TDLAS

December 31, 2023

1 Python translation to the TDLAS MATLAB code with annotation and validation

The script version of code contains individual py files, for function definitions, input definitions and main code. Here, they are combined in systematic order along with anootations on the equations and methods being used in the code

The variable and function names used in this script are the same as the ones used in MATLAB, the variable names may not be appropriate at some locations.

1.1 Input parameters definition

This section contains the definitions of parameters that are used in the computation

[1]:
```
# HITRAN database filename
HITRAN_filename       = "01_7000-7500_HITEMP2010_7443.2-7445.5.par"

# partition filename
PART_filename         = "q1.txt"

# minimum and maximum wave numbers in cm^-1
nu_1_min              = 7443.2
nu_1_max              = 7445.5

# number of terms between min ans max wave numbers to be considered
N_nu_range            = 3000

# total radial distance in cm and radial step size
total_radial_distance = 3.0
delta_x               = 0.01

# parameters for temperature and mole fraction fields construction-------------
# maximum flame temperature and ambient temperature
T_mag_uni_field       = A1 = 950.0
A2                    = 300.0

# location where flame temperature reaches half the maximum temperature
X0                    = 6.0*total_radial_distance/7.0
```

```
# gradient of the transition region
A3                    = 0.06

# maximum and ambient mole fraction of water vapour
x_mag_uni_field       = B1 = 0.095
B2                    = 0.028
```

Following are the constants used in the work

[2]:
```
# reference temperature
T0 = 296.0

# Plank's constant
h  = 6.62607004e-34

# speed of light in cm/s in vacuum
c  = 29979245800

# Boltzmann constant
k  = 1.38064852e-23

# molar mass of water
M  = 18.01

P  = 1 #  <----------- DOUBT

# Avogadro number
Na = 6.02214076e23
```

1.2 Importing libraries/modules

The needed modules and libraries are imported in this section

[3]:
```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from scipy.special import wofz     # Voigt function
```

1.3 Function definitions

1.3.1 HITRAN database reader function

This function was developed to read the Hi-resolution Tranmission database file for the chosen species of H2O. This will return the pandas dataframe with all the columns

[4]:
```
def HITRAN_reader(fname):

    # reading all file contents
    fid = open(fname,"r")
    lines = fid.readlines()

    # preparing lists to store line values
    molNo_list = []; isoNo_list = []; transitionWaveNo_list = []
    lineIntensity_list = []; einsteinACoeff_list = []; airBroadenedWidth_list =␣
↪[]
    selfBroadenedWidth_list = []; lowEState_list = []; tempCoeff_list = []
    pressureShift_list = []; upperVibQuanta_list = []; lowerVibQuanta_list = []
    upperLocalQuanta_list = []; lowerLocalQuanta_list = []; errorCodes_list = []
    referenceCodes_list = []; flagLineMixing_list = []
    upperStatisticalWeight_list = []; lowerStatisticalWeight_list = []


    # looping through the lines to read individual data
    for line in lines:
        # setting starting read position on the string
        idx = 0

        # reading molecule number
        molNo = int(float(line[idx:idx+2]))
        idx+=2

        # isotopologue number
        isoNo = int(float(line[idx:idx+1]))
        idx+=1

        # transition wavenumber / vaccum wavenumber
        transitionWaveNo = float(line[idx:idx+12])
        idx+=12

        # line intensity
        lineIntensity = float(line[idx:idx+10])
        idx+=10

        # einstein A-coefficient
        einsteinACoeff = float(line[idx:idx+10])
        idx+=10

        # air-broadened half width / air-broadened width
        airBroadenedWidth = float(line[idx:idx+5])
        idx+=5

        # self-broadened half width / self-broadened width
```

```
        selfBroadenedWidth = float(line[idx:idx+5])
        idx+=5

        # lower energy state
        lowEState = float(line[idx:idx+10])
        idx+=10

        # temperature dependence coefficient
        tempCoeff = float(line[idx:idx+4])
        idx+=4

        # pressure shift / air-pressure-induced line shift
        pressureShift = float(line[idx:idx+8])
        idx+=8

        # upper vibrational quanta / upper-state "global" quanta
        upperVibQuanta = line[idx:idx+15]
        idx+=15

        # lower vibrational quanta / lower-state "global" quanta
        lowerVibQuanta = line[idx:idx+15]
        idx+=15

        # upper local quanta / upper-state "local" quanta
        upperLocalQuanta = line[idx:idx+15]
        idx+=15

        # lower local quanta / lower-state "local" quanta
        lowerLocalQuanta = line[idx:idx+15]
        idx+=15

        # error codes / uncertainity indices
        errorCodes = line[idx:idx+6]
        idx+=6

        # reference codes / reference indices
        referenceCodes = line[idx:idx+12]
        idx+=12

        # flag for lineMixing / Flag
        flagLineMixing = line[idx:idx+1]
        idx+=1

        # upper statistical weight / statistical weight for the upper state
        upperStatisticalWeight = float(line[idx:idx+7])
        idx+=7
```

```
        # lower statistical weight / statistical weight for the lower state
        lowerStatisticalWeight = float(line[idx:idx+7])
        idx+=7

        # appending read values to the lists
        molNo_list.append(molNo)
        isoNo_list.append(isoNo)
        transitionWaveNo_list.append(transitionWaveNo)
        lineIntensity_list.append(lineIntensity)
        einsteinACoeff_list.append(einsteinACoeff)
        airBroadenedWidth_list.append(airBroadenedWidth)
        selfBroadenedWidth_list.append(selfBroadenedWidth)
        lowEState_list.append(lowEState)
        tempCoeff_list.append(tempCoeff)
        pressureShift_list.append(pressureShift)
        upperVibQuanta_list.append(upperVibQuanta)
        lowerVibQuanta_list.append(lowerVibQuanta)
        upperLocalQuanta_list.append(upperLocalQuanta)
        lowerLocalQuanta_list.append(lowerLocalQuanta)
        errorCodes_list.append(errorCodes)
        referenceCodes_list.append(referenceCodes)
        flagLineMixing_list.append(flagLineMixing)
        upperStatisticalWeight_list.append(upperStatisticalWeight)
        lowerStatisticalWeight_list.append(lowerStatisticalWeight)

        #  break

    # column names for pandas dataframe
    colNames = ["moleculeNumber","isotopologueNumber","transisionWaveNumber",
                "lineIntensity","einsteinACoefficient","airBroadenedWidth",
                "selfBroadenedWidth","lowerStateEnergy","temperatureDependence",
                ␣
↪"pressureShift","upperVibrationalQuanta","lowerVibrationalQuanta",
                "upperLocalQuanta","lowerLocalQuanta","errorCodes",
                "referenceCodes","flagForLineMixing","upperStatisticalWeight",
                "lowerStatisticalWeight"]

    # preparing dataframe
    fid = pd.DataFrame(np.
↪transpose([molNo_list,isoNo_list,transitionWaveNo_list,
                                        lineIntensity_list,einsteinACoeff_list,
                                        ␣
↪airBroadenedWidth_list,selfBroadenedWidth_list,
                                        ␣
↪lowEState_list,tempCoeff_list,pressureShift_list,
                                        upperVibQuanta_list,lowerVibQuanta_list,
```

```
                                                    ␣
↪upperLocalQuanta_list,lowerLocalQuanta_list,
                                                    ␣
↪errorCodes_list,referenceCodes_list,flagLineMixing_list,
                                                    ␣
↪upperStatisticalWeight_list,lowerStatisticalWeight_list]),
                        columns = colNames)

    # writing dataframe to csv file
    fid.to_csv("HITEMP_data.csv", index = None)

    # returning dataframe
    return fid
```

1.3.2 Partition function interpolator

This function interpolates the partition function values over a range of temperatures and obtains the interpolated value for the given temperature

[5]:
```
def Q_func(T, T_series, Q_series):
    """
    This function obtains the value of partition function for given temperature
    through linear interpolation

    T        - given input temperature
    T_series - series of temperature values from database
    Q_series - series of partition function values corresponding to each
               temperature in the database
    """

    return np.interp(T,T_series,Q_series)
```

1.3.3 Line strength function

This function computes the line strength using the following equation

$$S(T) = S(T_0)\frac{Q(T_0)}{Q(T)}\frac{T_0}{T}exp\left(\frac{-hcE"}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right)\frac{\left[1-exp\left(\frac{-hc\nu_0}{kT}\right)\right]}{\left[1-exp\left(\frac{-hc\nu_0}{kT_0}\right)\right]}$$

[6]:
```
def lineStrength(S0, nu0, Edd, T, fid_Q):
    """
    This function computes the line strength of a particular transition
    at a given temperature

    equation has been split into 4 parts for ease of programming
    """
```

```
    part_1 = Q_func(T0,fid_Q["T"],fid_Q["Q"])/Q_func(T,fid_Q["T"],fid_Q["Q"])
    part_2 = T0/T*np.exp(-h*c/k*Edd*(1/T - 1/T0))
    part_3 = 1 - np.exp(-h*c*nu0/k/T)
    part_4 = 1 - np.exp(-h*c*nu0/k/T0)

    S = S0*part_1*part_2*part_3/part_4

    return S
```

1.3.4 Spectral absorption coefficient function

This function computes the spectral absorption coefficient for a given x over all the wave numbers

Here, the a equation is given below, it describes the gausian half-width at half maximum value

$$a = 2\sqrt{log(2)}\frac{\nu - \nu_0}{\alpha_G}$$

the w equation which describes the lorenztian half-width at half maximum is given below

$$w = \sqrt{log(2)}\frac{\alpha_L}{\alpha_G}$$

Then the ϕ function value is computed with the equation described below

$$\phi(\nu) = \frac{2}{\alpha_G}\sqrt{\frac{log(2)}{\pi}}V(z) \quad \forall \quad z = a + wi$$

Finally, the value of spectral absorption coefficient is computed by the dot product of (line intensity, mole fraction and presure) and the ϕ function as given below

$$K(x) = (S(T) \times \chi \times P).\phi(\nu, T)$$

The name of the function is given as per the MATLAB code,

[7]:
```
def voigt(dat, nu0, s, delnu_g, delnu_l):
    """
    this function computes value of K (spectral absorption coefficient)
    at given X location for all wave numbers.

    The name of this program function is given  as per the matlab code
    """

    # computing difference between chosen wavenumber ranges and wave number
    # from the HITRAN database
    """ for this, the matrix is obtained by subtracting each element of one
    arrau over each other elements of the other array"""
    vv0 = nu0 - dat.reshape(dat.shape[0],1) #  it is (nu-nu0) in the equation
```

```
    # computing "a" equation from problem definition
    """
    DOUBT:
    here a 2 is missing in the code but present in the pblm definition
    """
    a = np.sqrt(np.log(2))*vv0/delnu_g

    # computing "w" equation from problem definition
    w = np.sqrt(np.log(2))*np.ones([dat.shape[0],1])*delnu_l/delnu_g

    # combining w and a into a complex function to feed it to voigt function
    z = a+w*1j

    # computing phi function
    """
    DOUBT:
    here a 2 is missing in the code but present in the pblm definition
    """
    phi = 1/delnu_g*np.sqrt(np.log(2)/np.pi)*wofz(z)

    # computing the K function in problem definition for current X value
    K = np.matmul(np.real(phi),s)

    return K
```

1.4 Computing the Non-uniform Absorption Spectra

Reading the HITRAN database and the partition function table

[8]:
```
# reading data from HITRAN file
fid_HITRAN = HITRAN_reader(HITRAN_filename)

# reading Partition function table
fid_Q = pd.read_csv(PART_filename, header = None, delim_whitespace = True,
                    names = ["T","Q"])
```

Extracting individual columns of data from the database and computing a range of wave numbers between the given min and max ranges

[9]:
```
# reading data from the database file
# center wavenumber
nu0  = fid_HITRAN["transisionWaveNumber"].to_numpy().astype("float64")
# reference line strength
s0   = fid_HITRAN["lineIntensity"].to_numpy().astype("float64")
# air-broadened width
g_a0 = fid_HITRAN["airBroadenedWidth"].to_numpy().astype("float64")
```

```
# self-broadened width
g_s0 = fid_HITRAN["selfBroadenedWidth"].to_numpy().astype("float64")
# lower state energy
Edd0 = fid_HITRAN["lowerStateEnergy"].to_numpy().astype("float64")
# temperature dependence exponent
n    = fid_HITRAN["temperatureDependence"].to_numpy().astype("float64")
# pressure shift coefficient
d0   = fid_HITRAN["pressureShift"].to_numpy().astype("float64")

# computing a range of wave numbers
dat1 = np.linspace(nu_1_min, nu_1_max, N_nu_range)
```

Filtering the entries from database based on the following criteria - line intensity should be greater than 10^{-30} - dropping extreme wave numbers

[10]:
```
# selecting the indices of entries with nu0 falling b/w extreme nu values and
# with line intensity <= 10^-30
index1 = (nu0 > nu_1_min) & (nu0 < nu_1_max)
index2 = s0 > 1e-30
index  = index1 & index2

nu1   = nu0[index]
s01   = s0[index]
g_a01 = g_a0[index]
g_s01 = g_s0[index]
Edd1  = Edd0[index]
n1    = n[index]
d01   = d0[index]
```

pressure is taken to be contstant, hence, multiplying the line strength with pressure and some conversion factor

[11]:
```
S0 = s01*2.479371939e19*P #  <-------------- DOUBT
```

Constructing the temperature and mole fraction profiles along with discretizing the x-locations

[12]:
```
# temperature and mole fraction fields construction----------------------------

# discretized radial distance
X = np.arange(0,total_radial_distance+delta_x,delta_x)

# non uniform temperature field
Tnon = A2+(A1-A2)/(1+np.exp((X-X0)/A3))

# non uniform mole fraction field
xnon = B2+(B1-B2)/(1+np.exp((X-X0)/A3))
```

Creating 2D matrices with size being the number of line strength entities and the number of x-locations, and computing the spatial step size

[13]:
```
# obtaining the size of s0 and Tnon for 2D array pre-allocations
ns = S0.shape[0]
nt = Tnon.shape[0] - 1 #  <----------------- DOUBT, nt+1 is actually nx

# preallocating 2d arrays
s       = np.zeros([nt,ns]) # line strength
d       = np.zeros([nt,ns]) # pressure shift coefficient
g_a     = np.zeros([nt,ns]) # air broadened width
g_s     = np.zeros([nt,ns]) # self broadened width
nu0_s   = np.zeros([nt,ns]) # shifted center-wavenumber
delnu_g = np.zeros([nt,ns]) # gaussian half-width at halft maximum
delnu_l = np.zeros([nt,ns]) # lorentzian half-width at halft maximum

# computing spatial step size
dx = np.diff(X)
```

Looping through all the filtered database entries and the x-locations and computing the following
- Pressure shift coefficient

$$\delta_p = \delta_0 \left(\frac{T_0}{T}\right)^{0.96}$$

- Air broadened width

$$\gamma_{air}(T) = \gamma_{air}(T_0) \left(\frac{T_0}{T}\right)^{n_{air}}$$

- Self broadened width

$$\gamma_{self}(T) = \gamma_{self}(T_0) \left(\frac{T_0}{T}\right)^{0.75}$$

- Shifted center wave number

$$\nu_0 = \nu + P(1-\chi)\delta_p$$

- Line strength with product of mole fraction and spatial step size

$$S(T) = S(T_0)\frac{Q(T_0)}{Q(T)}\frac{T_0}{T} exp\left(\frac{-hcE"}{k}\left(\frac{1}{T}-\frac{1}{T_0}\right)\right)\frac{\left[1-exp\left(\frac{-hc\nu_0}{kT}\right)\right]}{\left[1-exp\left(\frac{-hc\nu_0}{kT_0}\right)\right]}$$

$$S(T)\chi dx$$

- Gaussian half width at half maximum (1000 is a unit conversion factor for N_a and 10^4 for c in cm/s)

$$\alpha_G = \nu_0 \left(\frac{2N_a kTlog(2) \times 1000 \times 10^4}{mc^2}\right)^{\frac{1}{2}}$$

- Lorentzian half width at half maximum

$$\alpha_L = P\left(\chi\gamma_{self} + (1-\chi)\gamma_{air}\right)$$

[14]:
```
# looping through all x-locations and given line intensities
for i in range(ns):
    for j in range(nt):
        # getting current mole fraction value
```

```
        x = xnon[j]

        # computing the pressure shift coefficient
        d[j,i] = d01[i]*(T0/Tnon[j])**0.96

        # air broadened width
        g_a[j,i] = g_a01[i]*(T0/Tnon[j])**n1[i]

        # self broadened width
        g_s[j,i] = g_s01[i]*(T0/Tnon[j])**0.75

        # shifted center wave nuber
        nu0_s[j,i] = nu1[i] + P*(1-x)*d[j,i]

        # line strength
        s[j,i] = lineStrength(S0[i], nu0_s[j,i], Edd1[i], Tnon[j],␣
↪fid_Q)*dx[j]*x

        # gaussian HWHM
        delnu_g[j,i] = np.sqrt(2*k*np.log(2)*Na/c**2*1000*10**4)*nu0_s[j,i]*np.
↪sqrt(Tnon[j]/M)
        # delnu_g[j,i] = 0.5*7.162242257e-7*nu0_s[j,i]*np.sqrt(Tnon[j]/M)

        # lorentian HWHM
        delnu_l[j,i] = P*(x*g_s[j,i]+(1-x)*g_a[j,i])
```

Computing the absorption spectra

$$K(x) = P\chi(x)\sum_{i=1}^{N_x} S(T_i)\phi(\nu_i, T_i)$$

[15]:
```
# pre-allocating absorbance array for all wave numbers
"""
it is -ln(I(nu)/I_0)
"""
Absorbance = np.zeros([N_nu_range])

# computing absorbance coefficient K for each x and suming it up for total
for i in range(X.shape[0]-1): #  <-------------- DOUBT
    Absorbance += voigt(dat1, nu0_s[i,:], s[i,:], delnu_g[i,:], delnu_l[i,:])
```

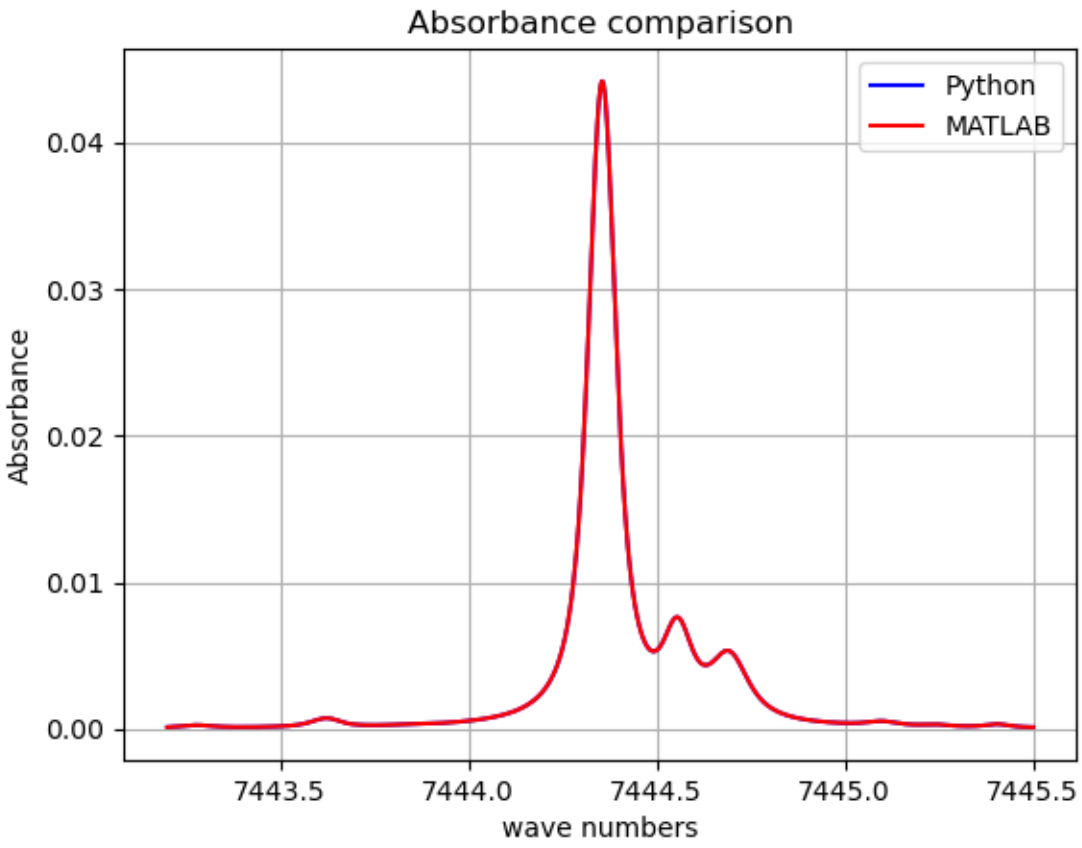
1.5 Post-processing

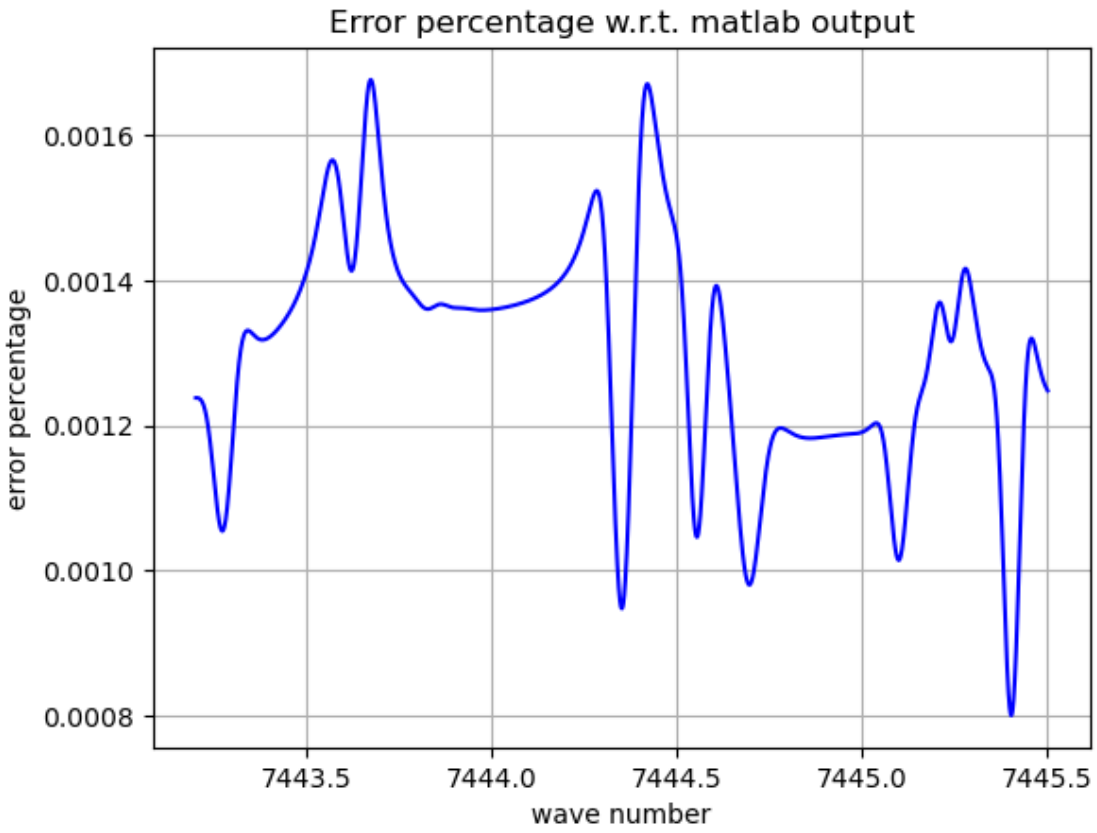
Preparing pandas dataframe with computed values, and compute error percentage with MATLAB output, then write computed values to a csv file

[16]:
```
# reading matlab output file
fid_mat = pd.read_csv("absorbance_matlab.csv", header = None,
                      names = ["wavenumber", "absorbance"])

# writing computed values to file along with matlab
fid_ab = pd.DataFrame(np.transpose([dat1, Absorbance]), columns = ["wavenumber",
                                                                   "absorbance"])
fid_ab["absorbance_matlab"] = fid_mat["absorbance"]
fid_ab["error_percentage"] =␣
 ↪abs((fid_ab["absorbance_matlab"]-fid_ab["absorbance"])/
 ↪fid_ab["absorbance_matlab"])*100.0
fid_ab.to_csv("absorbance_pythonOutput.csv", index = None)
```

Plotting comparison and error graphs

[17]:
```
# plotting absorbance graph
plt.figure()
plt.plot(dat1, Absorbance, '-b', label = "Python")
plt.plot(fid_mat["wavenumber"], fid_mat["absorbance"], '-r', label = "MATLAB")
plt.grid()
plt.legend()
plt.xlabel("wave numbers")
plt.ylabel("Absorbance")
plt.title("Absorbance comparison")
plt.savefig("absorbance.png", dpi = 150)

# plotting error percentage between matlab and python
plt.figure()
plt.plot(fid_ab["wavenumber"],fid_ab["error_percentage"], '-b')
plt.grid()
plt.xlabel("wave number")
plt.ylabel("error percentage")
plt.title("Error percentage w.r.t. matlab output")
plt.savefig("error.png", dpi = 150)

plt.show()
```


Absorbance comparison
Python
MATLAB
0.04
0.03
0.02
0.01
0.00
Absorbance
7443.5
7444.0
7444.5
7445.0
7445.5
wave numbers


Error percentage w.r.t. matlab output
error percentage
0.0016
0.0014
0.0012
0.0010
0.0008
7443.5
7444.0
7444.5
7445.0
7445.5
wave number

[ ]: