Table of Contents

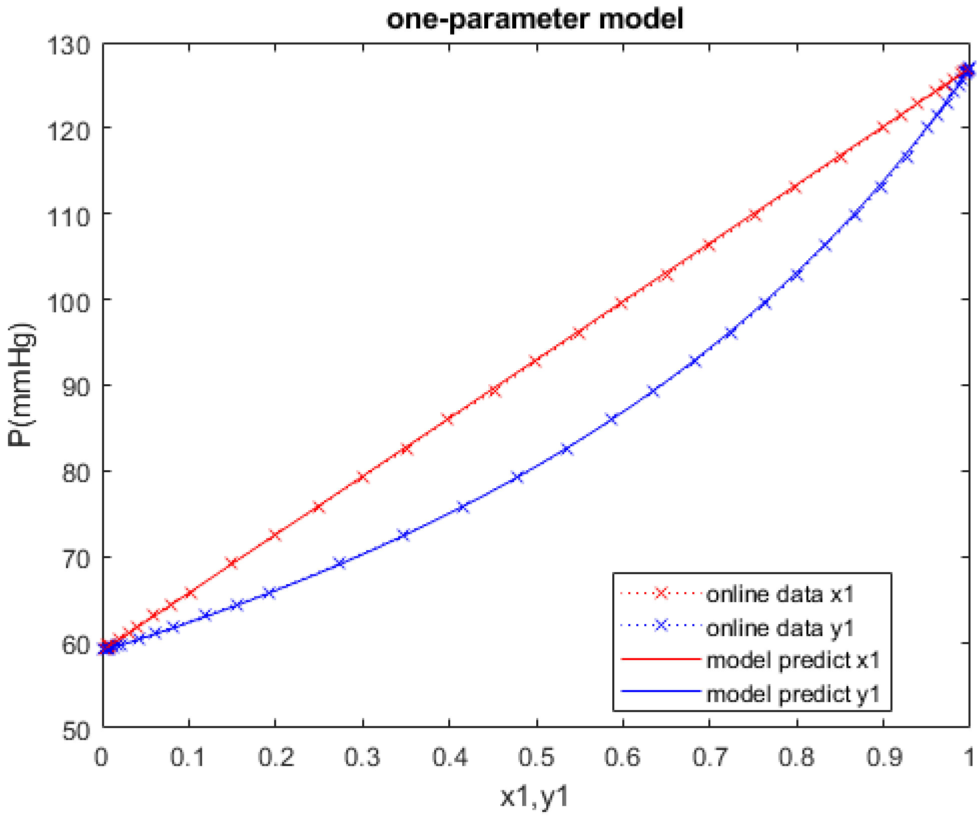

```
dat1 = load("C:\Users\buing\Documents\MATLAB\CBE
 562\meth(1)_eth(2).dat")
dat_rand = dat1;
dat1_rand_2 = dat1(4:40,2) + (- 0.002 +
 (0.004).*rand(length(dat1(4:40,2)),1));
dat1_rand_3 = dat1(2:38,3) + (- 0.002 +
 (0.004).*rand(length(dat1(2:38)),1));
dat_rand(4:40,2) = dat1_rand_2;
dat_rand(2:38,3) = dat1_rand_3;
dat = dat_rand;
Psat1_in = 127.04;
Psat2_in = 58.98;

P_1 = dat(:,1).*750;
x1 = dat(:,2);
y1 = dat(:,3);
x2 = 1.- dat(:,2);
y2 = 1.- y1;
%For Psat data, I took from CBE 311 database of excel sheet. I find
 the
%Psat data for methanol and ethanol at 25*C from excel sheet of
 Antoine.xlsx. This excel
% is introduced to us in CBE 311 as part of our learnings. The author
 of the book %
%create this database, and is reliable enough! It is given in mmHG,
 and convert
%to bar to fit P data from the website.
Psat1 = Psat1_in; %methanol(1) in bar
Psat2 = Psat2_in; %ethanol(2) in bar
%say this set of data is collected and we aren't sure about the
 activity
%model. Let's pick out a few CBE 311 activities model and build them
 as
% theta estimate model.
%we consider that these solutions could be modeled with modified
 Rault's
%Law/
%general form is P = x1g1Psat1 + x2g2Psat2
%our specialty lies in the activities coefficient embedded in gamma 1
 and 2,
%as different activities coefficient models will yield different
 gamma1 and
% 2 depending on the mole fraction.
```

```
%this is margules 1-parameter model:
%Ge/RT = A12x1x2
%ln(g1) = A12(x2)^2 => g1 = exp(A12(x2)^2)
%ln(g2) = A12(x1)^2 => g2 = exp(A12(x1)^2)
%in the full form:
%P = x1*exp(A12(x2)^2)*Psat1 + x2*exp(A12(x1)^2)*Psat2
% mathematically this seems complicated, so we could approach it
% differently
%gamma 1 and 2 by Rault's law definition is also gamma = yP/xPsat
%we could set up a set of gamma data and then use ln(g1) = A12(x2)^2
 or
%ln(g2) = A12(x1)^2. For our 1 parameter model, A12 should be equal to
 each
%other.
g1_data = y1.*P_1./(x1.*Psat1);
g2_data = y2.*P_1./(x2.*Psat2);
lng1 = log(g1_data);
Y1 = lng1;
X0_1 = x1.^2;
%lng2 = A12(x1^2) => Y = theta0*X01;
theta_est_1 = inv(X0_1'*X0_1)*X0_1'*Y1;
A12 = theta_est_1;
heis_theta_1 = eigs(X0_1'*X0_1);
%theta_est = A12
%back calculate g1 and g2
x1_pre = linspace(0.001,0.999,100);
x2_pre = 1.- x1_pre;
g1_pre = exp(theta_est_1*(x2_pre.^2));
g2_pre = exp(theta_est_1*(x1_pre.^2));
P1_pre = Psat1.*x1_pre.*g1_pre + Psat2.*x2_pre.*g2_pre;
y1_pre = g1_pre.*x1_pre.*Psat1./P1_pre;
%output


dat1 =

    0.0788    0.0010    0.0021
    0.0788    0.0010    0.0021
    0.0789    0.0020    0.0043
    0.0790    0.0030    0.0064
    0.0791    0.0040    0.0085
    0.0793    0.0060    0.0128
    0.0795    0.0080    0.0170
    0.0796    0.0100    0.0212
    0.0805    0.0200    0.0419
    0.0814    0.0300    0.0621
    0.0823    0.0400    0.0819
    0.0841    0.0600    0.1202
    0.0859    0.0800    0.1570
    0.0877    0.1000    0.1922
    0.0922    0.1500    0.2742
    0.0967    0.2000    0.3485
    0.1012    0.2500    0.4163
    0.1057    0.3000    0.4783
```

```
0.1102    0.3500    0.5353
0.1146    0.4000    0.5879
0.1191    0.4500    0.6365
0.1236    0.5000    0.6817
0.1281    0.5500    0.7237
0.1327    0.6000    0.7629
0.1372    0.6500    0.7996
0.1418    0.7000    0.8339
0.1463    0.7500    0.8662
0.1509    0.8000    0.8965
0.1555    0.8500    0.9249
0.1602    0.9000    0.9516
0.1620    0.9200    0.9618
0.1639    0.9400    0.9718
0.1657    0.9600    0.9814
0.1667    0.9700    0.9862
0.1676    0.9800    0.9909
0.1685    0.9900    0.9955
0.1687    0.9920    0.9964
0.1689    0.9940    0.9973
0.1691    0.9960    0.9982
0.1692    0.9970    0.9986
0.1693    0.9980    0.9991
0.1694    0.9990    0.9995
```

plot1

```
plot(x1,P_1,':xr')
hold on
plot(y1,P_1,':xb')
plot(x1_pre,P1_pre,'-r')
plot(y1_pre,P1_pre,'-b')
title('one-parameter model')
legend('online data x1','online data y1','model predict x1', 'model
 predict y1','location','best')
ylabel('P(mmHg)')
xlabel('x1,y1')
```



A12

```
A12 = theta_est_1;
```

Gaussian

```
heis_theta = eigs(X0_1'*X0_1);
GaussianX = heis_theta; %will fix later
```

Published with MATLAB® R2020a