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Fitting Data in *Mathematica*

There are two ways to fit data:
1. Fit[ ] command (less complicated)
Format:
Fit[data set, {x variable,y function}, x variable]
(2 examples below)

2. FindFit[ ] (more complicated)
Format:
FindFit[data, y function[x,a,b,c], {{a, min,max}, {b,min,max}}, {c,min,max}, x]
(1 example below)

We will use the Fit[ ] command in the example below.

Problem:
Consider the data below. We are told that the data is volume data (liters) as a function of pressure (atomospheres) taken at room temperature. We are also told that there is 1 mole of the gas and it is an inert gas. Our job is to fit the data.

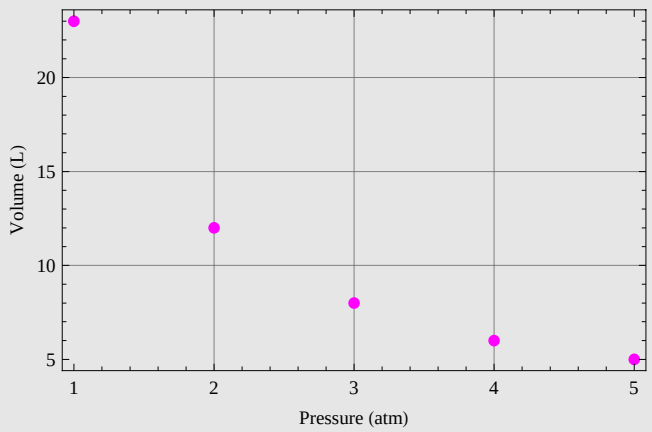
{pressure,volume}={{1, 23}, {2, 12}, {3, 8}, {4, 6}, {5, 5}}

What do we know?
1. data is volume as a function of pressure of gas
2. 1 mole of gas thus n =1
3. room temperature, so T~300K
4. inert gas, so we can probably use the Ideal Gas Law equation to fit the data

What we will do:
1. set the data equal to a variable
2. plot the data in a scatter plot to see if it looks like the ideal gas law. Recall that volume is inversely proportional to pressure

```
Clear[v, R, T, p, vdata]
vdata = {{1, 23}, {2, 12}, {3, 8}, {4, 6}, {5, 5}} (*list of data*)

(*plot data*)
vdataplot = ListPlot[vdata, Frame → True, GridLines → Automatic,
  PlotStyle → {RGBColor[1, 0, 1], PointSize[0.02`]},
  FrameLabel → {"Pressure (atm)", "Volume (L)"}]
  (*scatter plot of data*)
```

```
{{1, 23}, {2, 12}, {3, 8}, {4, 6}, {5, 5}}
```



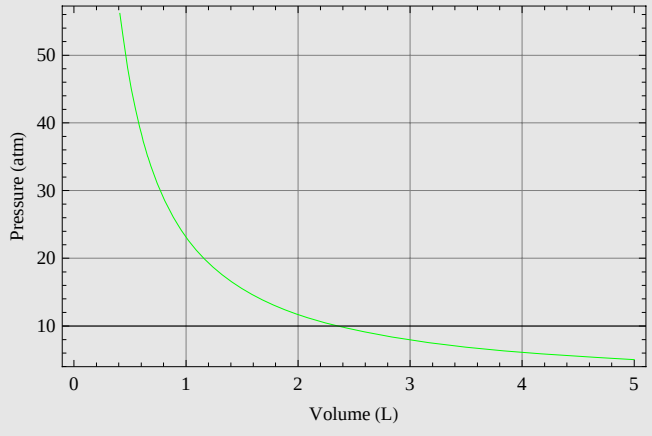
Note that from the plot that the volume looks like it is inversely proportional to pressure, similar to the ideal gas law. So we will try to fit the plot using the ideal gas law.

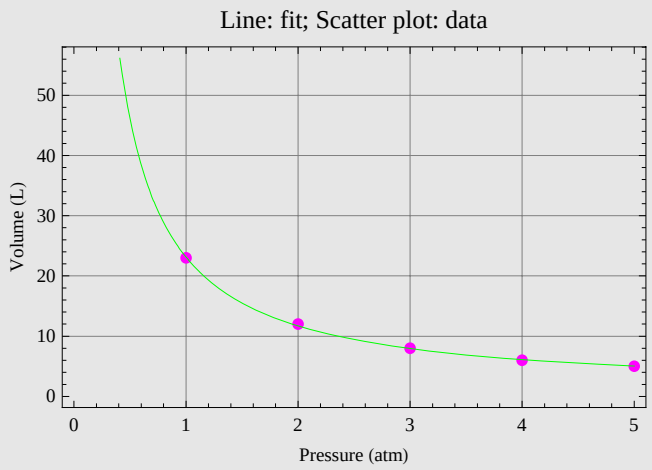
What we will do :

1. define the ideal gas law as a function
2. define the variables in the equation, i.e., R
3. Fit the data which will create an fitting equation. We use the Fit[ ] command
Fit[data set, {x variable,y function}, x variable]
4. Plot the fitting equation

```
(*Define equation*)
v[p_, n_, T_] := n R T / p (*Ideal gas law*)
(*Define variable*)
R = 0.08206;(*gas constant, units = atm L /(mol K)*)

(*define the fitting function*)
vfit = Fit[vdata, {p, v[p, 1, 300]}, p]
(*Fit[ ] command is used to fit the data set. Here,
we define the result of the Fit[ ] as a function called pfit*)
plotvfit = Plot[vfit, {p, 0, 5}, Frame → True,
  GridLines → Automatic, PlotStyle → {RGBColor[0, 1, 0]},
  FrameLabel → {"Volume (L)", "Pressure (atm)"}]
(*plotting the function pfit*)
Show[vdataplot, plotvfit,
 PlotLabel → "Line: fit; Scatter plot: data"]
(*showing the plots pplot and plotpfit on the same graph*)
```

$$\frac{23.0486}{p} + 0.0864887\, p$$





- Note that the fit is pretty good and the fitting function that was produced by the Fit[ ] command was not purely the ideal gas law.

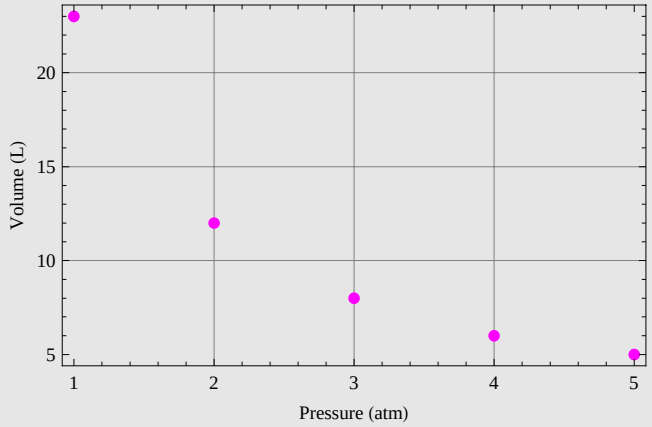
2. FindFit[ ] (more complicated)

Example :

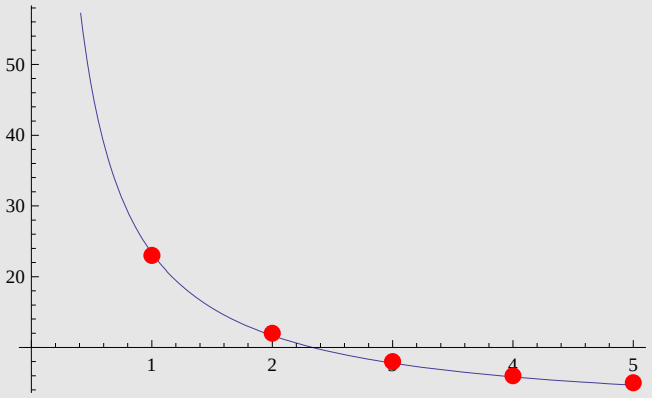
FindFit[data, y function[x, a, b, c], {{a, min, max}, {b, min, max}}, {c, min, max}, x]

```
Clear[v, R, T, p, vdata]
vdata = {{1, 23}, {2, 12}, {3, 8}, {4, 6}, {5, 5}} (*list of data*)

vdataplot = ListPlot[vdata, Frame → True, GridLines → Automatic,
  PlotStyle → {RGBColor[1, 0, 1], PointSize[0.02`]},
  FrameLabel → {"Pressure (atm)", "Volume (L)"}]
  (*scatter plot of data*)

(*Define variable*)
R = 0.08206;(*gas constant, units = atm L /(mol K)*)

(*define the fitting function*)
fitfuncv[p_] =
 n R T / p /. FindFit[vdata, n R T / p, {{n, 0, 10}, {T, 200, 400}}, p]
(*fitfunc2[x_]=a+b Exp[c x]/.
  FindFit[vdata,a+b Exp[c x],{{a,4,5},{b,4,5},{c,4,5}},x]*)
plotfit2 = Plot[fitfuncv[p], {p, 0, 5}, Epilog ->
   {RGBColor[1, 0, 0], AbsolutePointSize[8], Point /@ vdata}]
```

```
{{1, 23}, {2, 12}, {3, 8}, {4, 6}, {5, 5}}
```



$$\frac{23.3441}{p}$$



3. Other examples:

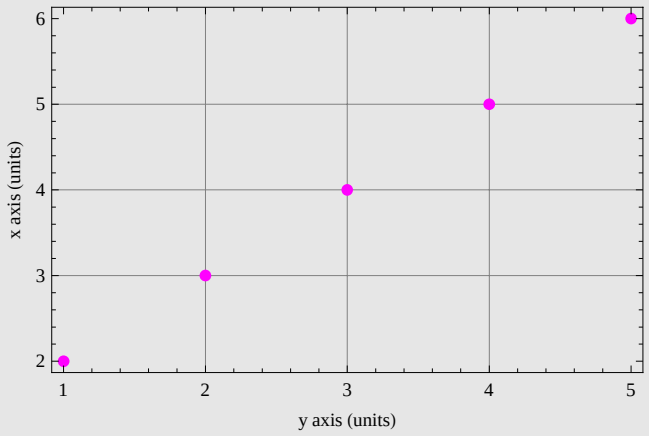
- **Example using the command: Fit[data set, {x variable,y function}, x variable]**

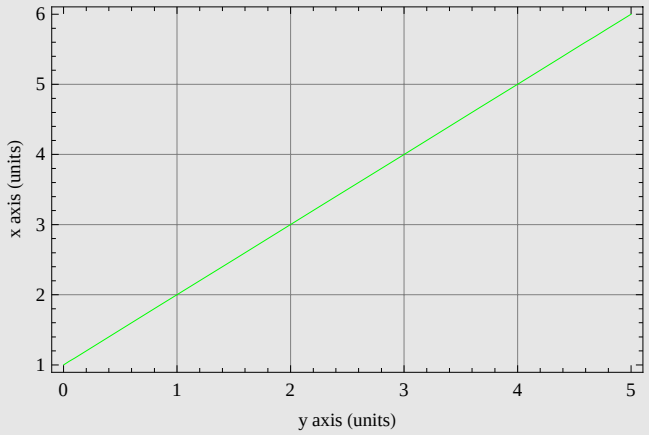
  Linear data

```
(*Define equation*)
linedata = {{1, 2}, {2, 3}, {3, 4}, {4, 5}, {5, 6}} (*list of data*)
(*define the fitting function*)
linefit = Fit[linedata, {1, x, x}, x]
(*Note that the function that we put in the fit command is y=
 x. Also note that the 1 that precedes the x is to tell
   the fit command that there can be a y-intercept*)

dataplot = ListPlot[linedata, Frame → True, GridLines → Automatic,
  PlotStyle → {RGBColor[1, 0, 1], PointSize[0.02`]},
  FrameLabel → {"y axis (units)", "x axis (units)"}]
  (*scatter plot of data*)
plotfit = Plot[linefit, {x, 0, 5}, Frame → True,
  GridLines → Automatic, PlotStyle → {RGBColor[0, 1, 0]},
  FrameLabel → {"y axis (units)", "x axis (units)"}]
(*plotting the function pfit*)
Show[dataplot, plotfit, PlotLabel → "Line: fit; Scatter plot: data"]
(*showing the plots pplot and plotpfit on the same graph*)
```

```
{{1, 2}, {2, 3}, {3, 4}, {4, 5}, {5, 6}}
```

```
1. + 1. x
```





Line: fit; Scatter plot: data