generate_datasets

September 29, 2024

1 Generate data sets for data fitting exercises

1.1 DMM

[39]:
```
import os
import socket
import matplotlib.pyplot as plt
import numpy as np
%matplotlib inline
```

1.2 Directory housekeeping

[40]:
```
# get the location of the 'intro_curve_fitting_python' directory on the local␣
↪machine;
# change into it or throw an error and force a kernel restart (in a jupyter␣
↪notebook)

# or edit the following to reflect the local machine name and preferred␣
↪directory
if not socket.gethostname() == 'apokalite': # local machine name
    basedir = input('Enter the full path of the directory␣
↪\'intro_curve_fitting_python\' on your machine.\n')
    if basedir == '':
        print('You must name a default directory. The kernel will now restart;␣
↪rerun this program.\n')
        quit()
else:
    basedir = '/home/david/gh/intro_curve_fitting_python' # preferred local␣
↪directory

try:
    os.chdir(basedir)
except:
    print('\nThat directory does not exist. The kernel will now restart; rerun␣
↪this program.\n')
    quit()
```

[41]:
```
# verify that expected data subdirectories exist; create them if not

# subdirectory for linear data
td = basedir+'/linear_data'
if not os.path.isdir(td):
    os.mkdir(td)

# subdirectory for exponential data
td = basedir+'/exponential_data'
if not os.path.isdir(td):
    os.mkdir(td)

# subdirectory for thermal denaturation data
td = basedir+'/thermal_denaturation_data'
if not os.path.isdir(td):
    os.mkdir(td)
```

1.3 Create noisy linear data sets

[42]:
```
# create linear data
# set the linear data directory:
datadir = basedir+'/linear_data'
```

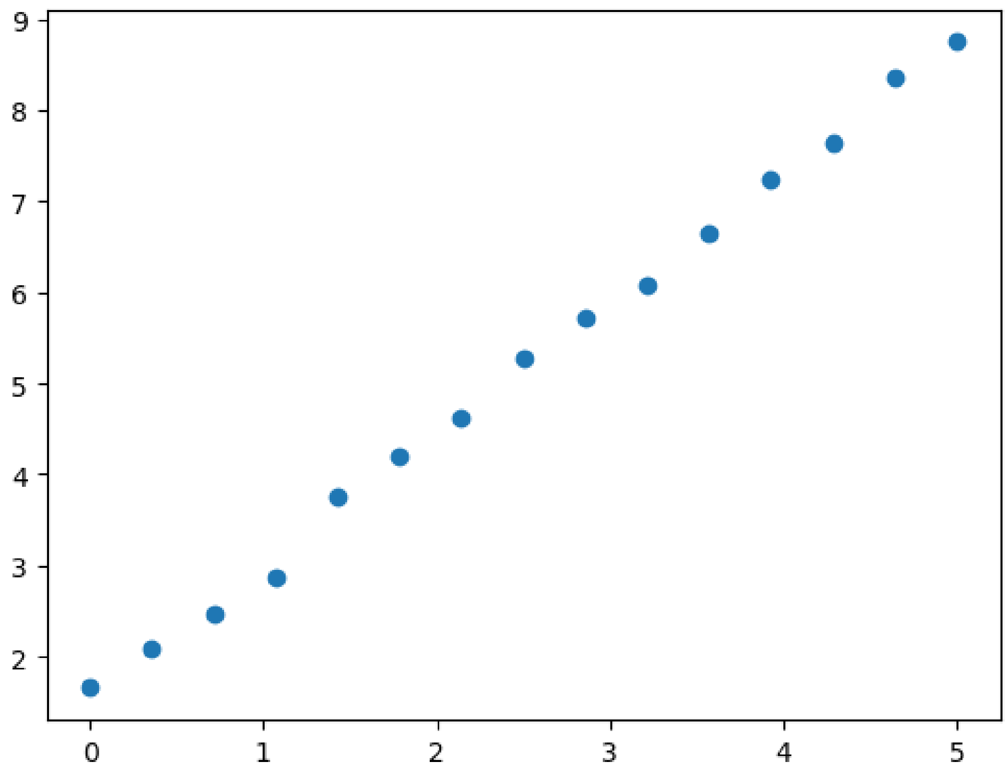
[43]:
```
# develop an algorithm

# randomly choose a slope between 0 and 5 and an intercept between -5 and +5
m = np.random.uniform(low=0, high=5)
b = np.random.uniform(low=-5, high=5)

# print the name of each variable,
# followed by its value as a floating point number with 2 decimal places
print(f'slope: %1.2f, intercept: %1.2f\n' % (m, b))
```

```
slope: 1.43, intercept: 1.58
```

[44]:
```
# create a linear data series

# create an array of 15 equally-spaced x values spanning 0 through 5
x = np.linspace(0,5,15)

# create the array of y values corresponding to y = mx + b
y = m*x + b

# add random normally distributed noise
# compute sigma = 0.02 * y(max) - y(min)
sigma = 0.02 * (np.max(y) - np.min(y))
```

```
# add random error from a normal distribution having mean=0 and sigma as defined
# to each element of y
y = np.random.normal(0, sigma, 15) + y
```

[45]:
```
# make and show a scatter plot
plt.scatter(x,y)
plt.show()
```

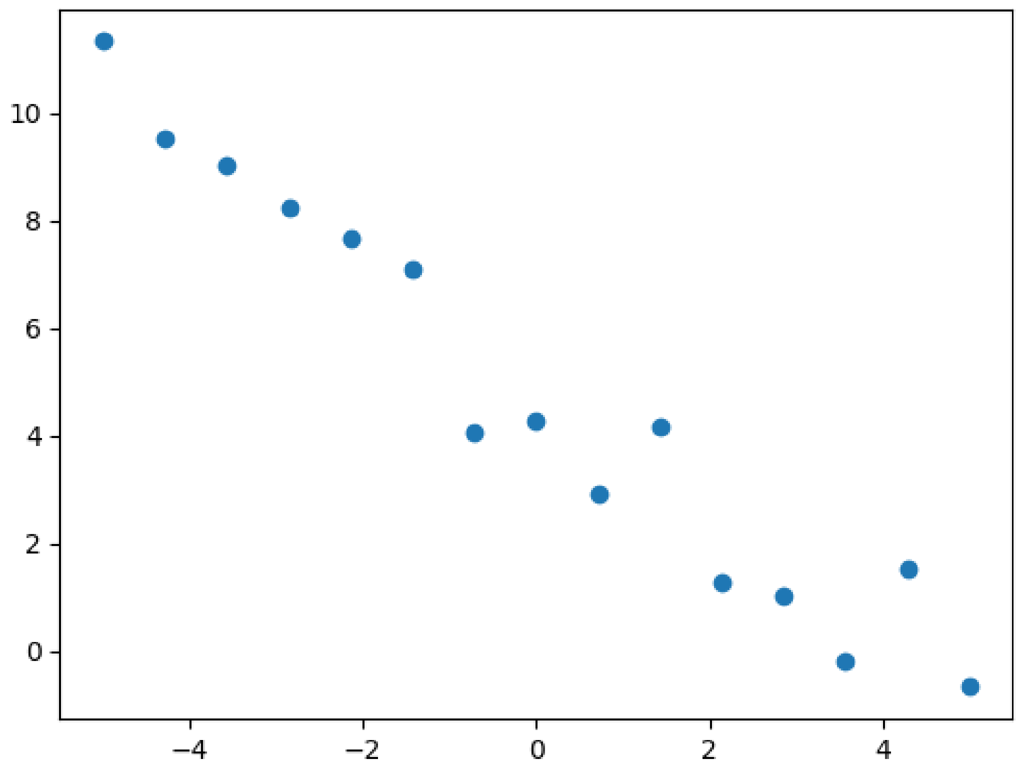


[46]:
```
# create a function that accomplishes all the number crunching given the␣
↪necessary input parameters

def mklineards(minx, maxx, minm, maxm, minb, maxb, dec, nump):
    # most variable names self-explanatory, except:
    # dec: decimal (fraction) value to multiply by (y(max)-y(min)) to
    # determine input sigma parameter to noise function
    # nump: 'number of points' to generate
    m = np.random.uniform(low=minm, high=maxm)
    b = np.random.uniform(low=minb, high=maxb)
    x = np.linspace(minx, maxx, nump)
    y = m * x + b
    y = y + np.random.normal(0, dec*(np.max(y) - np.min(y)), nump)
```

```
    return x,y
```

[47]:
```
# run the function with the following parameters:

minx = -5
maxx = 5
minm = -5
maxm = -0.01
minb = 0
maxb = 5
dec = 0.1
nump = 15

x,y = mklineards(minx, maxx, minm, maxm, minb, maxb, dec, nump)
```

[48]:
```
# make and show a scatter plot
plt.scatter(x,y)
plt.show()
```



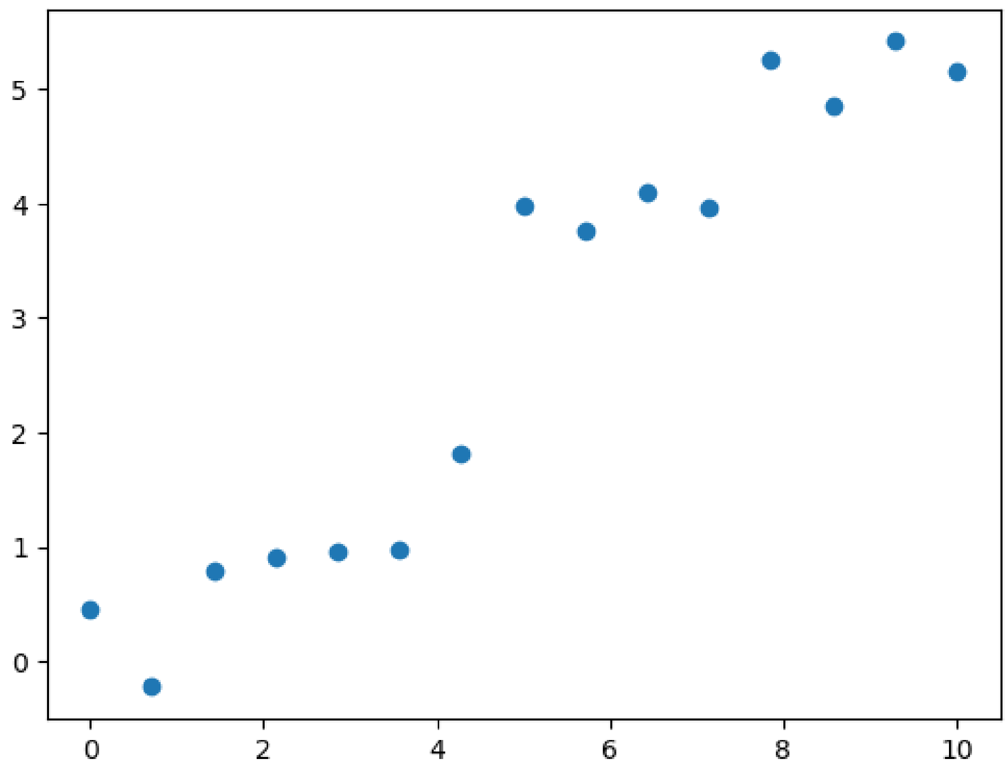
[49]:
```
# create a function to save the dataset to a csv file
def savexy(x,y,fn):
    # variable names self-explanatory, except:
```

```python
    # fn: filename, a string
    a = np.column_stack((x,y))
    ofn = datadir+'/'+fn
    np.savetxt(ofn, a, delimiter=",")
    return print(f'saved x, y dataset as \'{fn}\' in directory \'{datadir}\'\n')
```

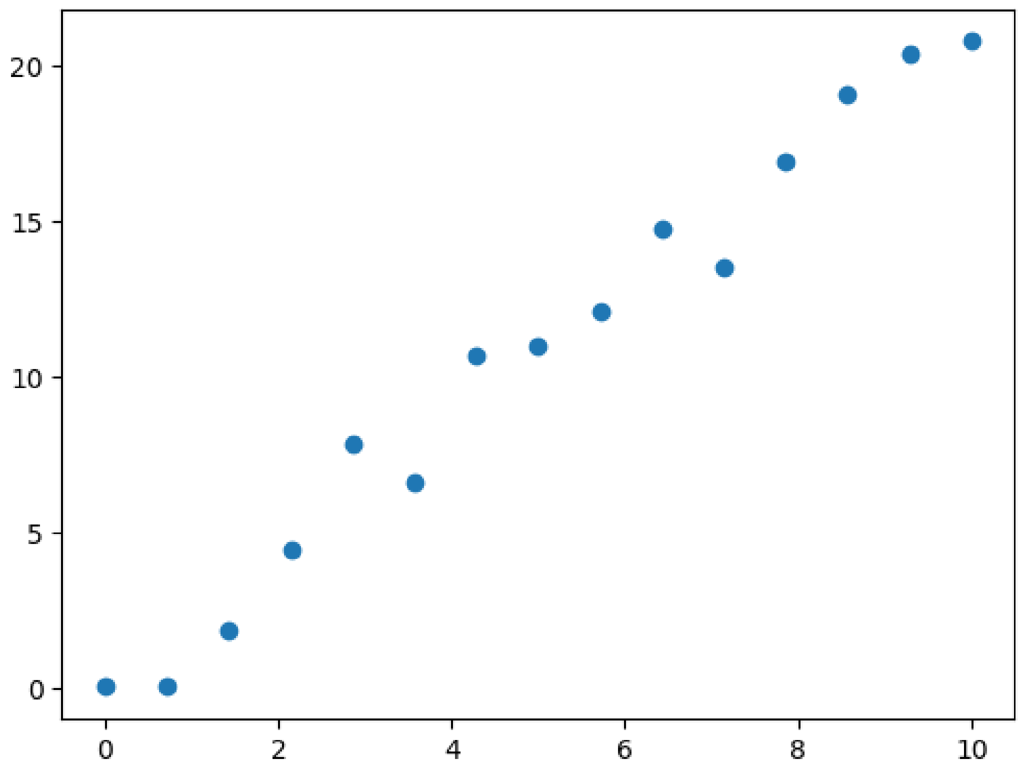
[50]:
```python
# save the data
savexy(x,y,'linear1.csv')
```

```
saved x, y dataset as 'linear1.csv' in directory
'/home/david/gh/intro_curve_fitting_python/linear_data'
```

[51]:
```python
# run the function two more times, with different parameters each time,
# saving the datasets along the way

minx = 0
maxx = 10
minm = 0
maxm = 1
minb = 0
maxb = 10
dec = 0.2
nump = 15

x,y = mklineards(minx, maxx, minm, maxm, minb, maxb, dec, nump)
plt.scatter(x,y)
plt.show()

savexy(x,y,'linear2.csv')

minx = 0
maxx = 10
minm = -10
maxm = 10
minb = -10
maxb = 10
dec = 0.05
nump = 15

x,y = mklineards(minx, maxx, minm, maxm, minb, maxb, dec, nump)
plt.scatter(x,y)
plt.show()

savexy(x,y,'linear3.csv')
```




```
saved x, y dataset as 'linear2.csv' in directory
'/home/david/gh/intro_curve_fitting_python/linear_data'
```




```
saved x, y dataset as 'linear3.csv' in directory
'/home/david/gh/intro_curve_fitting_python/linear_data'
```

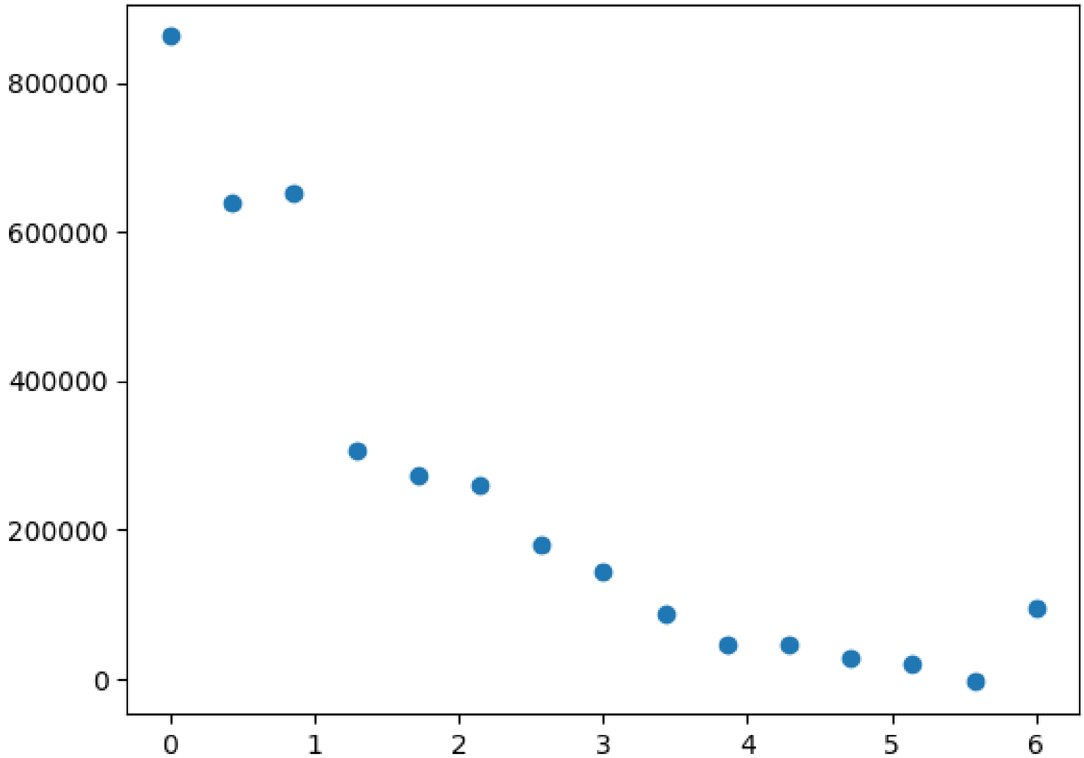
1.4 Create noisy exponential decay data sets

[52]:
```
# create exponential (decay) data
# set exponential data directory:
datadir = basedir+'/exponential_data'
```

[53]:
```
# develop the algorithm

# define an arbitrary exponential (assumed to be decay) function
# that goes to zero at large x
def expdf(x, k, A):
    return A * np.exp(k*x)

# choose a random value for k, the decay constant, in the range
# -1 <= k <= 0
k = np.random.uniform(low=-1, high=0)
print(f'k: %.3f (e.g., per second)\n' % (k))
```

```python
# given k, compute the lifetime
l = -1/k
print(f'lifetime: %.3f (e.g., seconds)\n' % (l))

# randomly choose maxx between 3 and 6 lifetimes
maxx = np.ceil(np.random.uniform(low=3*l, high=6*l))
print(f'maxx: %.3f (e.g., seconds)\n' % (maxx))

# randomly choose an A value on the interval 0, 1000000
A = np.random.uniform(low=1, high=1000000)

# create 15 uniformly spaced points between, and including, 0 and maxx
x = np.linspace(0, maxx, 15)

# create the corresponding y values
y = expdf(x,k,A)

# add random noise to the y values
dec = 0.05
nump = 15
y = y + np.random.normal(0, dec*(np.max(y) - np.min(y)), nump)

# scatter plot and show
plt.scatter(x,y)
plt.show()
```

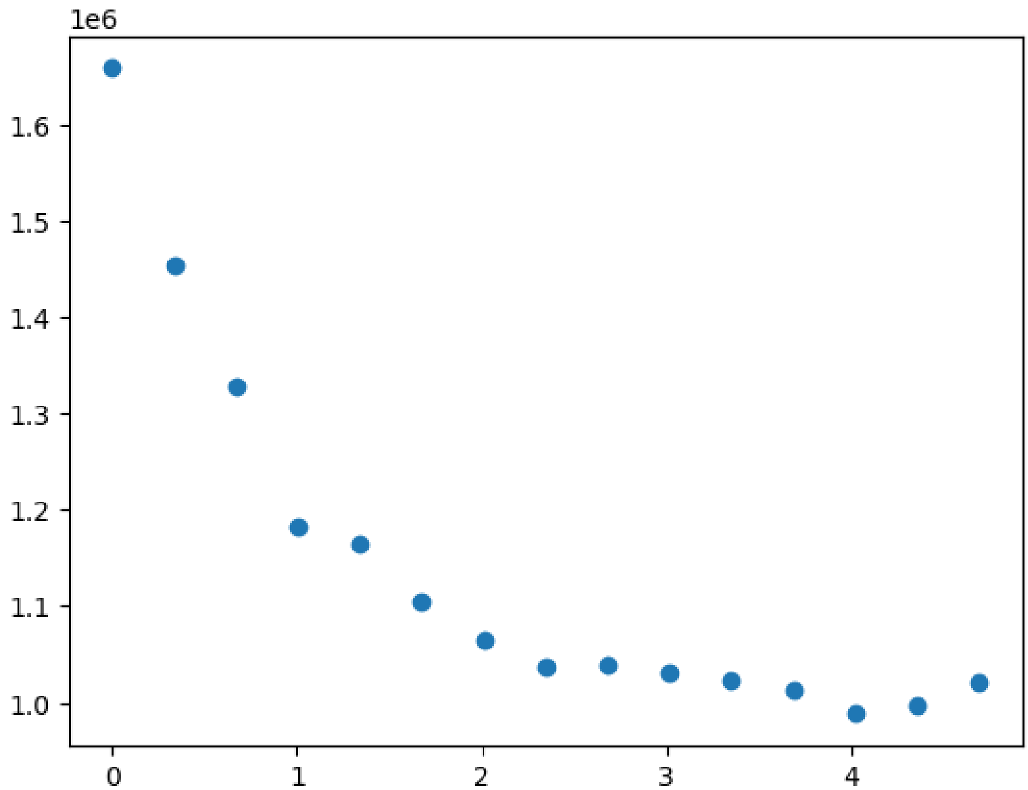
```
k: -0.612 (e.g., per second)

lifetime: 1.635 (e.g., seconds)

maxx: 6.000 (e.g., seconds)
```



[54]:
```
# create a function to implement the algorithm given the necessary input␣
↪parameters

def mkexpdecayds(mink, maxk, minxlifetimes, maxxlifetimes, minA, maxA, ylimit,␣
↪dec, nump):
    # in which:
    # mink, maxk are limits to the range in which to choose the decay constant
    # maxk assumed to be negative; see ylimit
    # minxlifetimes and maxxlifetimes are the minimum and maximum right-hand␣
↪most values
    # on the x axis, in multiples of the lifetime of the process
    # minA and maxA are limits to the range in which to choose the zero point␣
↪magnitude of the function
    # ylimit is the value of the function at large x
    # dec is the decimal (fraction) value to multiply by (y(max)-y(min)) to
    # determine the input parameter sigma in the noise function and
    # nump are the number of points to generate
    k = np.random.uniform(low=mink, high=maxk)
    maxx = -1/k * np.random.uniform(low=minxlifetimes, high=minxlifetimes)
    A = np.random.uniform(low=minA, high=maxA)
    x = np.linspace(0, maxx, nump)
```

```
    y = ylimit + A*np.exp(k*x)
    y = y + np.random.normal(0, dec*(np.max(y) - np.min(y)), nump)
    return x,y
```

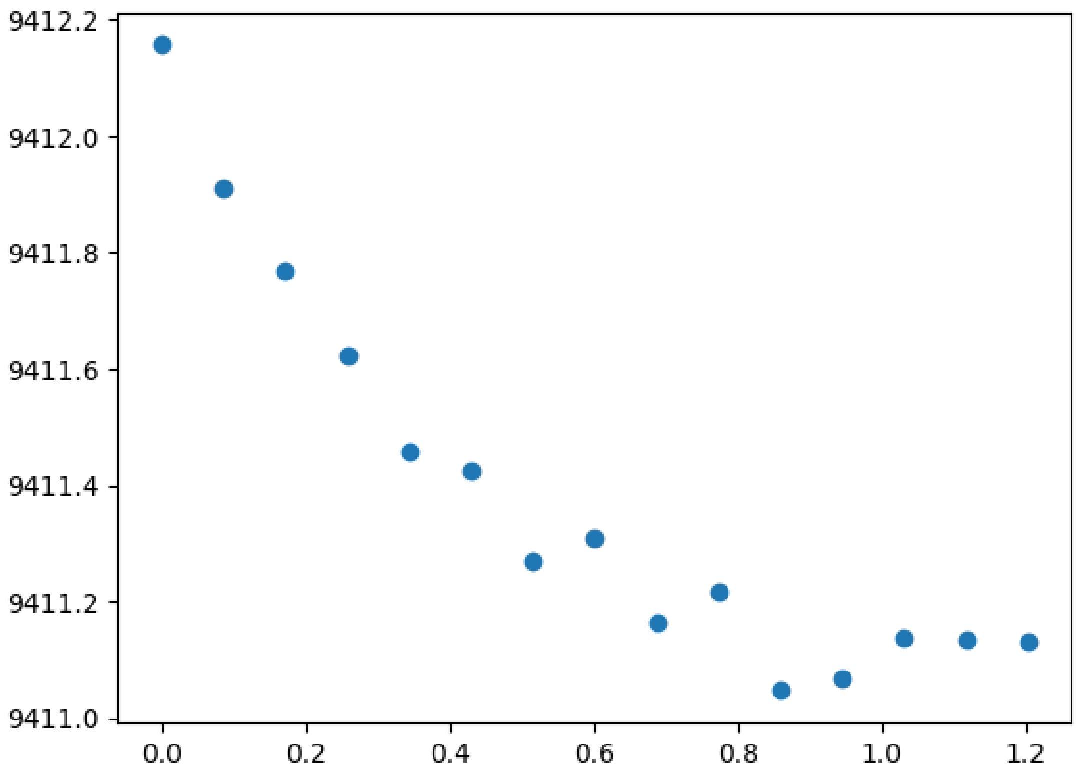
[55]:
```
mink=-1.1
maxk=-0.9
minxlifetimes=4.9
maxxlifetimes=5.1
minA=20000
maxA=1000000
ylimit=1000000
dec=0.02
nump=15

x,y = mkexpdecayds(mink, maxk, minxlifetimes, maxxlifetimes, minA, maxA,␣
 ↪ylimit, dec, nump)
plt.scatter(x,y)
plt.show()
savexy(x,y,'exponential1.csv')
```




```
saved x, y dataset as 'exponential1.csv' in directory
```

'/home/david/gh/intro_curve_fitting_python/exponential_data'

[56]:
```
mink=-10
maxk=-1
minxlifetimes=3
maxxlifetimes=5
minA=1
maxA=10
ylimit=9411
dec=0.05
nump=15

x,y = mkexpdecayds(mink, maxk, minxlifetimes, maxxlifetimes, minA, maxA,␣
 ↪ylimit, dec, nump)
plt.scatter(x,y)
plt.show()
savexy(x,y,'exponential2.csv')
```



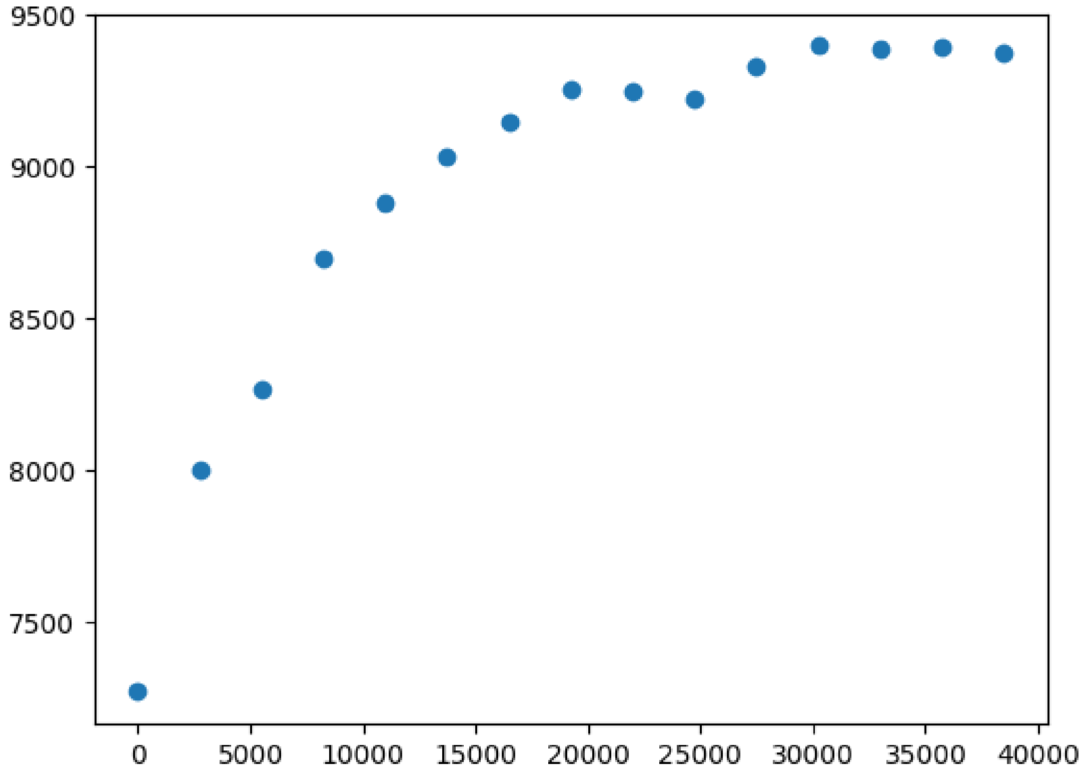

```
saved x, y dataset as 'exponential2.csv' in directory
'/home/david/gh/intro_curve_fitting_python/exponential_data'
```

[57]:

```
# make a slightly more interesting function just for fun:

def mkexpdecayds1(mink, maxk, minxlifetimes, maxxlifetimes, minA, maxA, ylimit,␣
 ↪dec, nump):
    # in which:
    # mink, maxk are limits to the range in which to choose the decay constant
    # maxk assumed to be negative; see ylimit
    # minxlifetimes and maxxlifetimes are the minimum and maximum right-hand␣
 ↪most values
    # on the x axis, in multiples of the lifetime of the process
    # minA and maxA are limits to the range in which to choose the zero point␣
 ↪magnitude of the function
    # ylimit is the value of the function at large x
    # dec is the decimal (fraction) value to multiply by (y(max)-y(min)) to
    # determine the input parameter sigma in the noise function and
    # nump are the number of points to generate
    k = np.random.uniform(low=mink, high=maxk)
    maxx = -1/k * np.random.uniform(low=minxlifetimes, high=minxlifetimes)
    A = np.random.uniform(low=minA, high=maxA)
    x = np.linspace(0, maxx, nump)
    y = ylimit + (1-A*np.exp(k*x)) # this line changed wrt parent
    y = y + np.random.normal(0, dec*(np.max(y) - np.min(y)), nump)
    return x,y
```

[58]:

```
mink=-0.001
maxk=-0.00001
minxlifetimes=5
maxxlifetimes=7
minA=1000
maxA=5000
ylimit=9411
dec=0.03
nump=15

x,y = mkexpdecayds1(mink, maxk, minxlifetimes, maxxlifetimes, minA, maxA,␣
 ↪ylimit, dec, nump)
plt.scatter(x,y)
plt.show()
savexy(x,y,'exponential3.csv')
```




```
saved x, y dataset as 'exponential3.csv' in directory
'/home/david/gh/intro_curve_fitting_python/exponential_data'
```