

```
In [97]: %matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import pandas as pd
from IPython.display import display
```

Curve Fitting

17.4 Use least-squares regression to fit a straight line to

x	6	7	11	15	17	21	23	29	29	37	39
y	29	21	29	14	21	15	7	7	13	0	3

Along with the slope and the intercept, compute the standard error of the estimate and the correlation coefficient. Plot the data and the regression line. If someone made an additional measurement of $x = 10$, $y = 10$, would you suspect, based on a visual assessment and the standard error, that the measurement was valid or faulty? Justify your conclusion.

given a set of n points X and Y we can form the linear fit line using:

$$a_1 = \frac{n \sum xy - \sum y \sum x}{n \sum x^2 - (\sum x)^2}$$

$$a_0 = \frac{\sum y - a_1 \sum x}{n}$$

A)

```
In [98]: """
Using Pandas dataframes, Set a dataframe "df" to hold:
X: x values
Y: y values
XY: x*y values
Y2: Square of y values
X2: Square of x values
"""

#setup initial data dictionary
data = {"X": [6,7,11,15,17,21,23,29,29,37,39], "Y": [29,21,29,14,21,15,7,7,13,0,3]}

#turn the data to pandas df
df = pd.DataFrame(data)
```

```
#calculate other columns using numpy
X = df["X"].to_numpy()
Y = df["Y"].to_numpy()
XY = np.multiply(X,Y)
X2 = np.multiply(X,X)
Y2 = np.multiply(Y,Y)

#add the calculated columns to df
df["XY"] = XY
df["X2"] = X2
df["Y2"] = Y2
```

In [99]:

```
#function to calculate STD
def std_calc(x,y):
    return (y-a0-(a1*x))**2

#dataframe "Sums" that hold summation of columns from df
Sums = pd.DataFrame({"X":df["X"].sum(),
                    "Y":df["Y"].sum(),
                    "XY":df["XY"].sum(),
                    "X2":df["X2"].sum(),
                    "Y2":df["Y2"].sum()
                    })

#get n and calculate a1,a0 using the formulas
n=df.shape[0]
a1 = (n*Sums["XY"]-Sums["Y"]*Sums["X"])/(n*Sums["X2"]-Sums["X"]**2)
a0 = (Sums["Y"]-a1*Sums["X"])/(n)

#calculate squared error for y (SE_y)
df["SE_y"] = df["Y"].apply(lambda y: (y-df["Y"].mean())**2)
df["std_div"] = df.apply(lambda d: std_calc(d['X'], d['Y']), axis=1)

#calculate f(x) evaluation for every x point for plotting
df['f(x)'] = df['X'].apply(lambda x: a1*x+a0)

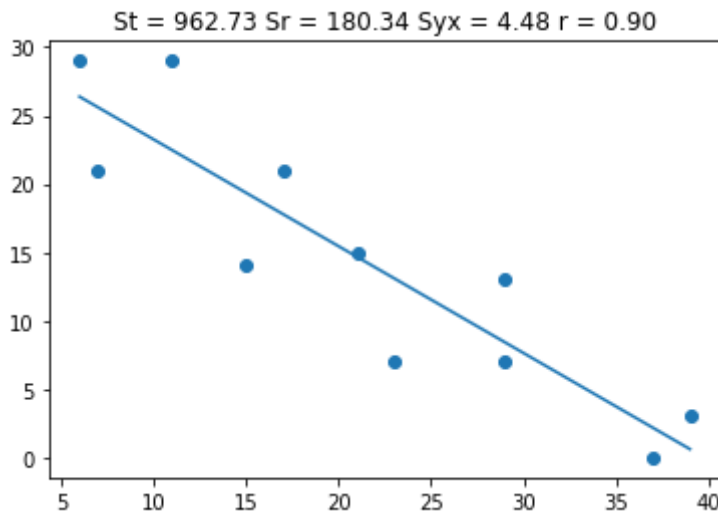
#calculation of measurements
St = df["SE_y"].sum()
Sr = df["std_div"].sum()
Syx = np.sqrt(Sr/(n-2))
r = np.sqrt((St-Sr)/St)
display(df)
```

	X	Y	XY	X2	Y2	SE_y	std_div	f(x)
0	6	29	174	36	841	211.570248	6.887373	26.375619
1	7	21	147	49	441	42.842975	21.114695	25.595073
2	11	29	319	121	841	211.570248	42.603206	22.472887
3	15	14	210	225	196	0.206612	28.629999	19.350701
4	17	21	357	289	441	42.842975	10.306618	17.789608
5	21	15	315	441	225	0.297521	0.110608	14.667422
6	23	7	161	529	49	55.570248	37.287251	13.106329
7	29	7	203	841	49	55.570248	2.025070	8.423050
8	29	13	377	841	169	2.115702	20.948474	8.423050
9	37	0	0	1369	0	208.933884	4.746636	2.178678

	X	Y	XY	X2	Y2	SE_y	std_div	f(x)
10	39	3	117	1521	9	131.206612	5.675903	0.617585

In [100...

```
#plotting
# (x,y) scatter plot
plt.scatter(df["X"],df["Y"])
# regression line plotting
plt.plot(df["X"],df["f(x)"])
# title with measurements, the ";" supresses unwanted output
plt.title(f"St = {St:0.2f} Sr = {Sr:0.2f} Syx = {Syx:0.2f} r = {r:0.2f}");
```



B)

Taking the measured values $x = 10$ and $y = 10$ we see that when x is subbed in $y = a_1x + a_0$ that we get $y = 23.253$.

Taking the absolute value difference between $y_{calculated}$ and $y_{measured}$ we get $|\Delta_y| = 13.253$.

$|\Delta_y|$ is greater that the Standard deviation, which we got to be $S_{x/y} = 4.48$, by approximately 2.9x **Therefore the measurement is likely to be wrong.**

17.9 Fit an exponential model to

x	0.4	0.8	1.2	1.6	2	2.3
y	800	975	1500	1950	2900	3600

Plot the data and the equation on both standard and semi-logarithmic graph paper.

Starting with:

$$y = \alpha_0 e^{(\alpha_1 x)}$$

Take natural log of both side:

$$\ln y = \ln \alpha_0 + \alpha_1 x$$

Taking

$$z = \ln y, a_0 = \ln \alpha_0, a_1 = \alpha_1$$

we get

$$z = xa_1 + a_0$$

using the same equation for linear fit to find a_0, a_1 then calculate α_0, α_1

In [101...

```

"""
Using Pandas dataframes, Set a dataframe "df" to hold:
X: x values
Y: y values
Z: natural log of y values
XZ: x*z values
X2: Square of x values
"""

#setup initial data dictionary
data = {"X":[0.4,0.8,1.2,1.6,2,2.3], "Y":[800,975,1500,1950,2900,3600]}

#turn the data to pandas df
df = pd.DataFrame(data)

#calculate other columns using numpy
X = df["X"].to_numpy()
Y = df["Y"].to_numpy()
df["Z"] = np.log(Y)
df["XZ"] = np.multiply(X, df["Z"])
df["X2"] = np.multiply(X, X)

#dataframe "Sums" that hold summation of columns from df
Sums = pd.DataFrame({"X": [df["X"].sum()],
                     "Y": [df["Y"].sum()],
                     "Z": [df["Z"].sum()],
                     "XZ": [df["XZ"].sum()],
                     "X2": [df["X2"].sum()]
                     })

#calculate linear constants
n=df.shape[0]
a1 = (n*Sums["XZ"]-Sums["Z"]*Sums["X"])/(n*Sums["X2"]-Sums["X"]**2)
a0 = (Sums["Z"]-a1*Sums["X"])/(n)

#find the exponential constants
alph0 = np.exp(a0)
alph1 = a1

#calculate f(x) evaluation for every x point for plotting
df['f(x)'] = df['X'].apply(lambda x : alph0 * np.exp(x*alph1))

#display the df table
display(df)

```

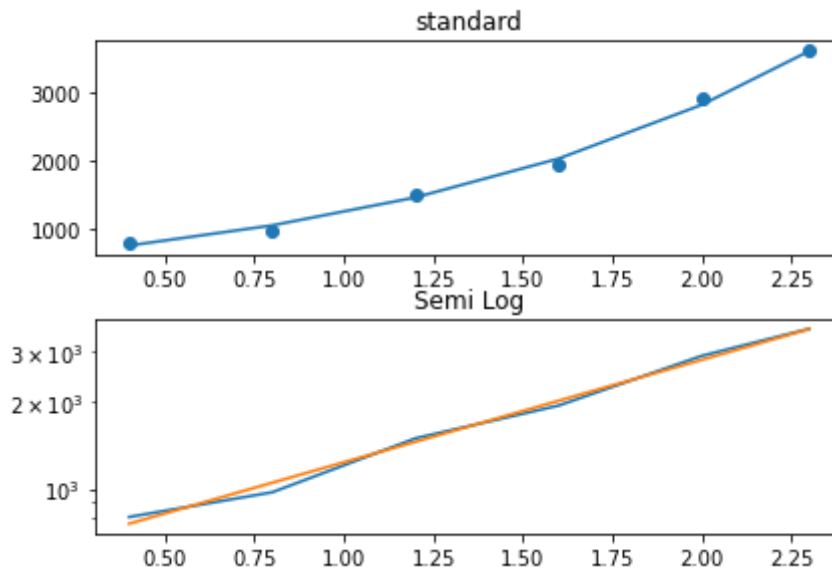
	X	Y	Z	XZ	X2	f(x)
0	0.4	800	6.684612	2.673845	0.16	758.362261
1	0.8	975	6.882437	5.505950	0.64	1052.182313
2	1.2	1500	7.313220	8.775864	1.44	1459.840075
3	1.6	1950	7.575585	12.120935	2.56	2025.440856

	X	Y	Z	XZ	X2	f(x)
4	2.0	2900	7.972466	15.944932	4.00	2810.178136
5	2.3	3600	8.188689	18.833985	5.29	3592.481694

In [102...

```
# Plotting
# init 2 plots
fig, (ax1, ax2) = plt.subplots(2)
fig.tight_layout()
# (x,y) scatter plot
ax1.scatter(df["X"],df["Y"])
ax2.semilogy(df["X"],df["Y"])
ax1.title.set_text("standard")

# regression line plotting
ax1.plot(df["X"],df["f(x)"])
ax2.semilogy(df["X"],df["f(x)"]);
ax2.title.set_text("Semi Log")
```



17.14 It is known that the data tabulated below can be modeled by the following equation

$$y = \left(\frac{a + \sqrt{x}}{b\sqrt{x}} \right)^2$$

Use a transformation to linearize this equation and then employ linear regression to determine the parameters a and b . Based on your analysis predict y at $x = 1.6$.

x	0.5	1	2	3	4
y	10.4	5.8	3.3	2.4	2

Take square root of both side:

$$\sqrt{(y)} = \frac{a + \sqrt{(x)}}{b\sqrt{(x)}}$$

Split the RHD fraction and simplify :

$$\frac{a + \sqrt{(x)}}{b\sqrt{(x)}} = \frac{a}{b\sqrt{(x)}} + \frac{\sqrt{(x)}}{b\sqrt{(x)}} = \frac{a}{b} \frac{1}{\sqrt{(x)}} + \frac{1}{b}$$

Putting all together:

$$\sqrt{(y)} = \frac{a}{b} \frac{1}{\sqrt{(x)}} + \frac{1}{b}$$

Taking

$$z = \sqrt{(y)}, w = \frac{1}{\sqrt{(x)}}, a_0 = \frac{1}{b}, a_1 = \frac{a}{b}$$

we get

$$z = wa_1 + a_0$$

In [103...

```

"""
Using Pandas dataframes, Set a dataframe "df" to hold:
X: x values
Y: y values
Z: sqrt(y) values
W: 1/sqrt(x) values
WZ: w*z values
W2: Squire of w values
"""

#setup initial data dictionary
data = {"X":[0.5,1,2,3,4], "Y":[10.4,5.8,3.3,2.4,2]}

#turn the data to pandas df
df = pd.DataFrame(data)

#calculate other columns using numpy
X = df["X"].to_numpy()
Y = df["Y"].to_numpy()
df["Z"] = np.sqrt(Y)
df["W"] = df["X"].apply(lambda x: 1/np.sqrt(x))
df["WZ"] = np.multiply(df["W"],df["Z"])
df["W2"] = np.multiply(df["W"],df["W"])

#dataframe "Sums" that hold summation of columns from df
Sums = pd.DataFrame({"X":[df["X"].sum()],
                    "Y":[df["Y"].sum()],
                    "Z":[df["Z"].sum()],
                    "W":[df["W"].sum()],
                    "WZ":[df["WZ"].sum()],
                    "W2":[df["W2"].sum()]
                    })

#calculate linear constants
n=df.shape[0]
a1 = (n*Sums["WZ"]-Sums["Z"]*Sums["W"])/(n*Sums["W2"]-Sums["W"]**2)
a0 = (Sums["Z"]-a1*Sums["W"])/(n)

```

```

#calculate f(x) evaluation for every x point for plotting
df['f(x)'] = df['W'].apply(lambda x: a1*x+a0)

#calculate a and b
b = 1/a0
a = a1*b

#calculate f(x) evaluation for every x point for plotting
df['f2(x)'] = df['X'].apply(lambda x: ((a+np.sqrt(x))/(b*np.sqrt(x)))**2)

# init 2 plots
fig, (ax1, ax2) = plt.subplots(2)
fig.tight_layout()

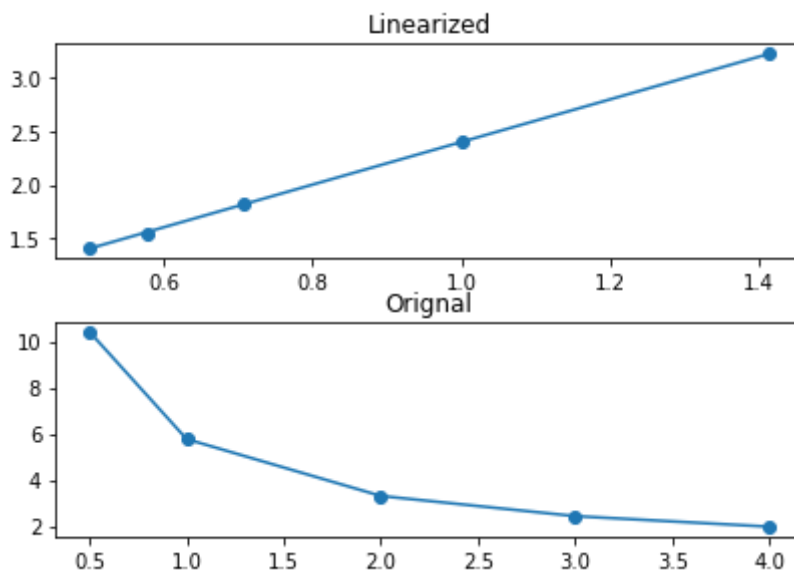
#Linear plot
# (x,y) scatter plot
ax1.scatter(df["W"],df["Z"])
# regression line plotting
ax1.plot(df["W"],df["f(x)"])
ax1.title.set_text("Linearized")

#original plot
# (x,y) scatter plot
ax2.scatter(df["X"],df["Y"])
# regression line plotting
ax2.plot(df["X"],df["f2(x)"])
ax2.title.set_text("Original")
display(df)
#find the prediction of x = 1.6
pred = lambda x:((a+np.sqrt(x))/(b*np.sqrt(x)))**2
print(f"the prediction of x = 1.6 is: \nf(1.6) = {float(pred(1.6)):.4f}")

```

	X	Y	Z	W	WZ	W2	f(x)	f2(x)
0	0.5	10.4	3.224903	1.414214	4.560702	2.000000	3.227079	10.414040
1	1.0	5.8	2.408319	1.000000	2.408319	1.000000	2.401914	5.769189
2	2.0	3.3	1.816590	0.707107	1.284523	0.500000	1.818433	3.306700
3	3.0	2.4	1.549193	0.577350	0.894427	0.333333	1.559942	2.433419
4	4.0	2.0	1.414214	0.500000	0.707107	0.250000	1.405851	1.976416

the prediction of x = 1.6 is:
 $f(1.6) = 3.9390$



Interpolation

In [104...

```
#method to calculate the fdd table
def fdd_table(X, Y):
    n = len(X)
    fdd_table= [[None for x in range(n)] for x in range(n)]

    #set initial column with given data
    for i in range(n):
        fdd_table[i][0]=Y[i]
    # calculate the fdd table
    for i in range(1,n):
        for j in range(n-i):
            fdd_table[j][i]=(fdd_table[j+1][i-1]-fdd_table[j][i-1])/(X[i+j]-X[j])

    #return fdd table as dataframe
    return pd.DataFrame(fdd_table)

def Newt_interpolate(X,Y,x_new,coeff):
    #initial values for the computational loop
    n = len(X)
    xterm = 1
    error = [None for _ in range(n)]
    iteration_res = [None for _ in range(n)]
    iteration_res[0] = coeff[0]

    #loop for newtown polynomial in order
    for i in range(1,n):
        xterm = xterm*(x_new - X[i-1])
        iteration_res[i] = iteration_res[i-1]+coeff[i]*xterm
        # error is the diffrence between the previous and current iteration
        error[i-1]=abs(iteration_res[i]-iteration_res[i-1])
    return (iteration_res[-1],pd.DataFrame({"Y":iteration_res,"Error":error}))
```

18.5 Given these data

x	1.6	2	2.5	3.2	4	4.5
f(x)	2	8	14	15	8	2

- (a) Calculate $f(2.8)$ using Newton's interpolating polynomials of order 1 through 3. Choose the sequence of the points for your estimates to attain the best possible accuracy.
- (b) Utilize Eq. (18.18) to estimate the error for each prediction.

In [105...

```
#set up the data and point x given
X=[1.6,2,2.5,3.2,4,4.5]
Y=[2,8,14,15,8,2]
x_given = 2.8

#find out the fdd table and get the first row since it contains the coeff of the
fdd = fdd_table(X,Y)
coeff = fdd[:1].values[0]
```



```
#get the final y interpolated and data frame containing y interpolated and the error
y_interp,error = Newt_interpolate(X,Y,x_given,coeff)
#display the fdd and y interpolated and the error for each order
display(fdd)
display(error)
```

	0	1	2	3	4	5
0	2	15.000000	-3.333333	-3.422619	1.847718	-0.481151
1	8	12.000000	-8.809524	1.011905	0.452381	NaN
2	14	1.428571	-6.785714	2.142857	NaN	NaN
3	15	-8.750000	-2.500000	NaN	NaN	NaN
4	8	-12.000000	NaN	NaN	NaN	NaN
5	2	NaN	NaN	NaN	NaN	NaN

	Y	Error
0	2.000000	18.000000
1	20.000000	3.200000
2	16.800000	0.985714
3	15.814286	0.212857
4	15.601429	0.066514
5	15.534914	NaN

In [106...

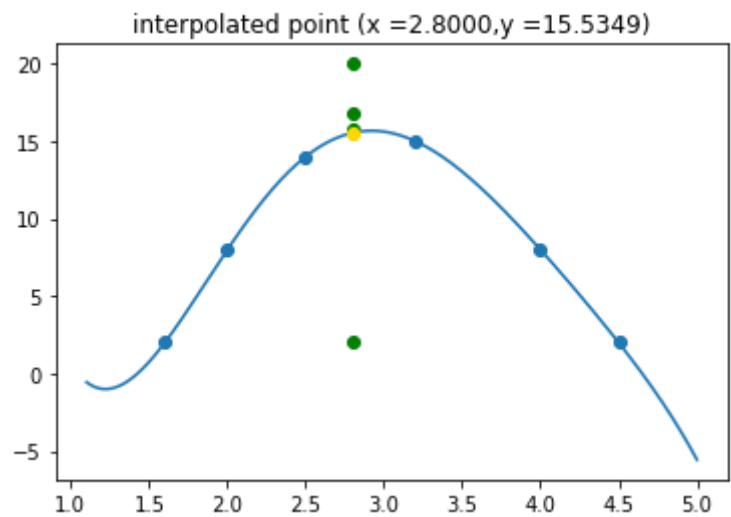
```
#plotting
plt.scatter(X,Y)

#plot all (x,y) where x is x given and y in set of y interpolated by Newton polynomial
#for each order except the last one in green
plt.scatter([x_given]*(len(X)-2),error["Y"].values[:-2],color="green")

#plot all (x,y) where x is x given and y in set of y interpolated by Newton polynomial
#of the highest order in gold and set it over every other plotted object for clarity
plt.scatter(x_given,y_interp,color="gold",zorder=3)

# sample a set of points (p,q) to plot the interpolated curve to graphically see it f
p = np.linspace(min(X)-.5, max(X)+.5, 1000)
q = [Newt_interpolate(X,Y,i,coeff)[0] for i in p]

plt.title(f"interpolated point (x ={x_given:0.4f},y ={y_interp:0.4f})")
plt.plot(p,q);
```



18.9 Use Newton’s interpolating polynomial to determine y at $x = 3.5$ to the best possible accuracy. Compute the finite divided differences as in Fig. 18.5 and order your points to attain optimal accuracy and convergence.

x	0	1	2.5	3	4.5	5	6
y	2	5.4375	7.3516	7.5625	8.4453	9.1875	12

In [107...

```
#set up the data and point x given
X=[0,1,2.5,3,4.5,5,6]
Y=[2,5.4375,7.3516,7.5625,8.4453,9.1875,12]
x_given = 3.5

#find out the fdd table and get the first row since it is contains the coeff of the
fdd = fdd_table(X,Y)
coeff = fdd[:1].values[0]

y_interp,error = Newt_interpolate(X,Y,x_given,coeff)

display(fdd)
display(error)
```

	0	1	2	3	4	5	6
0	2.0000	3.437500	-0.864573	0.145813	0.000010	-0.000003	7.901235e-07
1	5.4375	1.276067	-0.427133	0.145857	-0.000008	0.000001	NaN
2	7.3516	0.421800	0.083367	0.145827	-0.000001	NaN	NaN
3	7.5625	0.588533	0.447933	0.145822	NaN	NaN	NaN
4	8.4453	1.484400	0.885400	NaN	NaN	NaN	NaN
5	9.1875	2.812500	NaN	NaN	NaN	NaN	NaN
6	12.0000	NaN	NaN	NaN	NaN	NaN	NaN
	Y	Error					
0	2.000000	12.031250					

	Y	Error
1	14.031250	7.565017
2	6.466233	1.275867
3	7.742100	0.000043
4	7.742143	0.000015
5	7.742158	0.000005
6	7.742163	NaN

In [108...

```

#plotting
plt.scatter(X,Y)

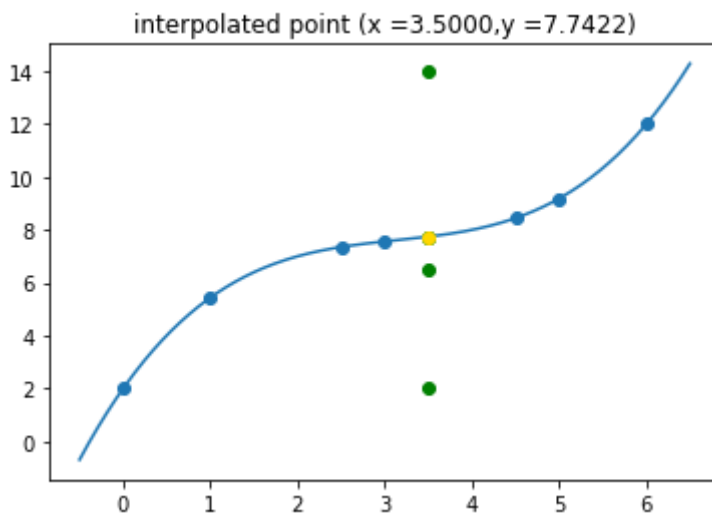
#plot all (x,y) where x is x given and y in set of y interpolated by Newton polynomi
#for each order except the last one in green
plt.scatter([x_given]*(len(X)-2),error["Y"].values[:-2],color="green")

#plot all (x,y) where x is x given and y in set of y interpolated by Newton polynomi
#of the highest order in gold and set it over every other plotted object for clarity
plt.scatter(x_given,y_interp,color="gold",zorder=3)

# sample a set of points (p,q) to plot the interpolated curve to graphically see it f
p = np.linspace(min(X)-.5, max(X)+.5, 1000)
q = [Newt_interpolate(X,Y,i,coeff)[0] for i in p]

plt.title(f"interpolated point (x ={x_given:0.4f},y ={y_interp:0.4f})")
plt.plot(p,q);

```



In []: