E31

November 14, 2022

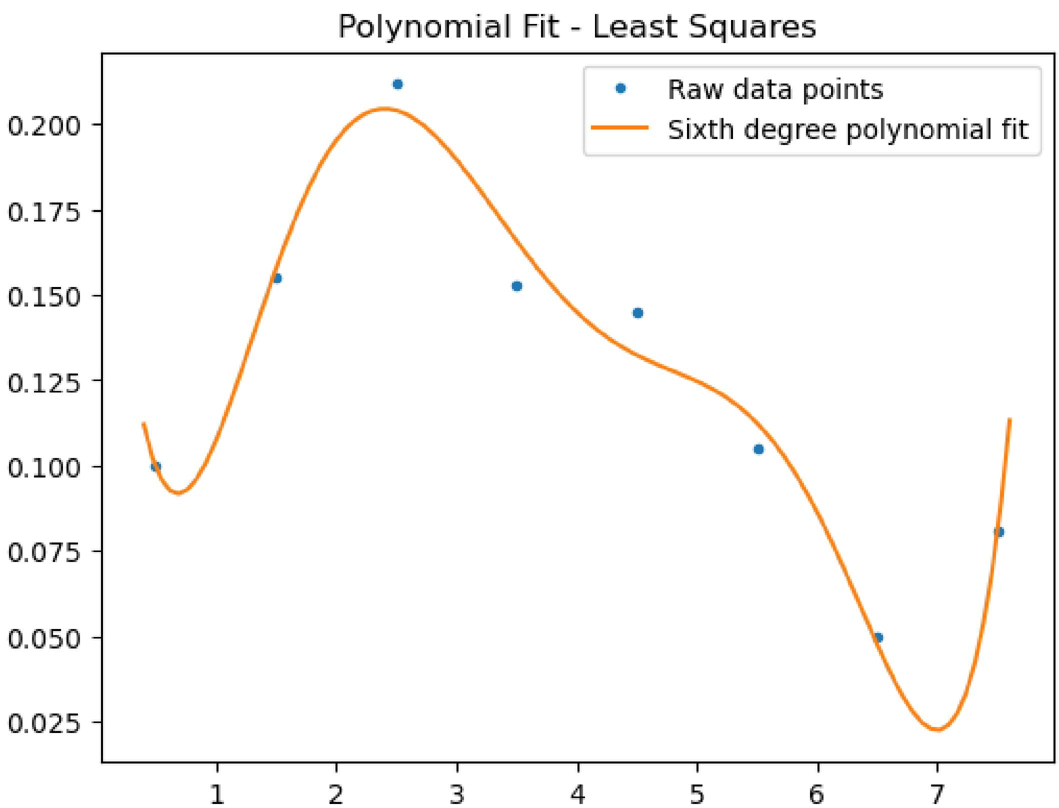
1 Exercise 31 - *Regularized Least Squares*

A colleague has measured a distribution. This distribution becomes part of a Monte Carlo simulation. To be able to work better with this distribution| you look for a suitable parameterization. You know that the distribution can be well described by a sixth-degree polynomial. However, the measurement is very noisy and your colleague was also only able to take eight pairs of values (x, y).

a) Fit a sixth degree polynomial to the data in the file `ex_a.csv` using the least squares method. State the resulting coefficients and plot the fitted polynomial and data.

[1]:
```
import numpy as np
import matplotlib.pyplot as plt
from numpy.linalg import inv, pinv
```

[2]:
```
x, y = np.genfromtxt('ex_a.csv', unpack=True, delimiter=',', skip_header=1)

def xn(x,n):
    return x**n



# design matrix
A = []
for i in range(7): A.append(xn(x,i))
A = np.array(A).T

# solution (coefficient) vector for least squares (weight matrix = unit matrix)
a = pinv(A.T@A)@A.T@y

x_ = np.linspace(x[0]-0.1, x[-1]+0.1, 100)
plt.plot(x,y, '.')
plt.plot(x_, np.polyval(np.flip(a), x_))     # coefficient vector in reverse␣
↪order for polyval-function
plt.legend(["Raw data points","Sixth degree polynomial fit"])
plt.title("Polynomial Fit - Least Squares")
plt.show()
```



Solution: The coefficients are

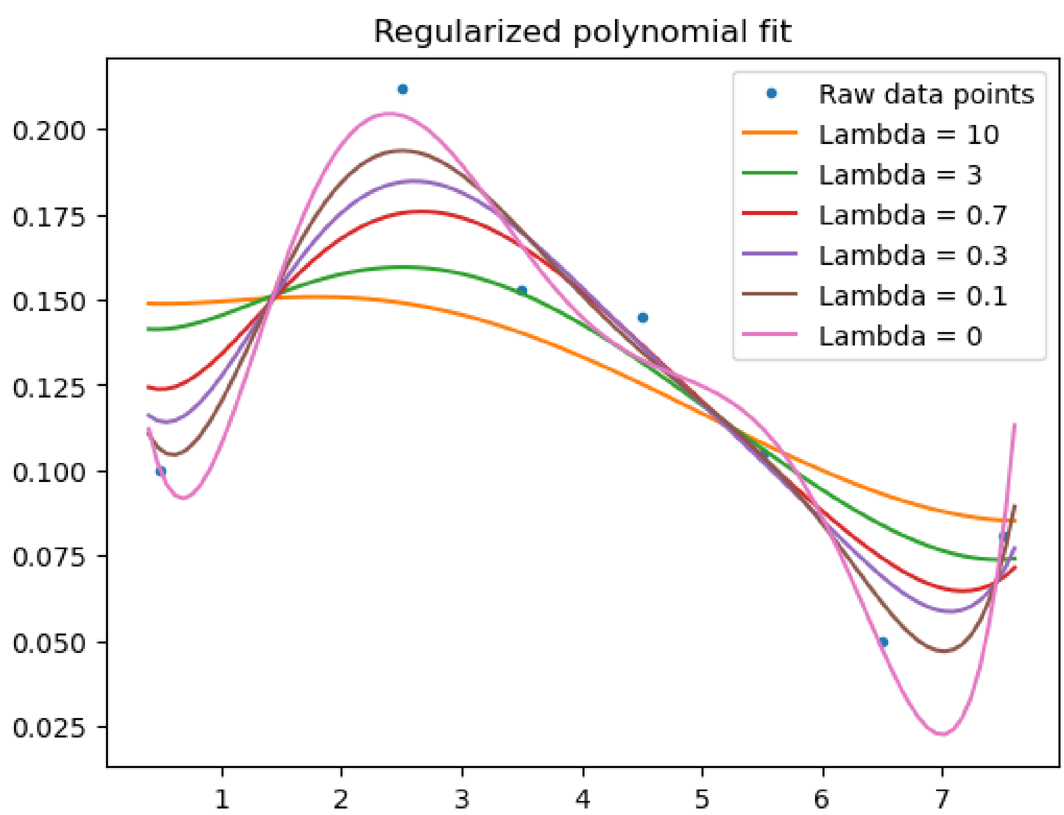
p_0	p_1	p_2	p_3	p_4	p_5	p_6
3.55e-04	-8.41e-03	7.69e-02	-3.37e-01	7.03e-01	-5.78e-01	2.50e-01

b) Fit a sixth degree polynomial to the data in the file `ex_a.csv` using the least squares method and additionally use the regularization via the second derivative ($\Gamma = \sqrt{\lambda} CA$). For the regularization strength use $\lambda \in (0.1, 0.3, 0.7, 3, 10)$. State the resulting coefficients and plot the fitted polynomial and the data.

We use $C = \begin{pmatrix} -1 & 1 & 0 & 0 & \cdots \\ 1 & -2 & 1 & 0 & \cdots \\ 0 & 1 & -2 & 1 & \cdots \\ \cdots & \cdots & 1 & -2 & 1 \\ \ldots & \cdots & \cdots & 1 & -1 \end{pmatrix}$.

[3]:
```
lam = [.1,.3,.7,3,10]
C = np.matrix([[-1,1,0,0,0,0,0,0],[1,-2,1,0,0,0,0,0],[0,1,-2,1,0,0,0,0],
               [0,0,1,-2,1,0,0,0],[0,0,0,1,-2,1,0,0],[0,0,0,0,1,-2,1,0]
             ,[0,0,0,0,0,1,-2,1],[0,0,0,0,0,0,1,-1]],dtype = "float64")
```

```
def reg(l):
    return inv(A.T@A + l*(C@A).T@(C@A))@A.T@y

a_reg = []
for i in range(len(lam)):
    a_reg.append(reg(lam[i]))


plt.plot(x,y, '.')
for i in range(len(lam)): plt.plot(x_, np.polyval(np.flip(a_reg)[i][0],x_))  #␣
↪a_reg is a matrix in a list, which results in tedious index management
plt.plot(x_, np.polyval(np.flip(a), x_))
plt.legend(["Raw data points", "Lambda = 10", "Lambda = 3", "Lambda = 0.7",␣
↪"Lambda = 0.3", "Lambda = 0.1", "Lambda = 0"])
plt.title("Regularized polynomial fit")
plt.show()
```



[4]:
```
print(a_reg)
```

```
[matrix([[ 1.77051516e-01, -2.90333213e-01,  3.75360675e-01,
         -1.77608015e-01,  3.94217777e-02, -4.20777821e-03,
          1.74225695e-04]]), matrix([[ 1.50746121e-01, -1.58077312e-01,
2.14314526e-01,
         -9.84996477e-02,  2.09125853e-02, -2.14507244e-03,
          8.61849490e-05]]), matrix([[ 1.42748957e-01, -8.72516595e-02,
1.22823253e-01,
         -5.43579871e-02,  1.09108334e-02, -1.06390109e-03,
          4.11723873e-05]]), matrix([[ 1.46435271e-01, -2.53253819e-02,
3.71732498e-02,
         -1.54747235e-02,  2.73169706e-03, -2.34332199e-04,
          8.27195513e-06]]), matrix([[ 1.50592612e-01, -8.00760585e-03,
1.09496192e-02,
         -4.81350343e-03,  7.81637373e-04, -5.87060020e-05,
          1.85143060e-06]])]
```

Table with regularized coefficients

	a_0	a_1	a_2	a_3	a_4	a_5	a_6
$\lambda = 0.1$	1.77e-01	-2.90e-01	3.75e-01	-1.77e-01	3.94e-02	-4.20e-03	1.74e-04
$\lambda = 0.3$	1.50e-01	-1.58e-01	2.14e-01	-9.84e-02	2.09e-02	-2.14e-03	8.61e-05
$\lambda = 0.7$	1.42e-01	-8.72e-02	1.22e-01	-5.43e-02	1.09e-02	-1.06e-03	4.11e-05
$\lambda = 3$	1.46e-01	-2.53e-02	3.71e-02	-1.54e-02	2.73e-03	-2.34e-04	8.27e-06
$\lambda = 10$	1.50e-01	-8.00e-03	1.09e-02	-4.81e-03	7.81e-04	-5.87e-05	1.85e-06

Your colleague makes the effort to produce 50 new measurements of the spectrum.

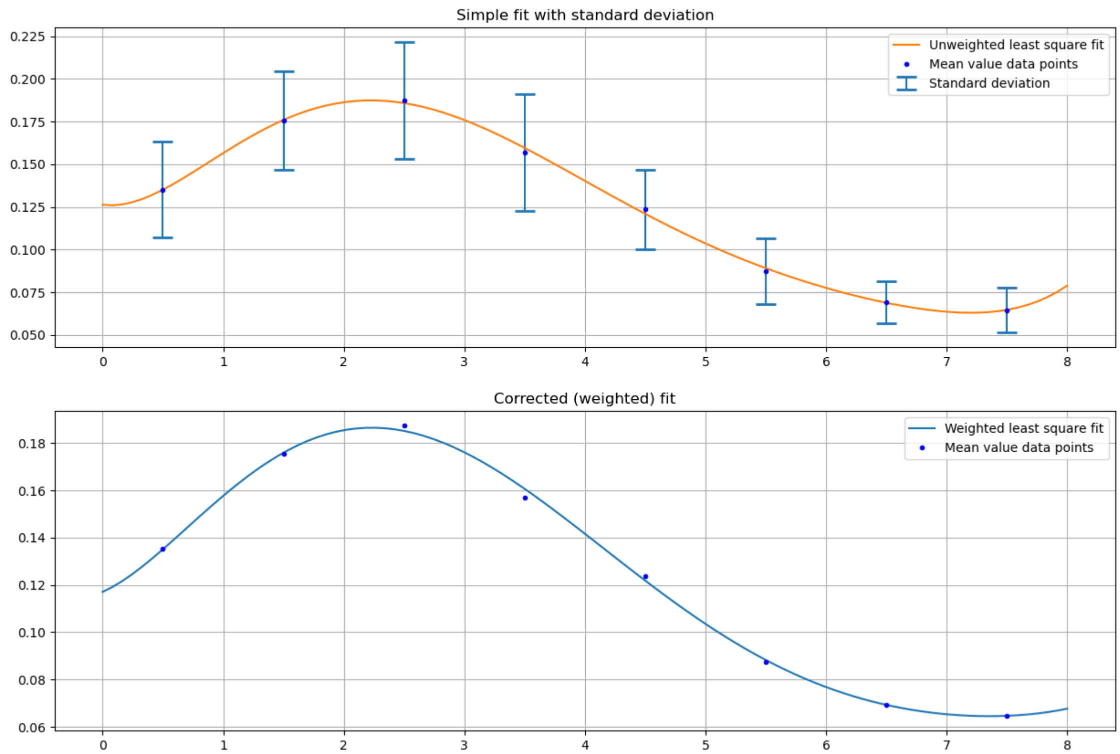
(c) Fit a sixth degree polynomial to the mean values of the data from the file ex_c.csv using the least squares method. Weight the calculated means with the uncertainty of the mean. Use these weights when fitting. Plot the fitted polynomial and the averaged data.

[5]:
```
data = np.genfromtxt('ex_c.csv', unpack=True, delimiter=',', skip_header=1)
x = data[0]
y = data[1:]
y = y.T  #the index now corresponds to the respective y_i

y_m = np.mean(y, axis=1)
y_s = np.std(y, axis=1)
```

We introduce the weight matrix $\mathbf{W}[\mathbf{y}] = \mathrm{Var}[\mathbf{y}]^{-1} = \begin{pmatrix} \frac{1}{\sigma_0^2} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sigma_1^2} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & \frac{1}{\sigma_n^2} \end{pmatrix}$

to get the general solution of the weighted least squares $\hat{a} = \left(A^\top W A\right)^{-1} A^\top W y$.

[6]:
```
W = np.diag(1/(y_s)**2)

# new design matrix
A = []
for i in range(7): A.append(xn(x,i))
A = np.array(A).T

# general (weighted) solution (coefficient vector)
a = pinv(A.T@W@A)@A.T@W@y_m

# for comparison: least squares without weights
p = np.polyfit(x, y_m, 6)

x_ = np.linspace(0,8,100)

fig, ax = plt.subplots(2, figsize=(15,10))
ax[0].grid()
ax[0].errorbar(x, y_m, yerr=y_s, capsize=8, lw=0, elinewidth=1.5, capthick=2)
ax[0].plot(x_, np.polyval(p, x_))     # least squares without weights
ax[0].plot(x, y_m, 'b.')
ax[0].legend(["Unweighted least square fit","Mean value data points", "Standard␣
↪deviation"])
ax[0].set_title("Simple fit with standard deviation")

ax[1].grid()
ax[1].plot(x_, np.polyval(np.flip(a), x_))
ax[1].plot(x, y_m, 'b.')
ax[1].set_title("Corrected (weighted) fit")
ax[1].legend(["Weighted least square fit","Mean value data points"])
plt.show()
```



Error bars represent the *(square-rooted)* reciprocal magnitude of the weights.

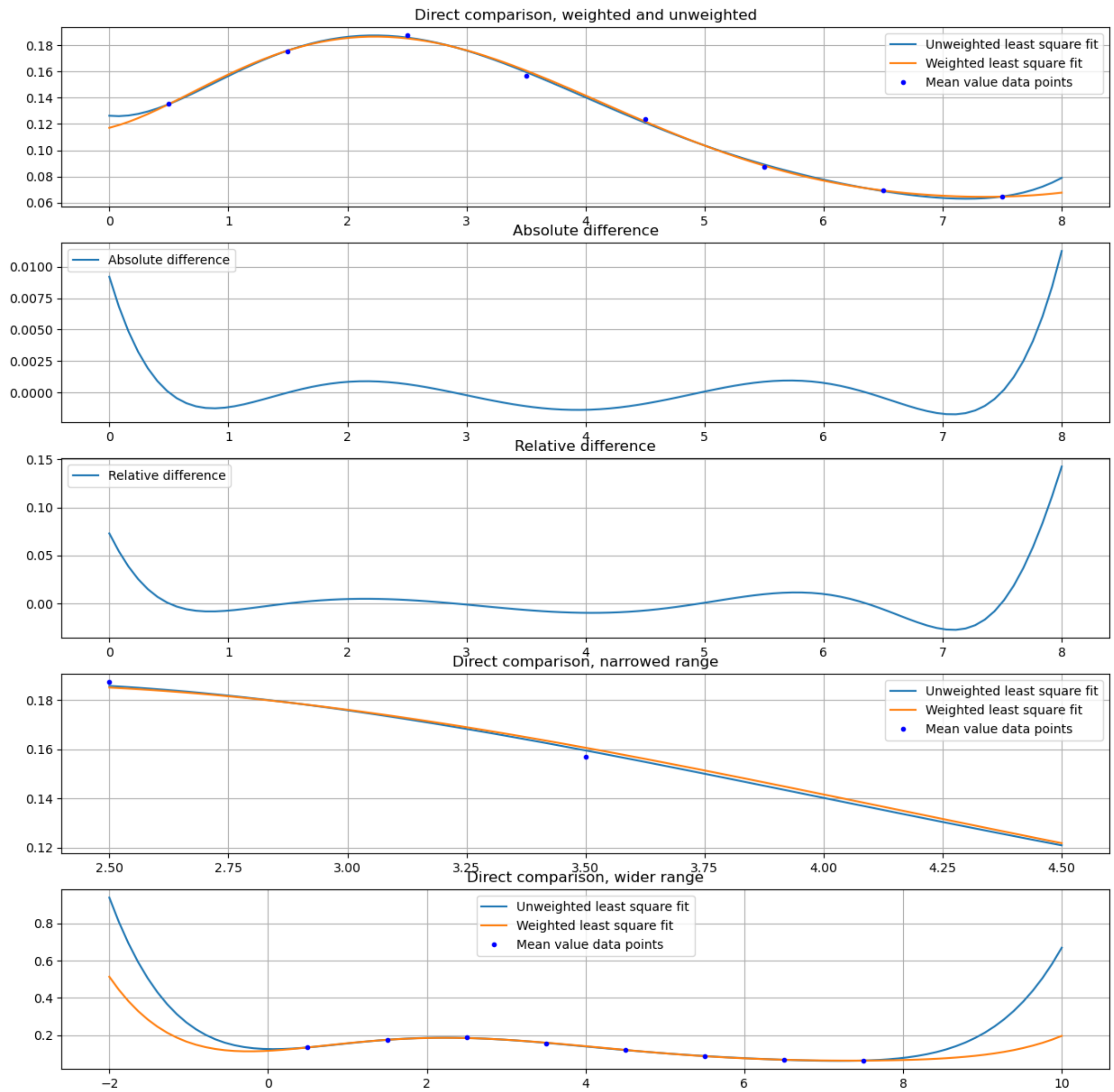
The two graphs are very similar. For comparison we calculate the absolute and relative deviation.

Absolute: $\Delta y(x) = y_u(x) - y_w(x) =: y_{abs}(x)$ with - y_u : *unweighted least squares* and - y_w : *weighted least squares*.

Relative: $\Delta \bar{y}(x) = \frac{y_u(x)-y_w(x)}{y_u(x)} =: y_{rel}(x)$

[7]:
```
fig, ax = plt.subplots(5, figsize=(15,15))
ax[0].plot(x_, np.polyval(p, x_))      # least squares without weights
ax[0].plot(x_, np.polyval(np.flip(a), x_))
ax[0].plot(x, y_m, 'b.')
ax[0].legend(["Unweighted least square fit", "Weighted least square fit","Mean␣
 ↪value data points"])
ax[0].set_title("Direct comparison, weighted and unweighted")
ax[0].grid()

ax[1].plot(x_, np.polyval(p, x_)-np.polyval(np.flip(a), x_))
ax[1].legend(["Absolute difference"])
ax[1].set_title("Absolute difference")
ax[1].grid()

ax[2].plot(x_, (np.polyval(p, x_)-np.polyval(np.flip(a), x_))/np.polyval(p, x_))
```

```python
ax[2].legend(["Relative difference"])
ax[2].set_title("Relative difference")
ax[2].grid()

x_s = np.linspace(2.5,4.5,100)
ax[3].plot(x_s, np.polyval(p, x_s))     # least squares without weights
ax[3].plot(x_s, np.polyval(np.flip(a), x_s))
ax[3].plot(x[2:4], y_m[2:4], 'b.')
ax[3].legend(["Unweighted least square fit", "Weighted least square fit","Mean␣
 ↪value data points"])
ax[3].set_title("Direct comparison, narrowed range")
ax[3].grid()

x__ = np.linspace(-2,10,100)
ax[4].plot(x__, np.polyval(p, x__))     # least squares without weights
ax[4].plot(x__, np.polyval(np.flip(a), x__))
ax[4].plot(x, y_m, 'b.')
ax[4].legend(["Unweighted least square fit", "Weighted least square fit","Mean␣
 ↪value data points"])
ax[4].set_title("Direct comparison, wider range")
ax[4].grid()
plt.show()
```



In the range of the data points, the relative deviation of the two polynomial fits (weighted and unweighted least squares) is not greater than 2.5%.

For a wider range of x-values we notice a dampened divergence towards infinity.

It is also noticeable that the *weighted least squares*-method doesn't necessarily guarantee a fit that is closer to the data points. It is rather smoothed out like the methods used previously.