

NMR

October 9, 2023

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[1]: import numpy as np
import pandas as pd
import sympy as sm
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit
from matplotlib_inline.backend_inline import set_matplotlib_formats
plt.style.use('seaborn-v0_8')
plt.rcParams |= {
    'text.usetex': True,
    'figure.figsize': (10, 4)
}
set_matplotlib_formats('svg', 'pdf')
```

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[2]: def smooth_data(data, window_size):
    return data.rolling(window=window_size, min_periods=1).mean()

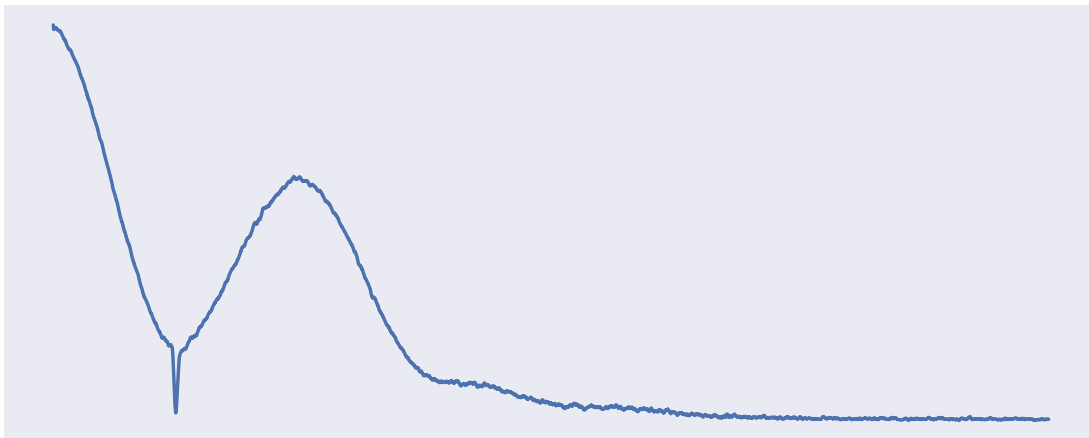
# Function for the decay exponential
def decay_func(t, A, k, C):
    return A * np.exp(-k * t) + C

t = sm.symbols('t')
def decay_func_sm(t, A, k, C):
    return A * sm.exp(-k * t) + C
```

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[3]: df = pd.read_csv('/Users/ammammar-imac/Documents/NMR/tek0004CH1H_OSE.csv')
df = df[19:]
df.columns = ['TIME', 'CH1']
```

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[4]: val = np.argmax(df.CH1)
plt.plot(df.TIME.iloc[val:], smooth_data(df.CH1.iloc[val:], 20))
plt.xticks([])
plt.yticks([])
plt.title("Decay fit for spin-echo and the original relaxation time for pure_↵water")
plt.show()
```

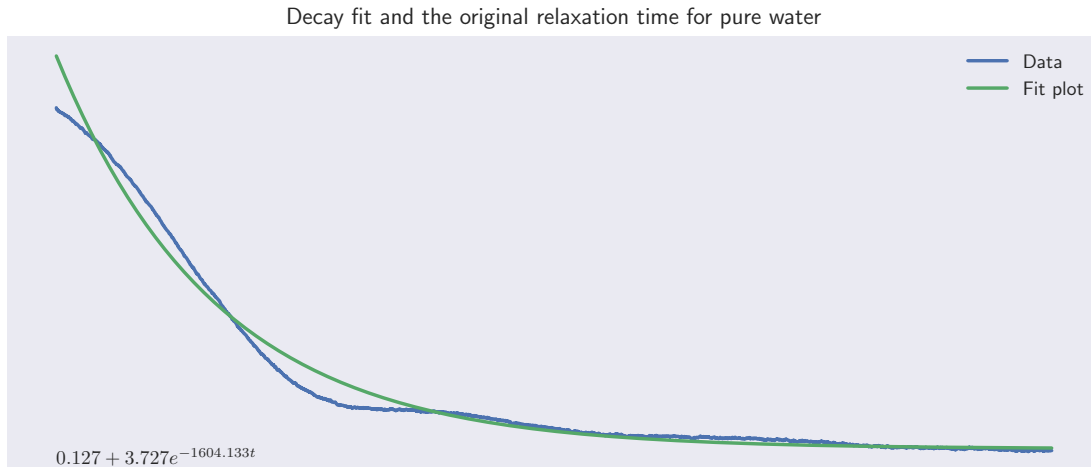
Decay fit for spin-echo and the original relaxation time for pure water



```
[5]: df = pd.read_csv('/Users/ammamr-imac/Downloads/NMR/tek0008ALLLLLLLL.csv')
df = df[19:]
df.columns = ['TIME', 'CH1']
val = np.argmax(df.CH1)
t_data = df.TIME.iloc[val:].astype(float)
y_data = smooth_data(df.CH1.iloc[val:], 50).astype(float)
params, covariance = curve_fit(decay_func, t_data, y_data)

[6]: plt.plot(df.TIME.iloc[val:], smooth_data(df.CH1.iloc[val:], 10), label='Data')
plt.plot(
    df.TIME.iloc[val:], decay_func(df.TIME.iloc[val:].astype(float), *params),
    label='Fit plot'
)

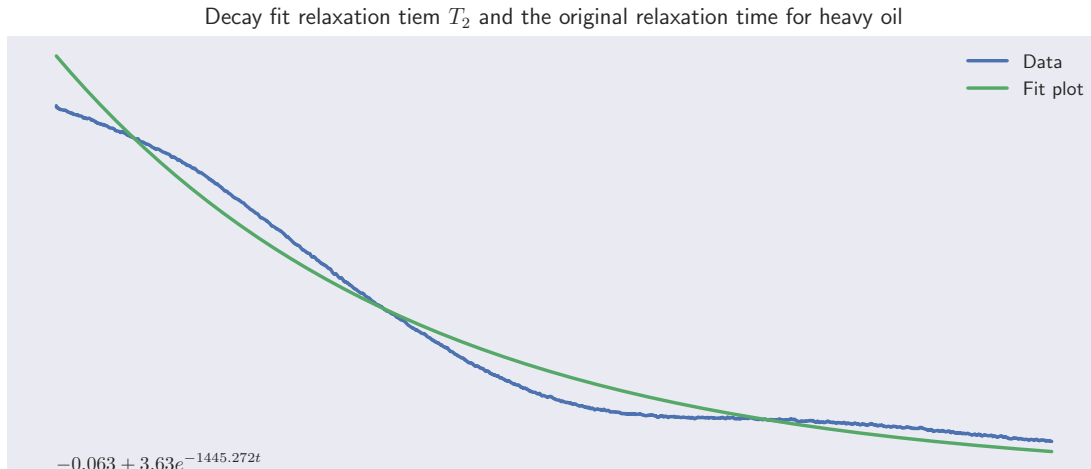
plt.xticks([])
plt.yticks([])
plt.text(0, 0, sm.latex(decay_func_sm(t, *[round(val, 3) for val in params])),
    mode='inline'))
plt.title("Decay fit and the original relaxation time for pure water")
plt.legend()
plt.show()
```



```
[7]: df = pd.read_csv('/Users/ammamr-imac/Documents/NMR/tek0001CH1.csv')
df = df[19:]
df.columns = ['TIME', 'CH1']
val = np.argmax(df.CH1)
t_data = df.TIME.iloc[val:].astype(float)
y_data = smooth_data(df.CH1.iloc[val:], 50).astype(float)
params, covariance = curve_fit(decay_func, t_data, y_data)
```

```
[8]: val = np.argmax(df.CH1)
plt.plot(df.TIME.iloc[val:], smooth_data(df.CH1.iloc[val:], 10), label='Data')
plt.plot(
    df.TIME.iloc[val:], decay_func(df.TIME.iloc[val:].astype(float), *params),
    label='Fit plot'
)

plt.xticks([])
plt.yticks([])
plt.text(0, 0, sm.latex(decay_func_sm(t, *[round(val, 3) for val in params])),
    mode='inline')
plt.title("Decay fit relaxation time $T_2$ and the original relaxation time for
    heavy oil")
plt.legend()
plt.show()
```



```
[9]: df = pd.read_csv('/Users/ammammar-imac/Documents/NMR/tek0009CHWSSS1.csv')
df = df[19:]
df.columns = ['TIME', 'CH1']
# fit plot
val = np.argmax(df.CH1)
t_data = df.TIME.iloc[val:].astype(float)
y_data = smooth_data(df.CH1.iloc[val:], 50).astype(float)
params, covariance = curve_fit(decay_func, t_data, y_data)
```

```
[10]: val = np.argmax(df.CH1)
plt.plot(df.TIME.iloc[val:], smooth_data(df.CH1.iloc[val:], 10),
         label='Data')
plt.plot(
    df.TIME.iloc[val:], decay_func(df.TIME.iloc[val:].astype(float), *params),
    label='Fit decay'
)

plt.xticks([])
plt.yticks([])
plt.text(0, 0, sm.latex(decay_func_sm(t, *[round(val, 3) for val in params])),
        mode='inline'))
plt.title("Decay fit for relaxation time  $T_2$  for salt water")
plt.legend()
plt.show()
```

Decay fit for relaxation time T_2 for salt water

