```
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, basinhopping, direct
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\ln^2} $
Here,
```

- \$\omega \$ represents the angular frequency of the system,
- \$\nu \$ is the ratio of the excitation frequency to the natural frequency (\$\nu = \frac{{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 [2]: 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 [3]: 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 [4]: 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 [5]: 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 [6]: min_Oerr = min(df1["J"])
    max_Oerr = max(df1["J"])
In [7]: bounds = [(min_Oerr, max_Oerr), (0, 0.03), (0, 1)]
```

Then we define the objective function

```
In [8]: 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 [9]: 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)

# one_mass_oscillator function: This is a function that should be replaced with actual model for calculating amplitudes.
# objective function function: This computes the sum of squared differences between the real amplitudes (amplitudes) and the calculating amplitudes and the calculating amplitudes.
```

We define the options and start the optimization process

```
In [10]: options = {
    "maxfun": 100000, #Maximum Function Evaluation
```

```
# Function Tolerance
             "ftol": 1e-9,
             "xtol": 1e-9,
                            #Variable Tolerance
             "stepmx": 10, #Controls Maximum Step size
             "eta": 0.25,
                            #Controls relative Step Size
             "gtol": 1e-5} #Gradient Tolerance
In [11]: J = np.array(df1["J"]) # measured frequency
         N = np.array(df1["N"]) # measured amplitude
In [12]: result = minimize(
             objective function,
             initial values,
             args=(J, N),
             method='Nelder-Mead',
             bounds=bounds,
             options=options)
         /tmp/ipykernel 1193528/2959858538.py:1: OptimizeWarning: Unknown solver options: maxfun, ftol, xtol, stepmx, eta, gtol
           result = minimize(
```

Then we can observe the results

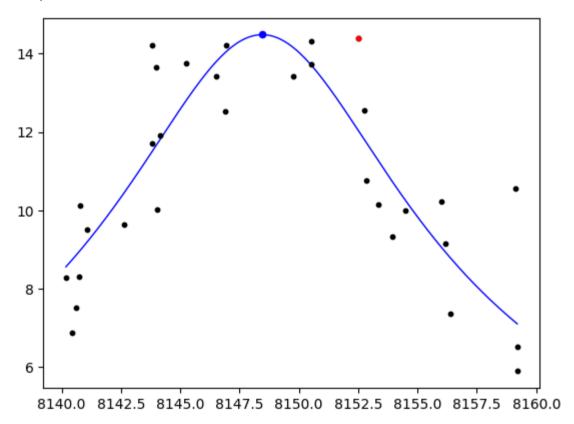
```
In [13]: # map optimized values to variables
    resonant_frequency = result.x[0]
    D = result.x[1]
    F = result.x[2]
    # predict the resonant amplitude with the fitted one mass oscillator.
    X_pred = np.linspace(min_Oerr, max_Oerr, 1000)
    ypred_one_mass_oscillator = one_mass_oscillator(result.x, X_pred)
    resonant_amplitude = max(ypred_one_mass_oscillator)
In [14]: result
```

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

```
In [15]: 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[15]: <matplotlib.collections.PathCollection at 0x14a9653ce390>



Task for the Project Work

Optimization of First Data Frame

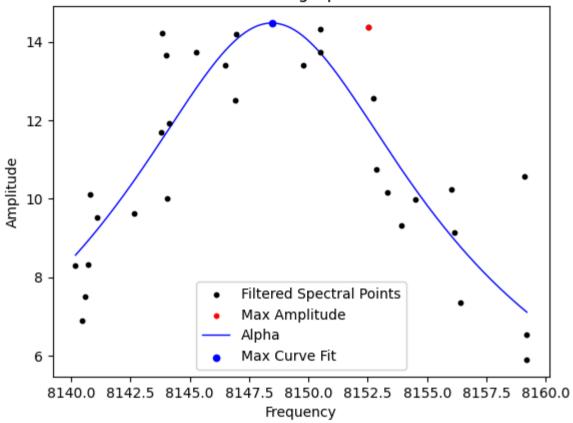
Using Global Optimizers

Using Dual Annealing

```
In [16]: 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 1193528/2542982551.py:6: RuntimeWarning: invalid value encountered in divide
 V = F / (np.sqrt((1 - nue**2) ** 2 + (4 * D**2 * nue**2)))
/tmp/ipykernel_1193528/2542982551.py:6: RuntimeWarning: divide by zero encountered 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/scipy/optimize/ numdiff.py:590: RuntimeWarning: invali
d value encountered in subtract
  df = fun(x) - f0
```

Dual Annealing Optimization



Optimized Parameters:

Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813

Force Amplitude: 0.02152990400035095 Resonant Amplitude: 14.479437222571885 Objective Function Value: 53.54144153462606

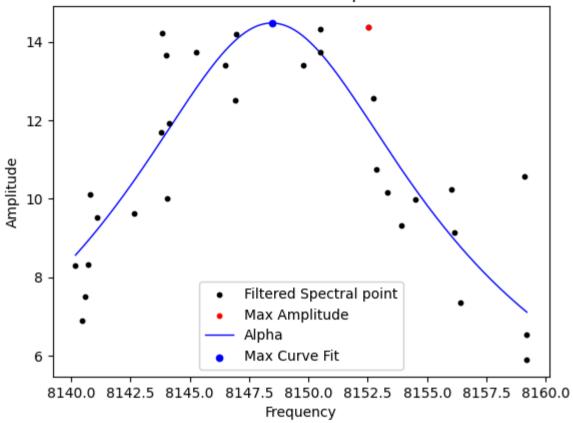
```
Out[16]: message: ['Maximum number of iteration reached']
success: True
status: 0
fun: 53.54144153462606
x: [ 8.148e+03 7.434e-04 2.153e-02]
nit: 1000
nfev: 6437
njev: 109
nhev: 0
```

Using Differencial Evolution

```
In [17]: 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
```

Differential Evolution Optimization



Optimized Parameters:

Resonant Frequency: 8148.45804766124
Damping Coefficient: 0.0007434644794704813

Force Amplitude: 0.02152990400035095 Resonant Amplitude: 14.479437222571885 Objective Function Value: 53.56531877262423

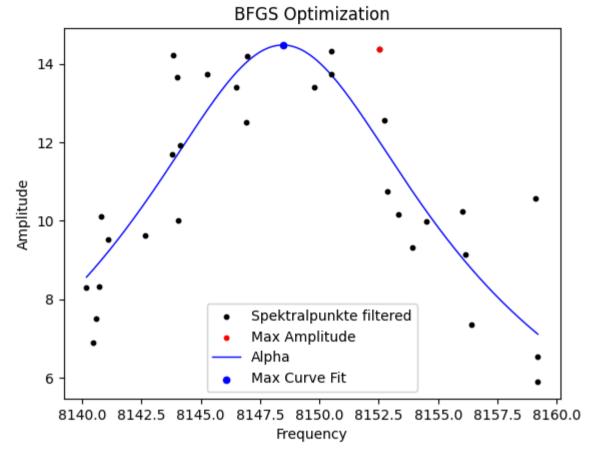
Using Local Optimizers

Using BFGS

```
In [18]: 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_1193528/996043608.py:1: OptimizeWarning: Unknown solver options: 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[18]:    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	Observations
Dual Annealing	Global	53.54144153462606	6437	1000	Achieves the best objective function value indicating a global optimum but requires the highest number of evaluations, making it less efficient computationally.
DifferntialEvolution	Global	53.54938461678095	2012	43	Provides a near-optimal solution with significantly fewer evaluations compared to Dual Annealing, making it a more computationally efficient global optimizer.
Nelder Mead	local	53.54144061205875	169	93	Achieves a near-optimal solution with the fewest evaluations, indicating high efficiency as a local optimizer.
L-BFGS-B	local	53.54144117175894	188	28	Quickly converges to a local optimum with a low number of evaluations and the fewest iterations , highlighting its efficiency in finding local optima.

In []:

Optimization of 2nd Data Frame

Using Global Optimizers

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

```
In [21]: 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 [22]: 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

Out[20]: 23

```
In [23]: min_Oerr = min(df2["J"])
max_Oerr = max(df2["J"])
```

```
In [24]: bounds = [(min_Oerr, max_Oerr), (0, 0.03), (0, 1)]
```

Then we define the objective function

options=options)

```
In [25]: 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 [26]: 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

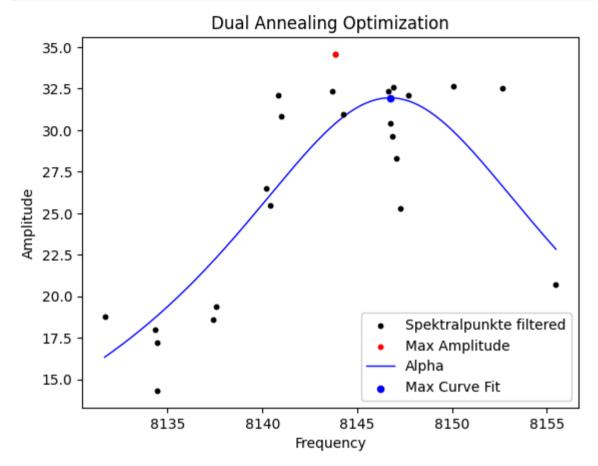
```
/tmp/ipykernel 1193528/2959858538.py:1: OptimizeWarning: Unknown solver options: maxfun, ftol, xtol, stepmx, eta, gtol
           result = minimize(
In [29]: # map optimized values to variables
         resonant frequency = result.x[0]
         D = result.x[1]
         F = result.x[2]
         # 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
                message: Optimization terminated successfully.
Out[29]:
                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 [30]: 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

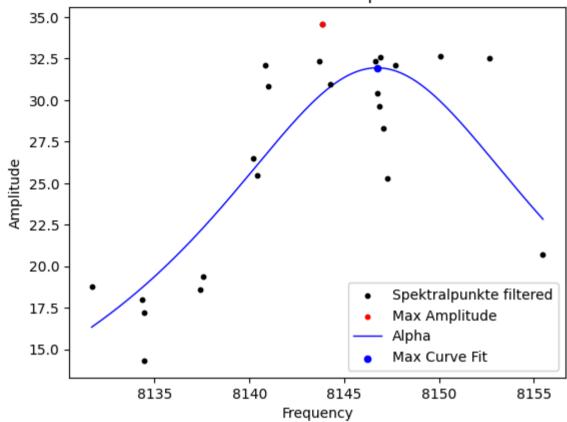
Resonant Amplitude: 31.94467402394625 Objective Function Value: 229.4092694161751

Using Differencial Evolution

```
In [31]: 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
```

Differential Evolution Optimization



Optimized Parameters:

Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854

Force Amplitude: 0.07020956698446057 Resonant Amplitude: 31.94467402394625

Objective Function Value: 229.4192718479083

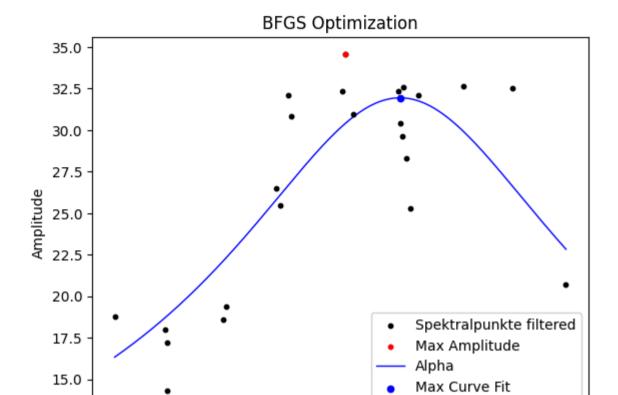
Using Local Optimizers

Using BFGS

```
In [32]: 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_1193528/2860355532.py:1: OptimizeWarning: Unknown solver options: xtol, stepmx, eta
result = minimize(
```



8140

8145

Frequency

8150

8155

Optimized Parameters:

Resonant Frequency: 8146.746051852071
Damping Coefficient: 0.0010989248372497854

8135

Force Amplitude: 0.07020956698446057 Resonant Amplitude: 31.94467402394625

Objective Function Value: 229.4092692624839

```
Out[32]: 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	Observations
Dual Annealing	Global	229.4092694161751	6181	1000	Finds the optimal solution with the highest number of evaluations and iterations.
DifferntialEvolution	Global	229.4192718479083	1778	37	Achieves a near-optimal solution with fewer evaluations and iterations compared to dual annealing.
Nelder Mead	Local	229.4092648339145	239	135	Efficiently converges to a near-optimal solution with minimal evaluations and iterations.
L-BFGS-B	local	229.4092692624839	180	45	Quickly reaches the optimal solution with the least number of evaluations and a moderate number of iterations.

Conclusion

The selection of an optimizer depends on the specific requirements of the problem at hand:

For Global Optimization: Dual Annealing achieves the best global optimum but is computationally expensive, while Differential Evolution provides a good balance between solution quality and computational efficiency.

For Local Optimization: Nelder-Mead is highly efficient in terms of evaluations, making it suitable for scenarios where computational resources are limited. L-BFGS-B is the fastest in terms of iterations, making it ideal for problems where quick convergence is critical.

The selection of an optimizer depends on the specific requirements of the problem.