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# Laboratory 14: Data Models and Graphing

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ENGR 1330 Laboratory 14 - In-Lab

In [2]:
```
# Preamble script block to identify host, user, and kernel
import sys
! hostname
! whoami
print(sys.executable)
print(sys.version)
print(sys.version_info)
```

```
DESKTOP-6HAS1BN
desktop-6has1bn\medra
C:\Users\medra\anaconda3\python.exe
3.8.5 (default, Sep  3 2020, 21:29:08) [MSC v.1916 64 bit (AMD64)]
sys.version_info(major=3, minor=8, micro=5, releaselevel='final', serial=0)
```

## Example 1

Consider the data below

| Methanol Mole Fraction (Liquid Phase) | Methanol Mole Fraction (Vapor Phase) |
|---|---|
| 1.0 | 1.0 |
| 0.882 | 0.929 |
| 0.765 | 0.849 |
| 0.653 | 0.764 |
| 0.545 | 0.673 |
| 0.443 | 0.575 |
| 0.344 | 0.471 |
| 0.25 | 0.359 |
| 0.159 | 0.241 |
| 0.072 | 0.114 |
| 0.0 | 0.0 |

Estimate the vapor mole fraction of methanol corresponding to the liquid mole fraction of methanol of x = 0.15.

Let's try a few different functional forms as a data model; first linear, then quadratic, and then a power-law model.

As a first step, lets import some minimal needed packages, and build a plotting function.

In [3]:
```
import matplotlib.pyplot as plt
def make2plot(listx1,listy1,listx2,listy2,strlablx,strlably,strtitle):
    mydata = plt.figure(figsize = (10,5)) # build a square drawing canvass from figure
    plt.plot(listx1,listy1, c='red', marker='v',linewidth=0) # basic data plot
    plt.plot(listx2,listy2, c='blue',linewidth=1) # basic model plot
    plt.xlabel(strlablx)
    plt.ylabel(strlably)
    plt.legend(['Observations','Model'])# modify for argument insertion
    plt.title(strtitle)
    plt.show()
    return
```

Next lets define some data models; linear, quadratic, and power-law

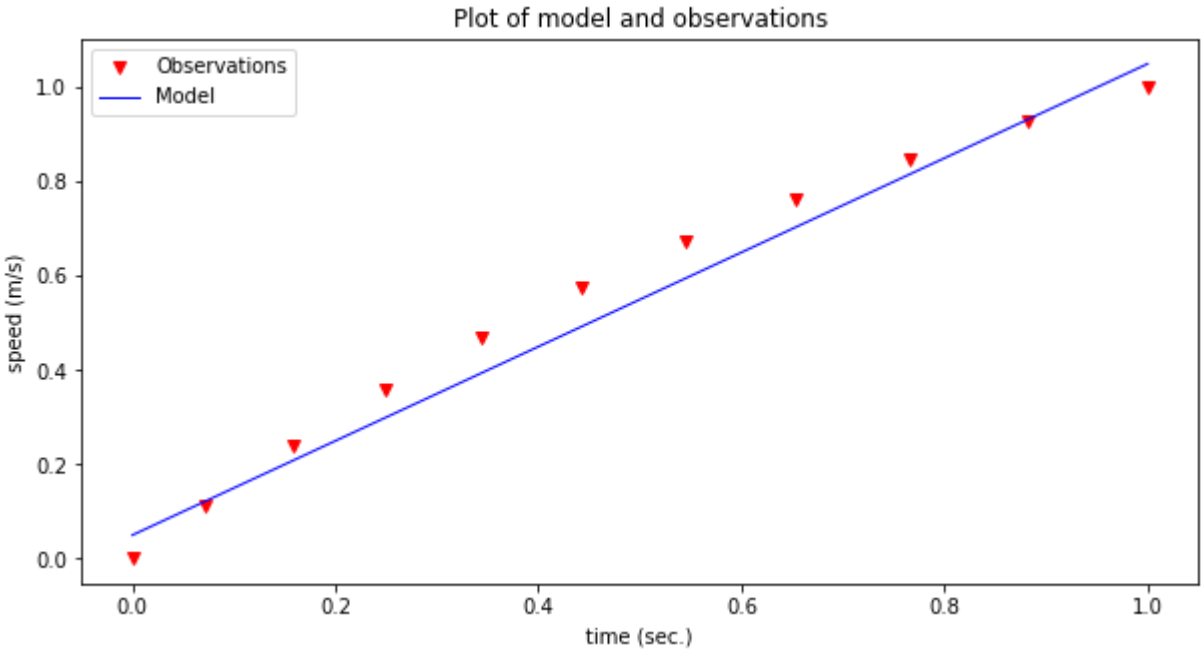
In [4]:
```
def linear(b0,b1,x):
    '''
    linear data model, b0,b1 are parameters
    return y = b0+b1*x
    '''
    linear=b0+b1*x
    return(linear)

def quadratic(b0,b1,b2,x):
    '''
    quadratic data model, b0,b1 are parameters
    return y = b0+b1*x+b2*x^2
    '''
    quadratic=b0+b1*x+b2*x**2
    return(quadratic)

def powerlaw(b0,b1,b2,x):
    '''
    power law data model
    return y = b0 + b1*x**b2'''
    powerlaw=b0+b1*x**b2
    return(powerlaw)

def residue(list1,list2,list3):
    '''
    compute residues
    list3 = list1 - list2
    return residuals in list3
    '''
    if len(list1)!=len(list2) or len(list1)!=len(list3):
        print('Lists unequal length, undefined operations')
        return
    for i in range(len(list1)):
        list3[i]=list1[i]-list2[i]
    return(list3)
```

Now lets make some model fits (trial-and-error); First the needed data

In [5]:
```
xtable = [1.0,0.882,0.765,0.653,0.545,0.443,0.344,0.25,0.159,0.072,0]
```

```
ytable = [1.0 ,0.929 ,0.849 ,0.764 ,0.673 ,0.575 ,0.471 ,0.359 ,0.241 ,0.114 ,0]
```

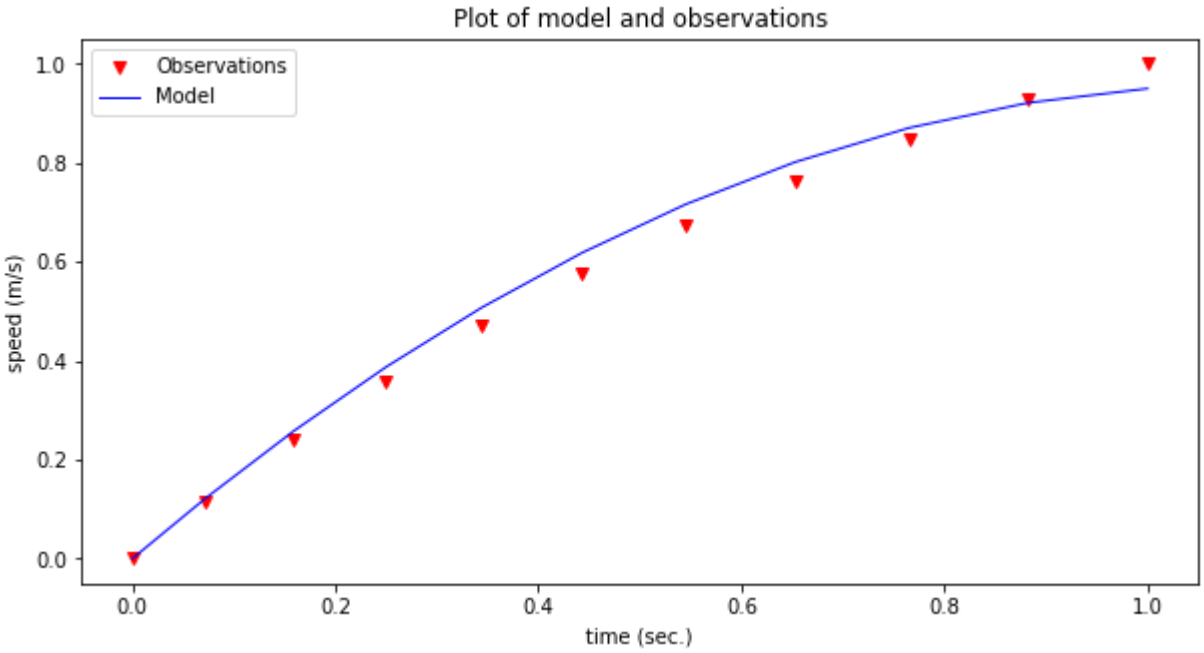
In [9]:
```
# Fit a data model - linear model
intercept=float(input('Enter b0 value'))
slope=float(input('Enter b1 value'))
# build a data model
modelYYY = [] # empty list
for i in range(len(xtable)):
    modelYYY.append(linear(intercept,slope,xtable[i]))
# Plotting results
make2plot(xtable,ytable,xtable,modelYYY,'time (sec.)','speed (m/s)','Plot of model and
```




In [10]:
```
# get the residues
resids = [0 for i in range(len(xtable))] # empty list
residue(ytable,modelYYY,resids)
print(sum(resids))
for i in range(len(resids)):
    resids[i]=resids[i]**2
print(sum(resids))
```

```
0.3119999999999997
0.03319199999999998
```

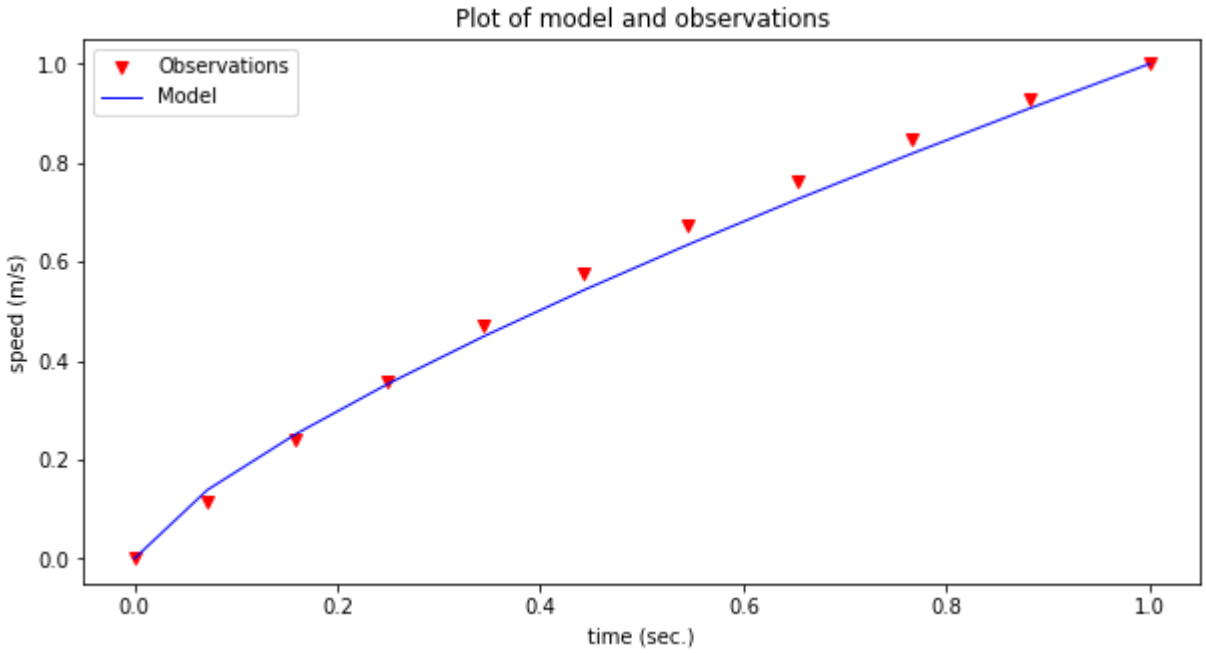
In [11]:
```
# Fit a data model - quadratic model
intercept=float(input('Enter b0 value'))
slope=float(input('Enter b1 value'))
curvature = float(input('Enter b2 value'))
# build a data model
modelYYY = [] # empty list
for i in range(len(xtable)):
    modelYYY.append(quadratic(intercept,slope,curvature,xtable[i]))
# Plotting results
make2plot(xtable,ytable,xtable,modelYYY,'time (sec.)','speed (m/s)','Plot of model and
```




In [12]:
```
# get the residues
resids = [0 for i in range(len(xtable))] # empty list
residue(ytable,modelYYY,resids)
print(sum(resids))
for i in range(len(resids)):
    resids[i]=resids[i]**2
print(sum(resids))
```

```
-0.17744359999999992
0.010656751633440004
```

In [13]:
```
# Fit a data model - power-law model
intercept=float(input('Enter b0 value'))
slope=float(input('Enter b1 value'))
exponent=float(input('Enter b2 value'))
# build a data model
modelYYY = [] # empty list
for i in range(len(xtable)):
    modelYYY.append(powerlaw(intercept,slope,exponent,xtable[i]))
# Plotting results
make2plot(xtable,ytable,xtable,modelYYY,'time (sec.)','speed (m/s)','Plot of model and
```




In [14]:
```
# get the residues
resids = [0 for i in range(len(xtable))] # empty list
residue(ytable,modelYYY,resids)
print(sum(resids))
for i in range(len(resids)):
    resids[i]=resids[i]**2
print(sum(resids))
```

```
0.14964279768159716
0.006498995544891791
```

Now choose which data model to use and make the estimate

In [15]:
```
xwant = float(input('Liquid Phase Mole Fraction'))
print('Estimated Vapor Phase Mole Fraction : ',round(quadratic(0.0,1.75,-.8,xwant),3))
```

```
Estimated Vapor Phase Mole Fraction :  0.245
```

In [16]:
```
xwant = float(input('Liquid Phase Mole Fraction'))

print('Estimated Vapor Phase Mole Fraction : ',round(powerlaw(0.0,1.0,0.75,xwant),3))
```

```
Estimated Vapor Phase Mole Fraction :  0.241
```

In [19]:
```
xwant = float(input('Liquid Phase Mole Fraction'))

print('Estimated Vapor Phase Mole Fraction : ',round(linear(0.05,1.0,xwant),3))
```

```
Estimated Vapor Phase Mole Fraction :  0.2
```

xwant = float(input('Liquid Phase Mole Fraction'))

print('Estimated Vapor Phase Mole Fraction : ',round(residue(0.0,1.0,0.75,xwant),3))

## Exercise 1

A meaningful modification is to make the estimate using all the models (you will have to use care in parameter names, but its an easy model!). It is left as an exercise.