Data Fitting

Exercise 3

Comparison between Polynomial and Natural Cubic Spline Interpolation

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1 Introduction

An imaginary chemistry experiment produces the following data set:

x_i	-1	-0.96	-0.86	-0.79	0.22	0.50	0.93
f_i	-1.000	-0.151	0.894	0.986	0.895	0.500	-0.306

The purpose of this exercise is to use these data points to compute and plot the interpolating polynomial together with the natural cubic spline, and to report what it is observed. My hypothesis is that there may be an unsatisfactory oscillating behavior in the polynomial interpolant, whereas the natural cubic spline will be stiffer with less tendency to oscillate because it is a piece-wise type of interpolation.

2 Tools

The following programming language and libraries have been used in this exercise:

- Python 3.7
- SciPy

The SciPy `interpolate` sub-package was used to compute the interpolating polynomial and the natural cubic spline:

- `scipy.interpolate.lagrange(x, y)`
- `scipy.interpolate.CubicSpline(x, y, bc_type)`

The following NumPy methods of the SciPy environment have been used in this exercise:

- `numpy.array(object)`
- `numpy.linspace(start, stop, num)`
- `numpy.polynomial.polynomial.Polynomial(poly)`
- `numpy.setprint_options(precision)`

The following Matplotlib methods of the SciPy environment have been used in this exercise to plot:

- `matplotlib.pyplot.plot(x, y, formatting, label)`
- `matplotlib.pyplot.legend()`
- `matplotlib.pyplot.show()`
- `matplotlib.pyplot.figure(dpi)`
- `matplotlib.pyplot.ylim(miny, maxy)`
- `matplotlib.pyplot.xlabel(name)`
- `matplotlib.pyplot.ylabel(name)`

3 Computation and plotting

The exercise asks to compute the interpolating polynomial of the given data set. To do so, I first create two arrays in Python containing the data points using `np.array` and a linear space from -1 to 1 containing 1000 points. These values are finally passed to the `lagrange` method which returns the *Lagrange* interpolating polynomial (`poly = lagrange(x, y)`).

The following are coefficients the interpolating polynomial retrieved with `Polynomial(poly).coef`:

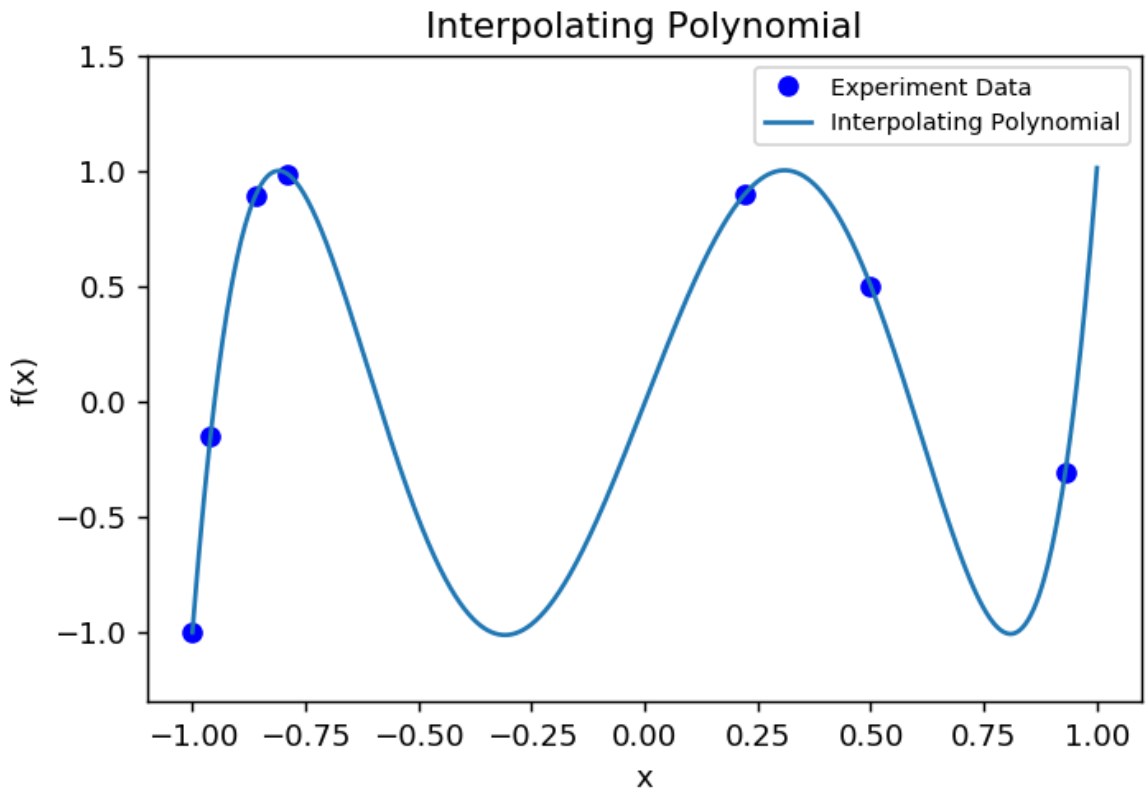
- 4.3649939020826437e-02
- 1.6076695441034385e+01
- -4.8402059220598259e-02
- -2.0100476671430044e+01
- 1.6880653327119008e-02
- 5.0294636999940936e+00
- -6.4460635283115466e-03

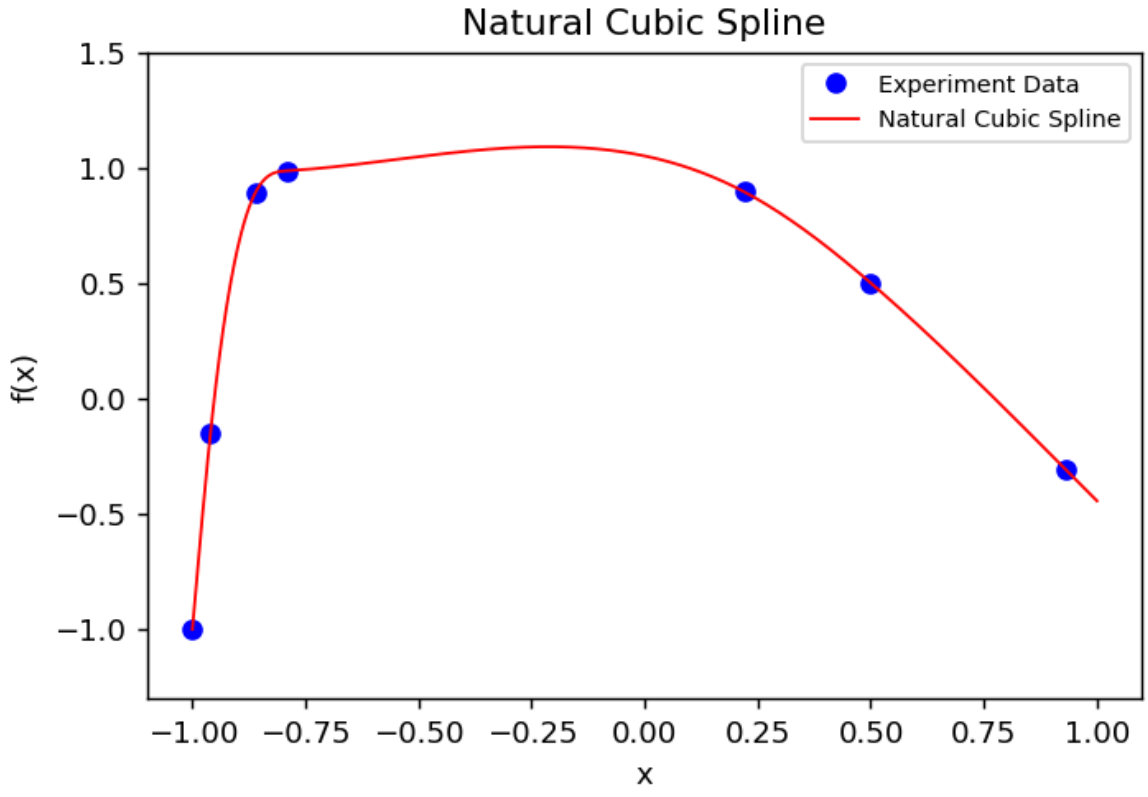
The polynomial of the 6th degree in the *power* form is:

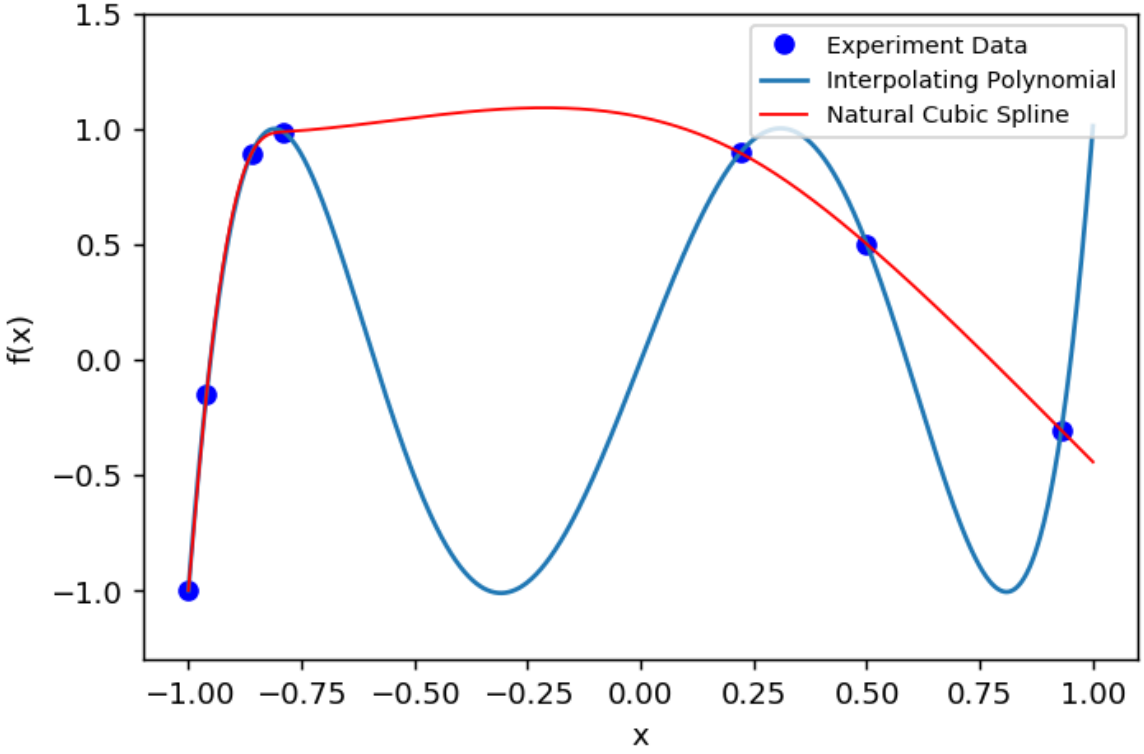
$$0.04365005085x^6 + 16.0766955610565x^5 - 0.048402197837630x^4 - 20.10047681678335740x^3 + 0.016880699153672132 0x^2 + 5.029463735952404423200x - 0.006446071786954468800$$

In order to calculate the natural cubic spline I use the built-in SciPy method `CubicSpline(x, y, bc_type)` and use "Natural" for the `bc_type`. The coefficients are the following:

[[−8.0654538905002710e+021.4844899135604635e+022.5130673577722442e+02−7.2398801257531864e−011.2138819568393451e+005.0415317855085340e−01][−8.5265128291212022e−14−9.6785446686003496e+01−5.2250749279189527e+015.2366523402757015e−01−1.6700184440756460e+00−6.5035760033060053e−01][2.2515472622480029e+011.8644054755039885e+013.7404351585205808e+001.1953927535924665e−01−1.0382774667893093e+00−1.6879827592230572e+00][−1.0000000000000000e+00−1.5100000000000000e−018.9400000000000002e−019.8599999999999999e−018.9500000000000002e−015.0000000000000000e−01]]


Interpolating Polynomial
Experiment Data
Interpolating Polynomial
f(x)
x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


Natural Cubic Spline
Experiment Data
Natural Cubic Spline
f(x)
x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00


Experiment Data
Interpolating Polynomial
Natural Cubic Spline
f(x)
x
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

4 Observations

The natural cubic spline is a much more accurate representation than the *Lagrange* function which appears inconsistent with several *ups and downs*.

Since the natural cubic spline is a type of piece-wise interpolation, the graph passes through the experiment data points with low-degree polynomials. Since we only use low-degree polynomials, we eliminate the excessive oscillations that are present in the interpolating polynomial.