In [138…
```
import numpy as np
import warnings
import pandas as pd
import matplotlib.pyplot as plt
from scipy.optimize import minimize
from scipy.optimize import differential_evolution,shgo,dual_annealing, ba
seed = 123
```

Project: One-Mass Oscillator Optimization

Introduction

In this project, you will apply various optimization algorithms to fit a one-mass oscillator model to real-world data. The objective is to minimize the sum of the squared residuals between the model predictions and the observed amplitudes of a one-mass oscillator system across different frequencies.

One-Mass Oscillator Model

The one-mass oscillator is characterized by the following equation, representing the amplitudes of the system:

$$ V(\omega) = \frac{F}{\sqrt{(1 - \nu^2)^2 + 4D^2\nu^2}} $$
Here,

- $ \omega $ represents the angular frequency of the system,
- $ \nu $ is the ratio of the excitation frequency to the natural frequency ($ \nu = \frac{\omega_{\text{err}}}{\omega_{\text{eig}}} $),
- $ D $ is the damping ratio,
- $ F $ is the force applied to the system.

The goal of the project is to determine the optimal values for the parameters $ \omega_{\text{eig}} $, $ D $, and $ F $ that result in the best fit of the one-mass oscillator model to the observed amplitudes.

Load the real world data

- we have two different measurements
- J represents the measured frequencies
- N represents the measured amplitudes

In [139…
```
df1 = pd.read_pickle("df1.pkl")
df2 = pd.read_pickle("df2.pkl")
# Printing the lengths of the DataFrames
print("Length of df1:", len(df1))
print("Length of df2:", len(df2))
```

```
Length of df1: 33
Length of df2: 66
```

Low amplitudes distort the fit and are negligible therefore we define a lower threshold for N

In [140…

```
threshold = 0.4
df1.sort_values("N")
max_N = max(df1["N"])
df1 = df1[df1["N"]>=threshold*max_N]

# checking the lengths of the DataFrames again
print("Length of df1:", len(df1))
print("Length of df2:", len(df2))
```

```
Length of df1: 31
Length of df2: 66
```

We extract the frequency value for maximum value of the amplitude. This serves as the initial value for one decision variable.

In [141…

```
df_max=df1[df1["N"]==max(df1["N"])]
initial_Oeig = df_max["J"].values[0]
max_N = df_max["N"].values[0]
```

We also have to define the other two initial guesses

In [142…

```
initial_D = 0.006
initial_F = 0.120

initial_values = [initial_Oeig, initial_D, initial_F]
```

Additionally we define the bounds for the decision variables

In [143…

```
min_Oerr = min(df1["J"])
max_Oerr = max(df1["J"])
```

In [144…

```
bounds = [(min_Oerr, max_Oerr), (0, 0.03), (0, 1)]
```

Then we define the objective function

In [145…

```
def one_mass_oscillator(params, Oerr) -> np.ndarray:
    # returns amplitudes of the system
    # Defines the model of a one mass oscilator
    Oeig, D, F = params
    nue = Oerr / Oeig
    V = F / (np.sqrt((1 - nue**2) ** 2 + (4 * D**2 * nue**2)))
    return V
```

In [146…

```
def objective_function(params, Oerr, amplitudes) -> np.ndarray:
    # objective function to compare calculated and real amplitudes
    return np.sum((amplitudes - one_mass_oscillator(params, Oerr)) ** 2)
```

We define the options and start the optimization process

In [147…
```
options = {
    "maxfun": 100000, #Maximum Function Evaluation
    "ftol": 1e-9,     # Function Tolerance
    "xtol": 1e-9,     #Variable Tolerance
    "stepmx": 10,     #Controls Maximum Step size
    "eta": 0.25,      #Controls relative Step Size
    "gtol": 1e-5}     #Gradient Tolerance
```

In [148…
```
J = np.array(df1["J"]) # measured frequency
N = np.array(df1["N"]) # measured amplitude
```

In [149…
```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    method='Nelder-Mead',
    bounds=bounds,
    options=options)
```

```
/tmp/ipykernel_975535/2959858538.py:1: OptimizeWarning: Unknown solver o
ptions: maxfun, ftol, xtol, stepmx, eta, gtol
  result = minimize(
```

Then we can observe the results

In [150…
```
# map optimized values to variables
resonant_frequency = result.x[0]
D = result.x[1]
F = result.x[2]
# predict the resonant amplitude with the fitted one mass oscillator.
X_pred = np.linspace(min_Oerr, max_Oerr, 1000)
ypred_one_mass_oscillator = one_mass_oscillator(result.x, X_pred)
resonant_amplitude = max(ypred_one_mass_oscillator)
```

In [151…
```
result
```

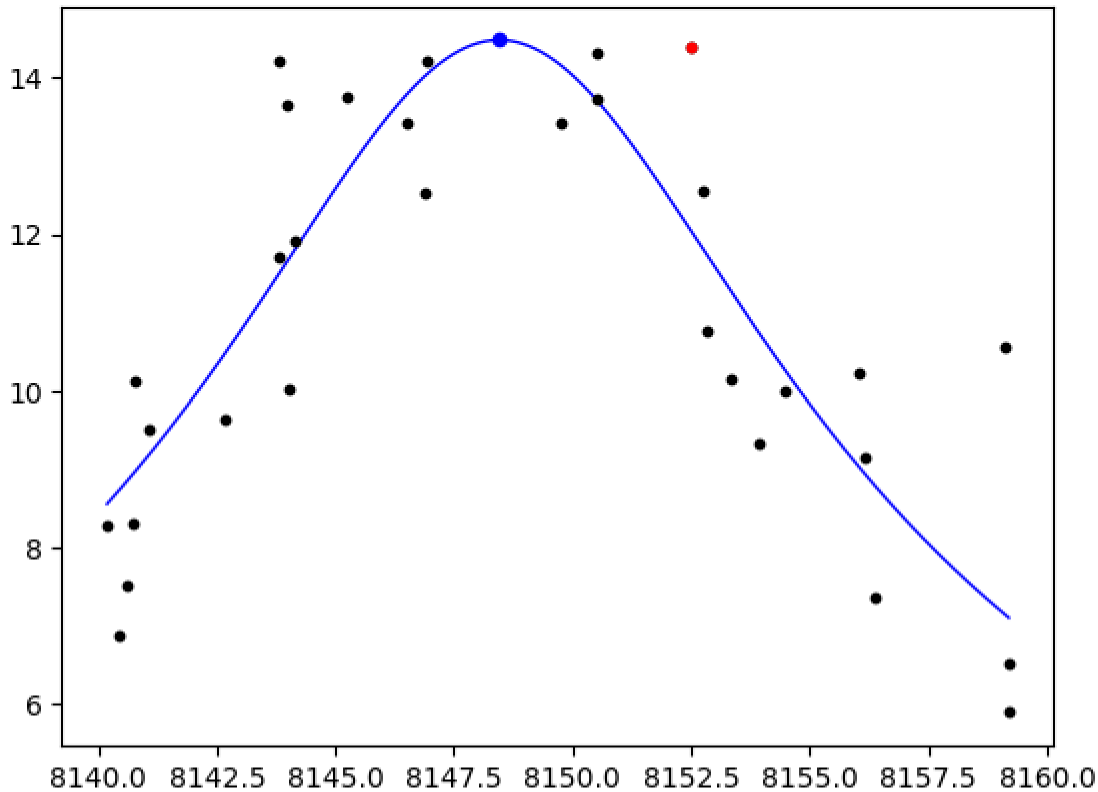
Out[151]:
```
       message: Optimization terminated successfully.
       success: True
        status: 0
           fun: 53.54144061205875
             x: [ 8.148e+03  7.435e-04  2.153e-02]
           nit: 93
          nfev: 169
 final_simplex: (array([[ 8.148e+03,  7.435e-04,  2.153e-02],
                       [ 8.148e+03,  7.435e-04,  2.153e-02],
                       [ 8.148e+03,  7.435e-04,  2.153e-02],
                       [ 8.148e+03,  7.435e-04,  2.153e-02]]), array([
 5.354e+01,  5.354e+01,  5.354e+01,  5.354e+01]))
```

Finally, we can plot the optimized fit and the real values

In [152…
```
plt.scatter(
    df1["J"],
    df1["N"],
```

```
    color="black",
    label="Spektralpunkte filtered",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
        X_pred,
        ypred_one_mass_oscillator,
        label="Alpha",
        color="blue",
        linewidth=1,
    )
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)
```

Out[152]: `<matplotlib.collections.PathCollection at 0x14a73828a810>`



Task for the Project Work

Optimization of First Data Frame

Using Global Optimizers

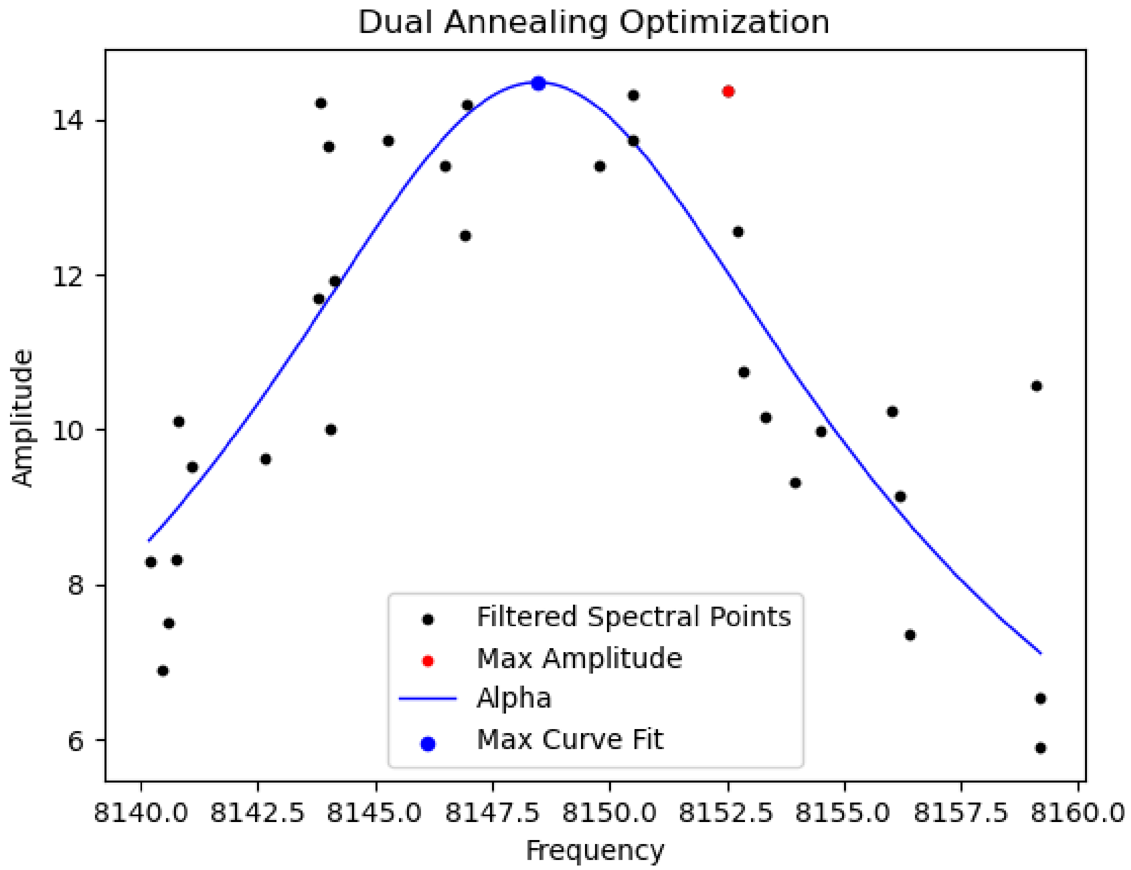
Using Dual Annealing

In [153…

```
result = dual_annealing(
    objective_function,
    bounds=bounds,
    args=(J, N),
    maxiter=1000,  # Maximum number of iterations
    seed=123,  # Seed for reproducibility
)

# Plotting
plt.scatter(
    df1["J"],
    df1["N"],
    color="black",
    label="Filtered Spectral Points",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Dual Annealing Optimization")
plt.show()

print("Optimized Parameters:")
```

```
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```

```
/tmp/ipykernel_975535/2542982551.py:6: RuntimeWarning: invalid value enc
ountered in divide
  V = F / (np.sqrt((1 - nue**2) ** 2 + (4 * D**2 * nue**2)))
/tmp/ipykernel_975535/2542982551.py:6: RuntimeWarning: divide by zero en
countered in divide
  V = F / (np.sqrt((1 - nue**2) ** 2 + (4 * D**2 * nue**2)))
/global/mambaforge/envs/py311-pyspotseven/lib/python3.11/site-packages/s
cipy/optimize/_numdiff.py:590: RuntimeWarning: invalid value encountered
in subtract
  df = fun(x) - f0
```




```
Optimized Parameters:
Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813
Force Amplitude: 0.02152990400035095
Resonant Amplitude: 14.479437222571885
Objective Function Value: 53.54144153462606
```

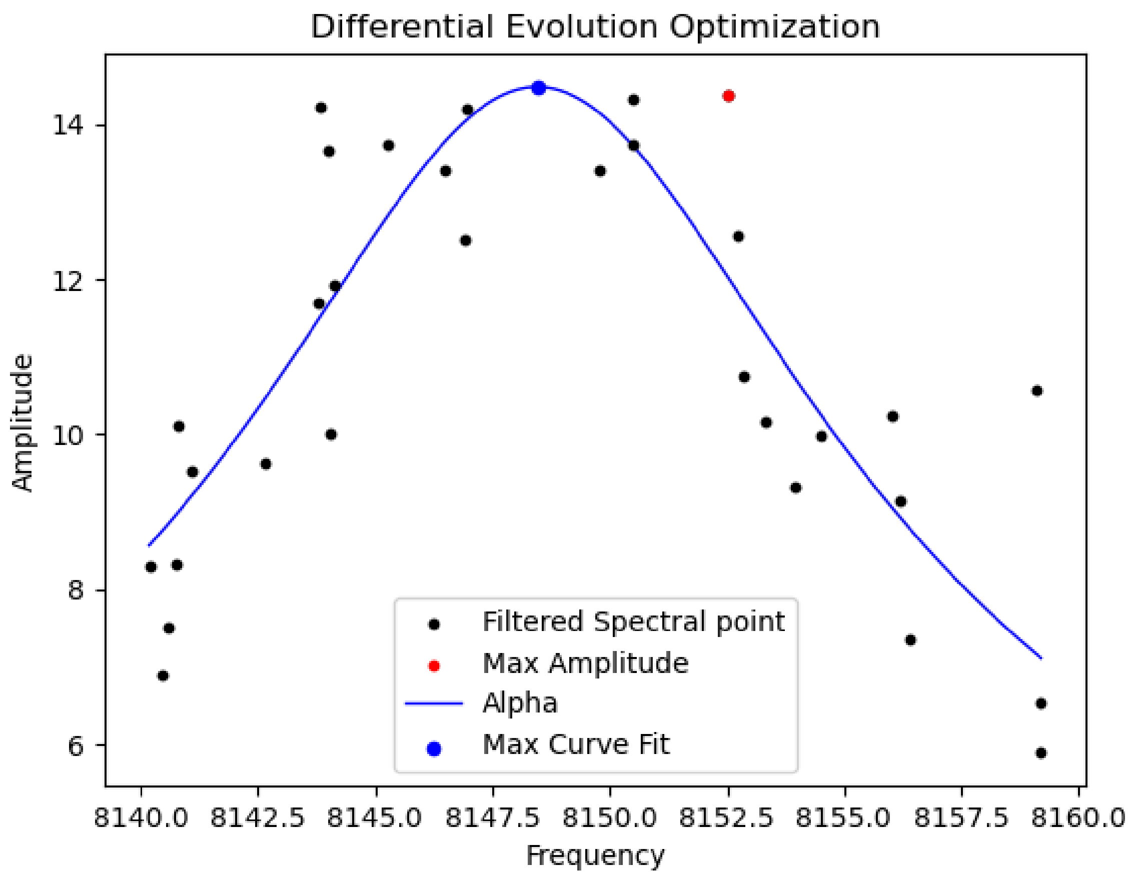
Out[153]:

```
 message: ['Maximum number of iteration reached']
 success: True
  status: 0
     fun: 53.54144153462606
       x: [ 8.148e+03  7.434e-04  2.153e-02]
     nit: 1000
    nfev: 6437
    njev: 109
    nhev: 0
```

Using Differencial Evolution

In [154…

```
result = differential_evolution(
    objective_function,
    bounds=bounds,  # Define bounds for each parameter
    args=(J, N),
    maxiter=1000,  # Maximum number of iterations
    seed=123,  # Seed for reproducibility
)

# Plotting
plt.scatter(
    df1["J"],
    df1["N"],
    color="black",
    label="Filtered Spectral point",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Differential Evolution Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```




```
Optimized Parameters:
Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813
Force Amplitude: 0.02152990400035095
Resonant Amplitude: 14.479437222571885
Objective Function Value: 53.56531877262423
```

Out[154]:

```
          message: Optimization terminated successfully.
          success: True
              fun: 53.56531877262423
                x: [ 8.148e+03  7.435e-04  2.153e-02]
              nit: 43
             nfev: 2012
       population: [[ 8.148e+03  7.456e-04  2.155e-02]
                    [ 8.148e+03  7.444e-04  2.149e-02]
                    ...
                    [ 8.148e+03  7.573e-04  2.184e-02]
                    [ 8.148e+03  7.644e-04  2.199e-02]]
population_energies: [ 5.357e+01  5.371e+01 ...  5.377e+01  5.373e+01]
              jac: [-1.305e+00  6.588e-01  1.656e+00]
```

Using Local Optimizers

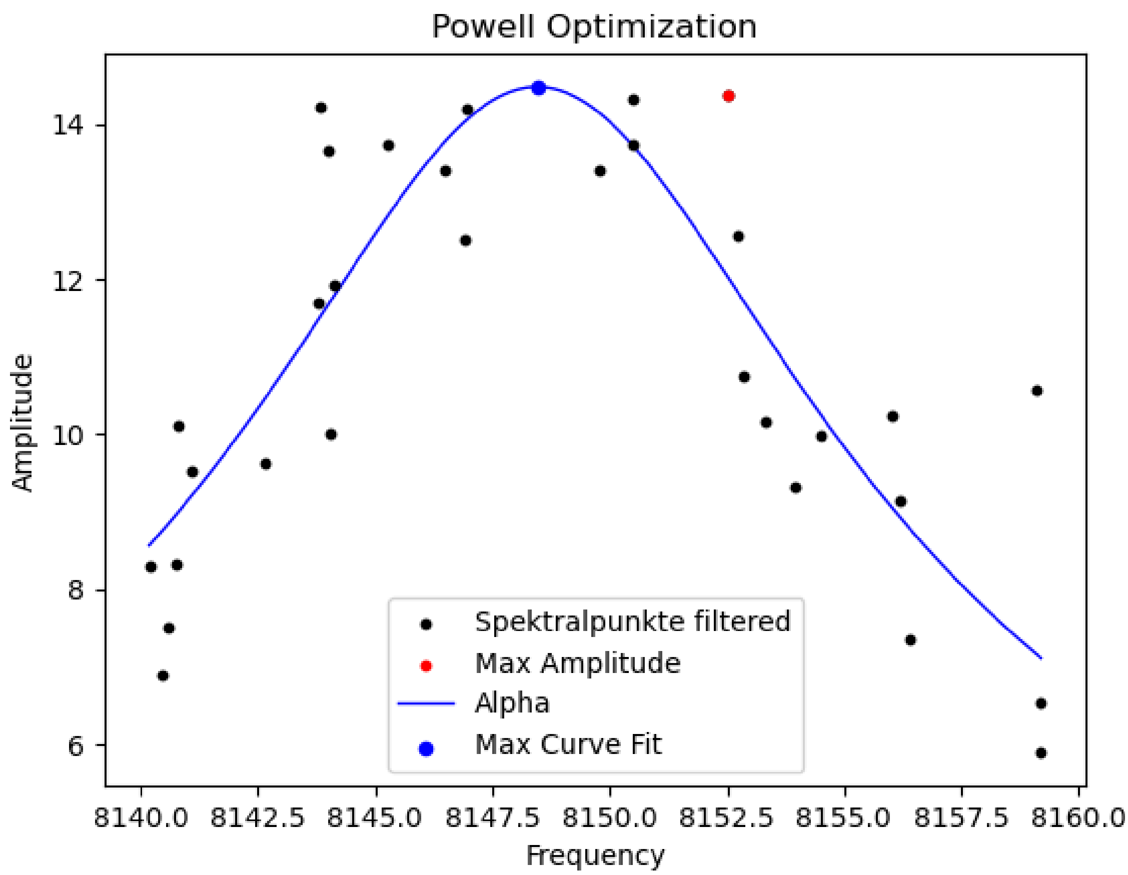
Using Conjugate Gradient

In [155…

```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    method='powell',
    options=options,
bounds=bounds)
# Plotting
```

```
plt.scatter(
    df1["J"],
    df1["N"],
    color="black",
    label="Spektralpunkte filtered",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Powell Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```

```
/tmp/ipykernel_975535/2450881691.py:1: OptimizeWarning: Unknown solver o
ptions: maxfun, stepmx, eta, gtol
  result = minimize(
```




```
Optimized Parameters:
Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813
Force Amplitude: 0.021529904000035095
Resonant Amplitude: 14.479437222571885
Objective Function Value: 53.54144059016111
```

Out[155]:

```
  message: Optimization terminated successfully.
  success: True
   status: 0
      fun: 53.54144059016111
        x: [ 8.148e+03  7.435e-04  2.153e-02]
      nit: 11
    direc: [[ 1.978e+00 -1.935e-03 -3.893e-02]
            [-1.091e+00 -1.473e-05 -1.175e-04]
            [ 5.034e-08  6.736e-10 -1.229e-08]]
     nfev: 693
```

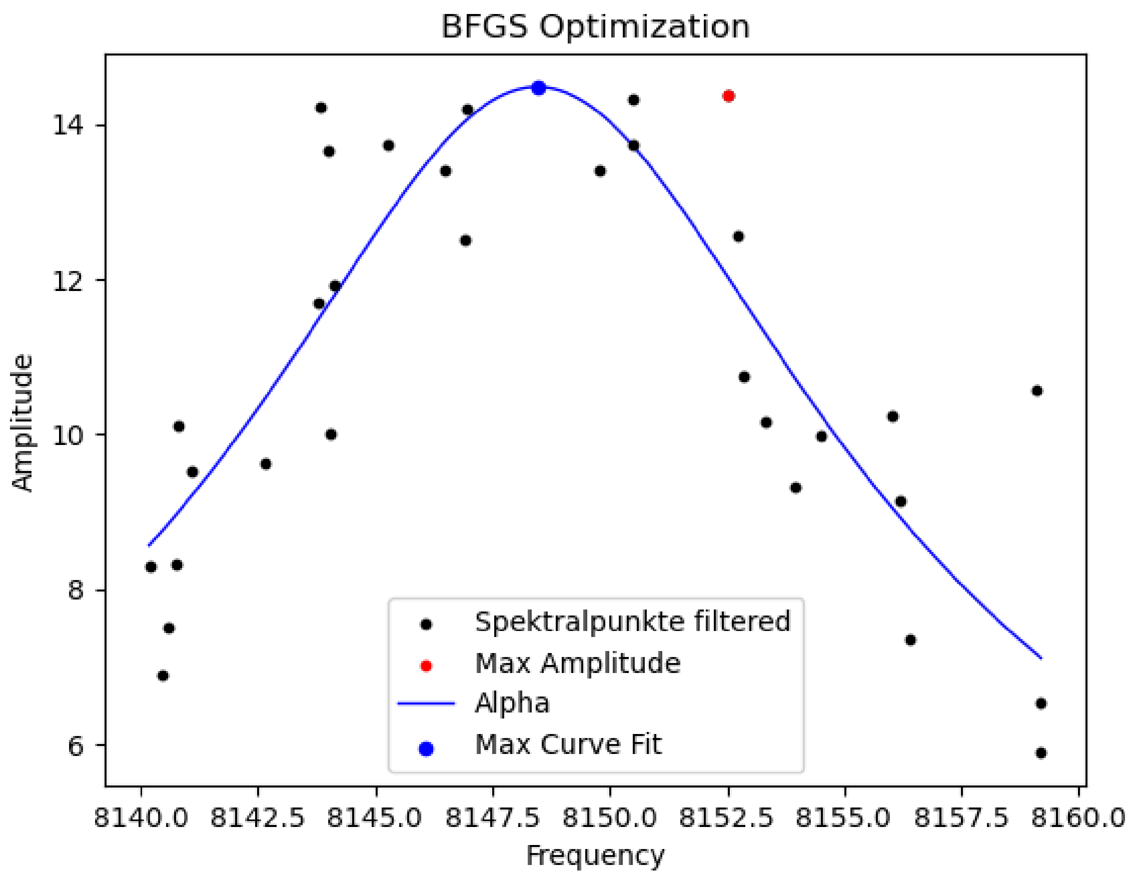
Using BFGS

In [157…

```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    method='L-BFGS-B',
    bounds=bounds,
    options=options)
result
# Plotting
plt.scatter(
    df1["J"],
    df1["N"],
    color="black",
```

```
    label="Spektralpunkte filtered",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("BFGS Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```

```
/tmp/ipykernel_975535/996043608.py:1: OptimizeWarning: Unknown solver op
tions: xtol, stepmx, eta
  result = minimize(
```




```
Optimized Parameters:
Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813
Force Amplitude: 0.02152990400035095
Resonant Amplitude: 14.479437222571885
Objective Function Value: 53.54144117175894
```

Out[157]:

```
  message: CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
  success: True
   status: 0
      fun: 53.54144117175894
        x: [ 8.148e+03  7.434e-04  2.153e-02]
      nit: 28
      jac: [ 1.419e-03  1.073e+01 -1.476e-01]
     nfev: 188
     njev: 47
 hess_inv: <3x3 LbfgsInvHessProduct with dtype=float64>
```

Comparision of different Optimisers

Optimizer	Scope(local/Global optimizer)	Objective Function Value	Number of Evaluations	Number of Iterations	Obser
Dual Annealing	Global	53.54144153462606	6437	1000	Achie global optimu the mo functio evalua
DifferntialEvolution	Global	53.54938461678095	2012	43	Finds optima solutio fewer

Optimizer	Scope(local/Global optimizer)	Objective Function Value	Number of Evaluations	Number of Iterations	Obser
					evalua than d annea
Powell's	Local	53.54144059016111	693	11	Powell metho efficie finds a optima solutio a lowe numbe iteratio compa Dual Annea but it r find th absolu solutio
Nelder Mead	local	53.54144061205875	169	93	Efficie finds a optima solutio fewer iteratio
L-BFGS-B	local	53.54144117175894	188	28	Quickl conve a loca optimu the lea numbe iteratio

Conclusion

The table highlights the trade-off between finding the absolute best solution (global optimum) and the computational cost of the optimization algorithm. Methods that guarantee the global optimum require significant processing power, while faster approaches might settle for very good solutions that aren't necessarily the absolute best. The optimal choice depends on the specific problem and the importance placed on finding the absolute best solution versus efficiency.

Optimization of 2nd Data Frame

Using Global Optimizers

In [158…

```
df1 = pd.read_pickle("df1.pkl")
df2 = pd.read_pickle("df2.pkl")
# Printing the lengths of the DataFrames
print("Length of df1:", len(df1))
```

```
print("Length of df2:", len(df2))
```

```
Length of df1: 33
Length of df2: 66
```

In [159…

```
threshold = 0.4
df2.sort_values("N")
max_N = max(df2["N"])
df2 = df2[df2["N"]>=threshold*max_N]
len(df2)
```

Out[159]: 23

We extract the frequency value for maximum value of the amplitude.
This serves as the initial value for one decision variable.

In [160…

```
df_max=df2[df2["N"]==max(df2["N"])]
initial_Oeig = df_max["J"].values[0]
max_N = df_max["N"].values[0]
```

We also have to define the other two initial guesses

In [161…

```
initial_D = 0.006
initial_F = 0.120

initial_values = [initial_Oeig, initial_D, initial_F]
```

Additionally we define the bounds for the decision variables

In [162…

```
min_Oerr = min(df2["J"])
max_Oerr = max(df2["J"])
```

In [163…

```
bounds = [(min_Oerr, max_Oerr), (0, 0.03), (0, 1)]
```

Then we define the objective function

In [164…

```
def one_mass_oscillator(params, Oerr) -> np.ndarray:
    # returns amplitudes of the system
    # Defines the model of a one mass oscilator
    Oeig, D, F = params
    nue = Oerr / Oeig
    V = F / (np.sqrt((1 - nue**2) ** 2 + (4 * D**2 * nue**2)))
    return V
```

In [165…

```
def objective_function(params, Oerr, amplitudes) -> np.ndarray:
    # objective function to compare calculated and real amplitudes
    return np.sum((amplitudes - one_mass_oscillator(params, Oerr)) ** 2)
```

We define the options and start the optimization process

In [166…

```
options = {
    "maxfun": 100000,
    "ftol": 1e-9,
    "xtol": 1e-9,
```

```
    "stepmx": 10,
    "eta": 0.25,
    "gtol": 1e-5}
J = np.array(df2["J"]) # measured frequency
N = np.array(df2["N"]) # measured amplitude
```

In [167…

```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    method='Nelder-Mead',
    bounds=bounds,
    options=options)
```

```
/tmp/ipykernel_975535/2959858538.py:1: OptimizeWarning: Unknown solver o
ptions: maxfun, ftol, xtol, stepmx, eta, gtol
  result = minimize(
```

In [168…

```
# map optimized values to variables
resonant_frequency = result.x[0]
D = result.x[1]
F = result.x[2]
# predict the resonant amplitude with the fitted one mass oscillator.
X_pred = np.linspace(min_Oerr, max_Oerr, 1000)
ypred_one_mass_oscillator = one_mass_oscillator(result.x, X_pred)
resonant_amplitude = max(ypred_one_mass_oscillator)
result
```

Out[168]:

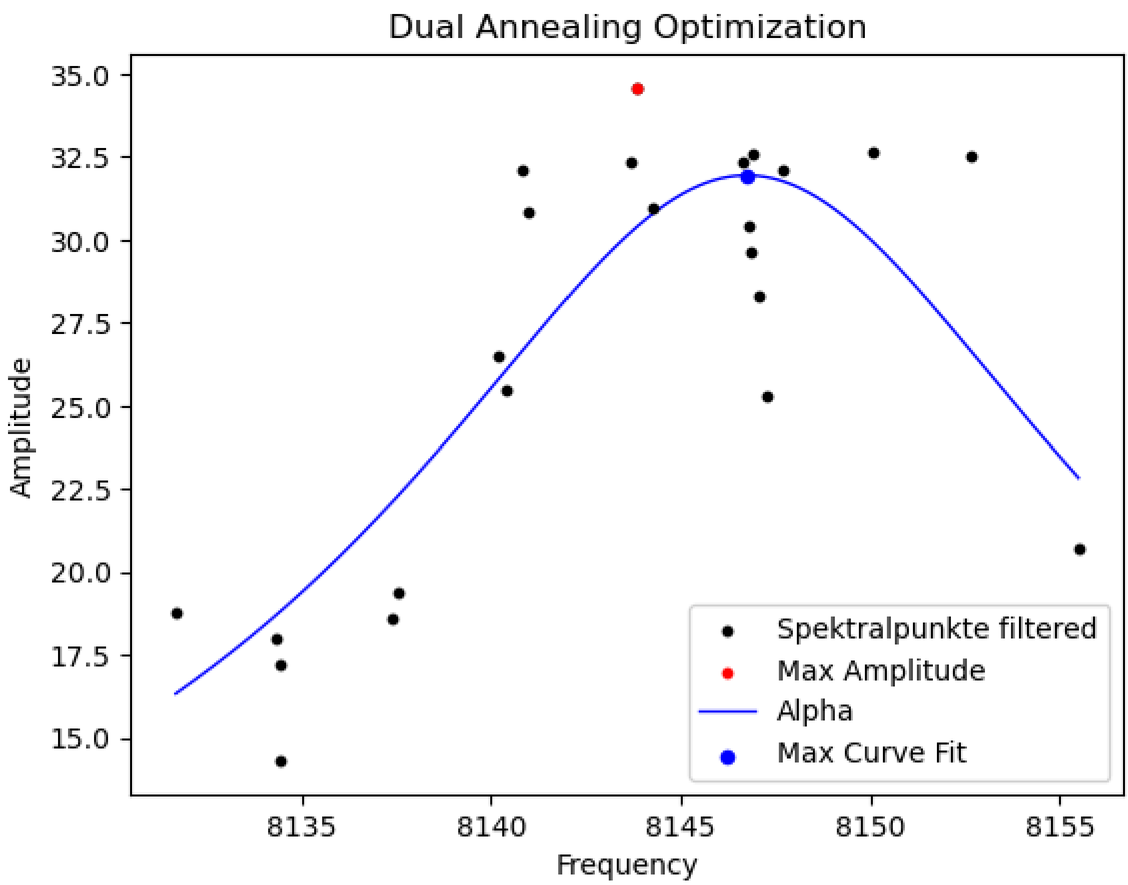
```
       message: Optimization terminated successfully.
       success: True
        status: 0
           fun: 229.4092648339145
             x: [ 8.147e+03  1.099e-03  7.021e-02]
           nit: 135
          nfev: 239
 final_simplex: (array([[ 8.147e+03,  1.099e-03,  7.021e-02],
                       [ 8.147e+03,  1.099e-03,  7.021e-02],
                       [ 8.147e+03,  1.099e-03,  7.021e-02],
                       [ 8.147e+03,  1.099e-03,  7.021e-02]]), array([
 2.294e+02,  2.294e+02,  2.294e+02,  2.294e+02]))
```

Using Dual Annealing

In [169…

```
result = dual_annealing(
    objective_function,
    bounds=bounds,
    args=(J, N),
    maxiter=1000,  # Maximum number of iterations
    seed=123,  # Seed for reproducibility
)

# Plotting
plt.scatter(
    df2["J"],
    df2["N"],
    color="black",
    label="Spektralpunkte filtered",
    zorder=5,
    s=10,
```

```
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Dual Annealing Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```



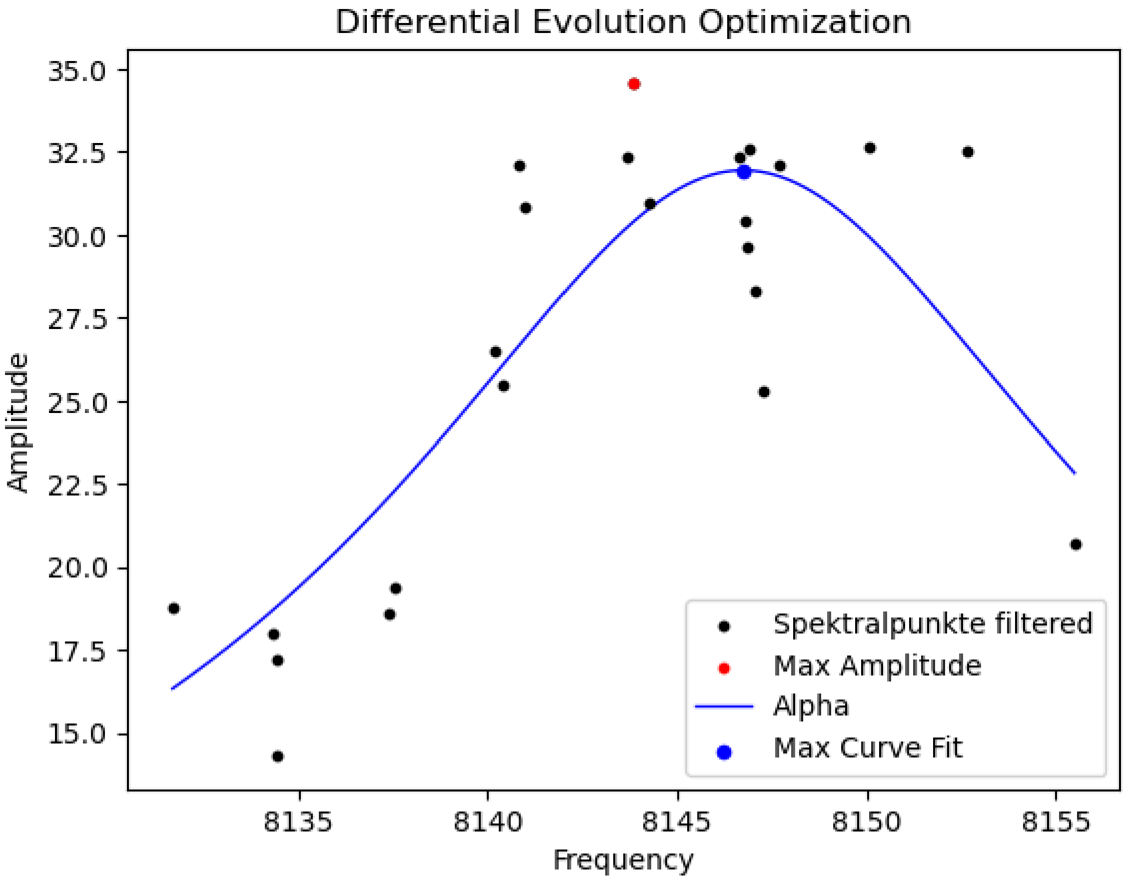

```
Optimized Parameters:
Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854
Force Amplitude: 0.07020956698446057
Resonant Amplitude: 31.94467402394625
Objective Function Value: 229.4092694161751
```

Out[169]:
```
 message: ['Maximum number of iteration reached']
 success: True
  status: 0
     fun: 229.4092694161751
       x: [ 8.147e+03  1.099e-03  7.020e-02]
     nit: 1000
    nfev: 6181
    njev: 45
    nhev: 0
```

Using Differencial Evolution

In [170…
```
result = differential_evolution(
    objective_function,
    bounds=bounds,  # Define bounds for each parameter
    args=(J, N),
    maxiter=1000,  # Maximum number of iterations
    seed=123,  # Seed for reproducibility
)

# Plotting
plt.scatter(
    df2["J"],
    df2["N"],
    color="black",
    label="Spektralpunkte filtered",
```

```
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Differential Evolution Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```




```
Optimized Parameters:
Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854
Force Amplitude: 0.07020956698446057
Resonant Amplitude: 31.94467402394625
Objective Function Value: 229.4192718479083
```

Out[170]:

```
             message: Optimization terminated successfully.
             success: True
                 fun: 229.4192718479083
                   x: [ 8.147e+03  1.101e-03  7.035e-02]
                 nit: 37
                nfev: 1778
          population: [[ 8.147e+03  1.102e-03  7.043e-02]
                       [ 8.147e+03  1.109e-03  7.042e-02]
                       ...
                       [ 8.147e+03  1.178e-03  7.560e-02]
                       [ 8.147e+03  1.097e-03  7.063e-02]]
 population_energies: [ 2.294e+02  2.299e+02 ...  2.351e+02  2.303e+02]
                 jac: [ 7.201e-01 -1.267e+00 -4.011e+00]
```

Using Local Optimizers

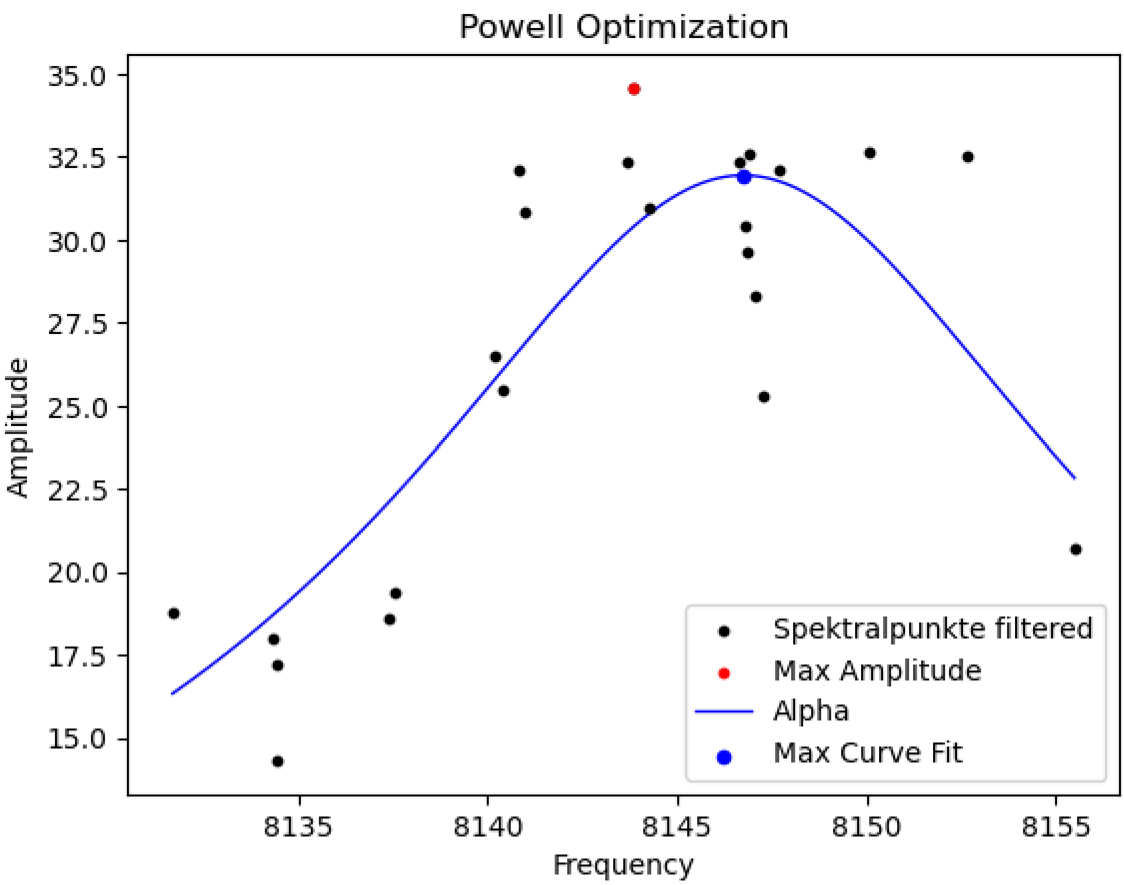
Using Conjugate Gradient

In [171…

```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    method='powell',
    options=options,
bounds=bounds)
```

```
# Plotting
plt.scatter(
    df2["J"],
    df2["N"],
    color="black",
    label="Spektralpunkte filtered",
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("Powell Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```

```
/tmp/ipykernel_975535/110192510.py:1: OptimizeWarning: Unknown solver op
tions: maxfun, stepmx, eta, gtol
  result = minimize(
```




```
Optimized Parameters:
Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854
Force Amplitude: 0.07020956698446057
Resonant Amplitude: 31.94467402394625
Objective Function Value: 229.4092648056204
```

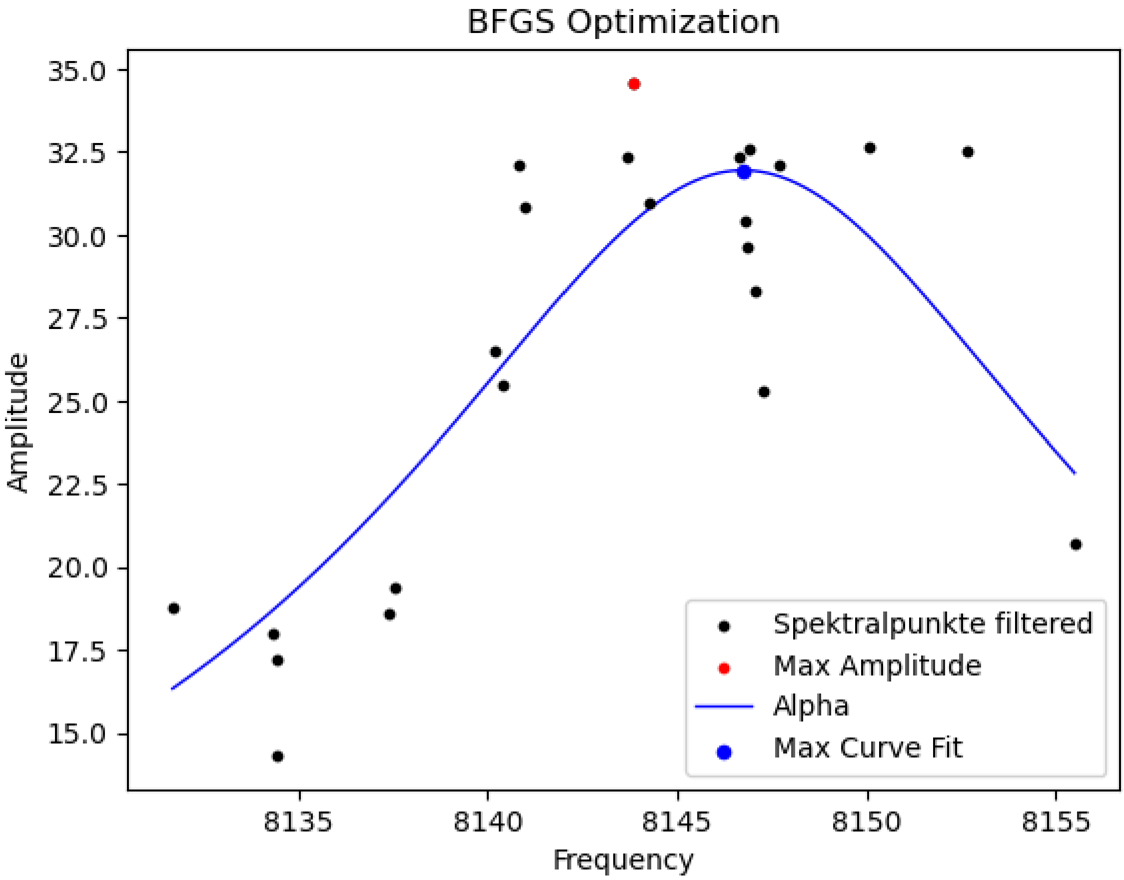
Out[171]:
```
 message: Optimization terminated successfully.
 success: True
  status: 0
     fun: 229.4092648056204
       x: [ 8.147e+03  1.099e-03  7.021e-02]
     nit: 9
   direc: [[-2.151e+00 -5.559e-04 -2.909e-02]
           [ 1.226e+00 -3.584e-05 -5.327e-04]
           [-1.653e-02 -2.415e-06 -2.265e-04]]
    nfev: 586
```

Using BFGS

In [172…
```
result = minimize(
    objective_function,
    initial_values,
    args=(J, N),
    bounds=bounds,
    options=options)
result
# Plotting
plt.scatter(
    df2["J"],
    df2["N"],
    color="black",
    label="Spektralpunkte filtered",
```

```
    zorder=5,
    s=10,
)
# color the max amplitude point red
plt.scatter(
    initial_Oeig,
    max_N,
    color="red",
    label="Max Amplitude",
    zorder=5,
    s=10,
)

plt.plot(
    X_pred,
    ypred_one_mass_oscillator,
    label="Alpha",
    color="blue",
    linewidth=1,
)
plt.scatter(
    resonant_frequency,
    resonant_amplitude,
    color="blue",
    label="Max Curve Fit",
    zorder=10,
    s=20,
)

plt.legend()
plt.xlabel("Frequency")
plt.ylabel("Amplitude")
plt.title("BFGS Optimization")
plt.show()

print("Optimized Parameters:")
print(f"Resonant Frequency: {resonant_frequency}")
print(f"Damping Coefficient: {D}")
print(f"Force Amplitude: {F}")
print(f"Resonant Amplitude: {resonant_amplitude}")
print(f"Objective Function Value: {result.fun}")
result
```

```
/tmp/ipykernel_975535/2860355532.py:1: OptimizeWarning: Unknown solver o
ptions: xtol, stepmx, eta
  result = minimize(
```




```
Optimized Parameters:
Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854
Force Amplitude: 0.07020956698446057
Resonant Amplitude: 31.94467402394625
Objective Function Value: 229.4092692624839
```

Out[172]:

```
  message: CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH
  success: True
   status: 0
      fun: 229.4092692624839
        x: [ 8.147e+03  1.099e-03  7.020e-02]
      nit: 20
      jac: [ 1.154e-03  8.419e+00 -1.765e-01]
     nfev: 180
     njev: 45
 hess_inv: <3x3 LbfgsInvHessProduct with dtype=float64>
```

Comparision of different Optimisers

Optimizer	Scope(local/Global optimizer)	Objective Function Value	Number of Evaluations	Number of Iterations	Obse
Dual Annealing	Global	229.4092694161751	6181	1000	Finds optim soluti the hi numb evalua and iterati
DifferntialEvolution	Global	229.4192718479083	1778	37	Achie near-(

Optimizer	Scope(local/Global optimizer)	Objective Function Value	Number of Evaluations	Number of Iterations	Obse
					soluti fewer evalua and it compa dual annea
Nelder Mead	Local	229.4092648339145	239	135	Efficie conve a near optim soluti minim evalua and iterati
Powell's	local	229.4092648056204	586	9	Powel metho efficie finds a optim soluti a lowe numb iterati compa Dual Annea but it find th absolu soluti
L-BFGS-B	local	229.4092692624839	180	45	Quick reach optim soluti the lea numb evalua and a mode numb iterati

Conclusion

Based on the table, there's a trade-off between finding the absolute best solution (global optimum) and the efficiency of the optimization algorithm. Algorithms that guarantee a global optimum (like Dual Annealing) require more evaluations and iterations. Conversely, faster algorithms (like Nelder-Mead or Powell's method) might converge to very good solutions (local optima) but potentially miss the absolute best.