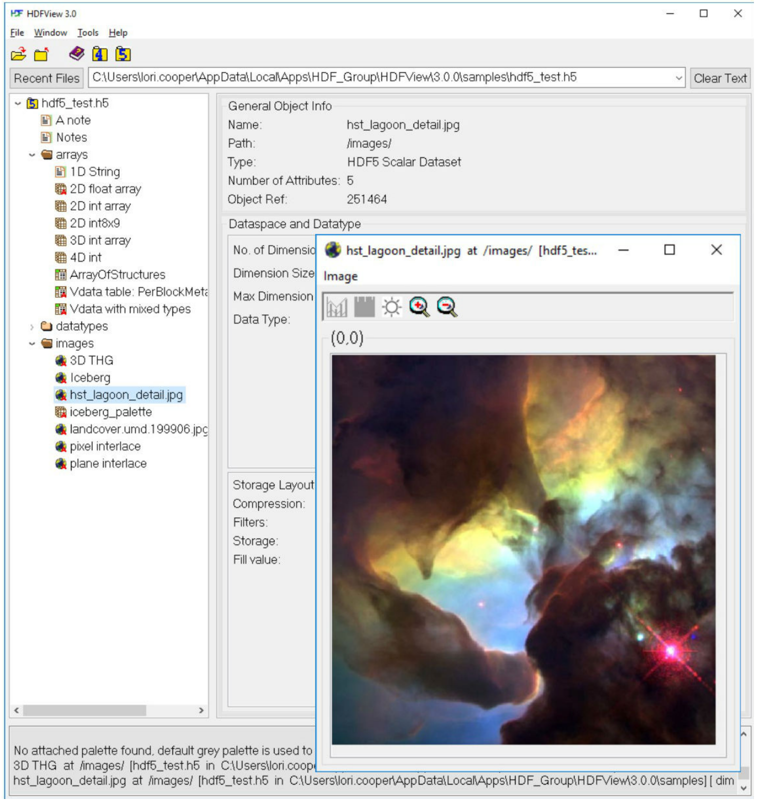

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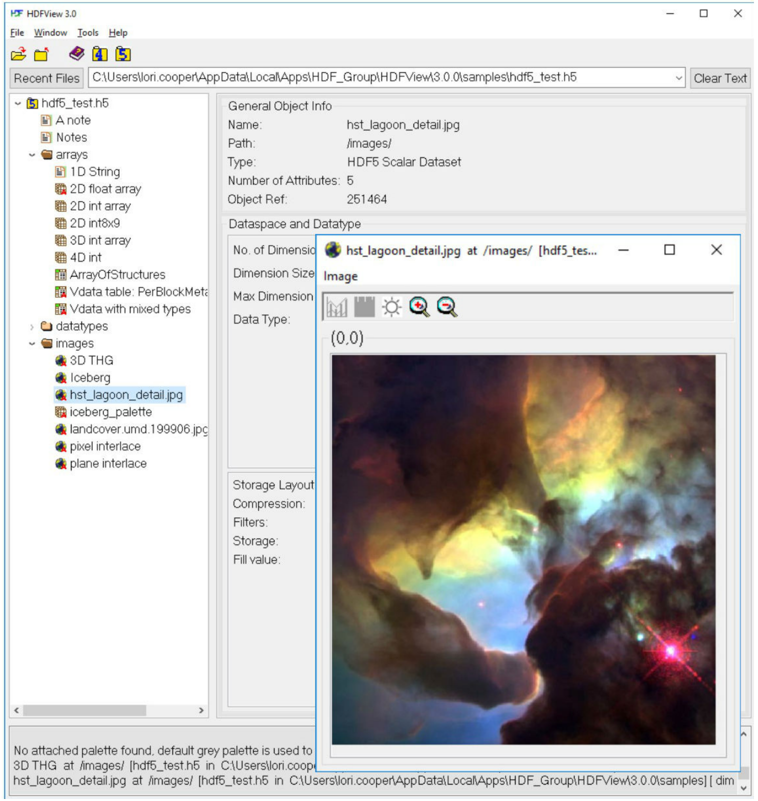

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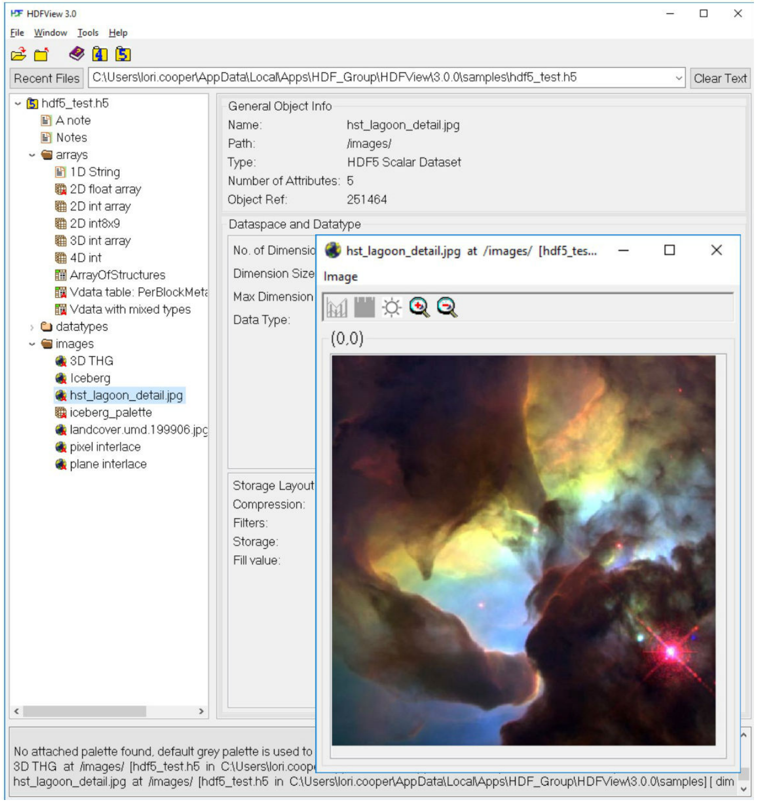

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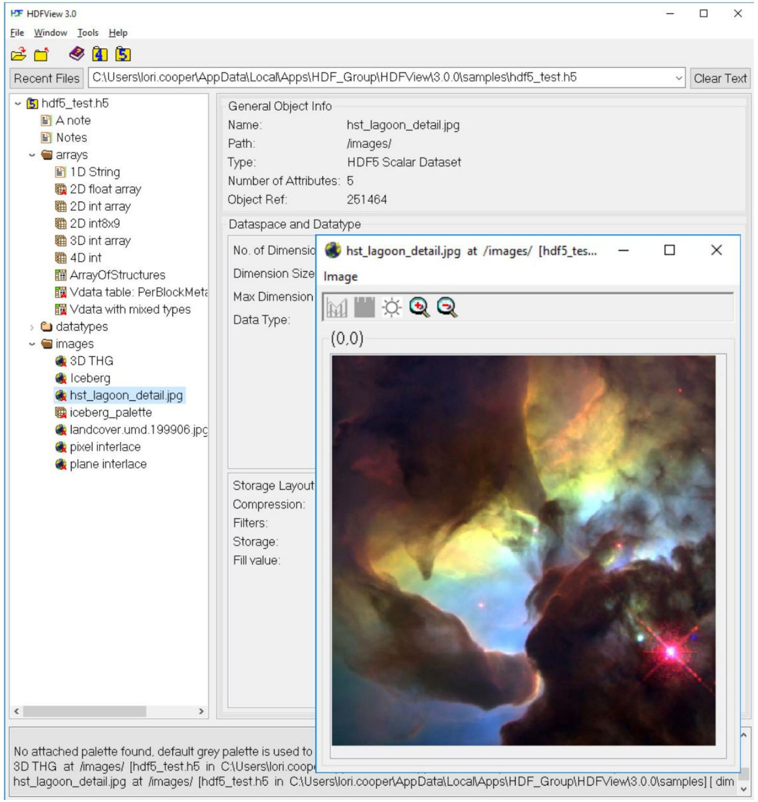

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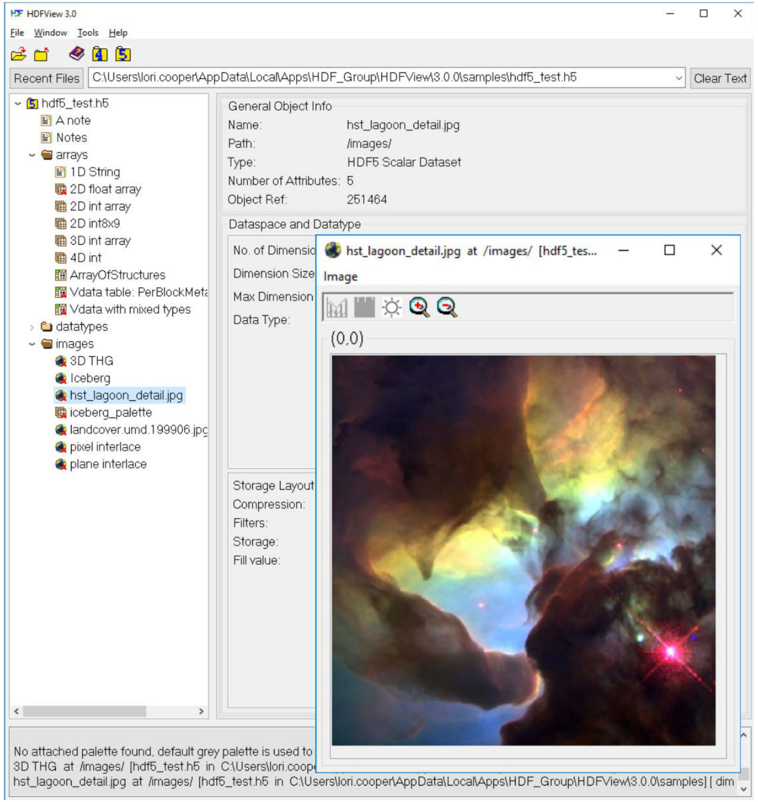

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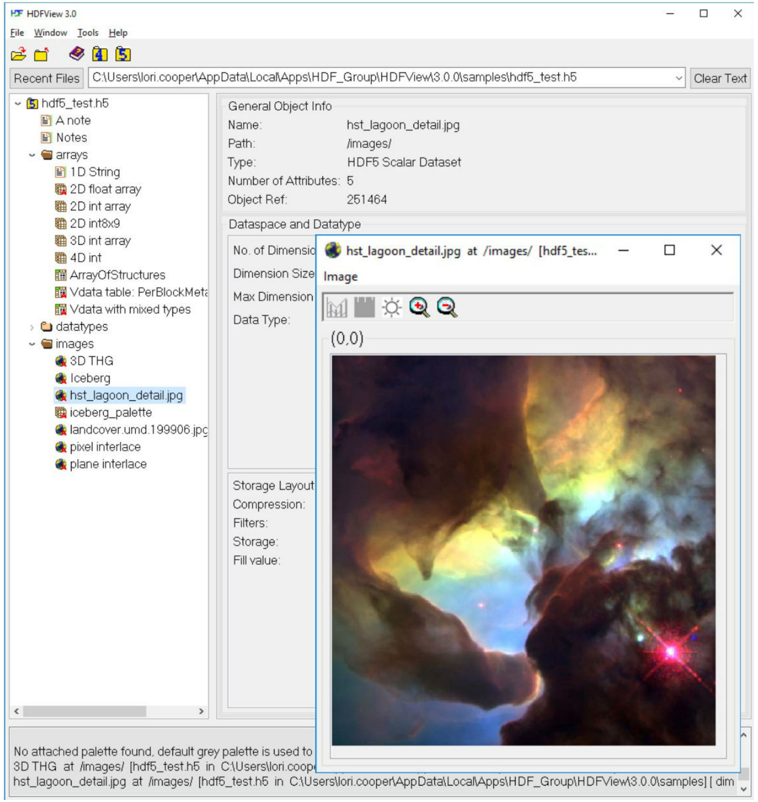

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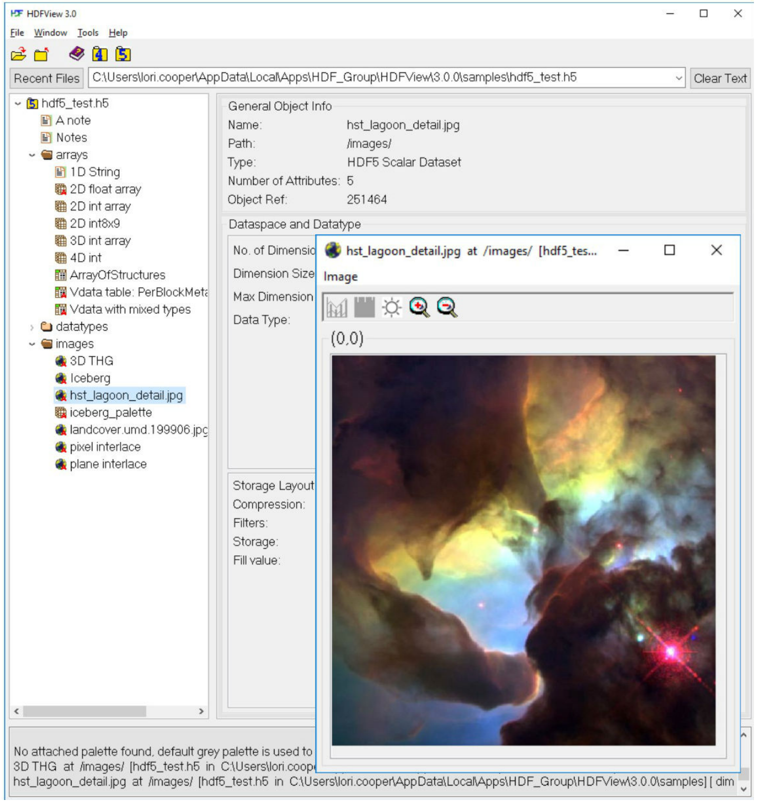
- > *Python and HDF5*, Andrew Collette, ISBN: 9781449367831 (2013)



iog to h5

- Based on `` `iog.so` ``, `` `iog_reader.py` ``, requiring `` `h5py` `` python package
  - iog2h5_2pt.py: convert 2pt iog files to h5
  - iog2h5_3pt.py: convert 3pt iog files to h5

> provided on demand