

```

load BOHnet
BOHdataset;
avgParticleAu = nanmean(BOHdataset.pAu);% replacing missing particle sizes with average values
avgParticlePd = nanmean(BOHdataset.pPd);

BOHdataset.pAu(isnan(BOHdataset.pAu)) = avgParticleAu;
BOHdataset.pPd(isnan(BOHdataset.pPd)) = avgParticlePd;
BOHdataset.PrepMethod(ismissing(BOHdataset.PrepMethod)) = "DP";
SurfaceArea = grpstats(BOHdataset(:,{'CeO2Type','SA'}), 'CeO2Type'); %Averaging the surface area
%disp(SurfaceArea)
BOHdataset = grouptransform(BOHdataset,"CeO2Type","meanfill","SA");

BOHdataset.SA;

%for i = 1:height(SurfaceArea) %i.e for each class
    % BOHdataset.SA(BOHdataset.CeO2Type == i & isnan(BOHdataset.SA)) = SurfaceArea.mean_SA(i);

%end
DPrepMethod = dummyvar(BOHdataset.PrepMethod);
DCeO2Type = dummyvar(BOHdataset.CeO2Type);
%DCE2PrepMethod = dummyvar(BOHdataset.CeO2PrepMethod);
DSolvent = dummyvar(BOHdataset.Solvent);
%DPlanes = dummyvar(BOHdataset.ActivePlane);

%DCE2PrepMethod = array2table(DCE2PrepMethod);
DCeO2Type = array2table(DCeO2Type);
DPrepMethod = array2table(DPrepMethod);
DSolvent = array2table(DSolvent);

BOHdataset1 = [BOHdataset, DCeO2Type, DPrepMethod, DSolvent];

BOHdataset1.PrepMethod = [];
BOHdataset1.CeO2Type = [];
BOHdataset1.CeO2PrepMethod = [];
BOHdataset1.Solvent = [];

inputs1 = removevars(BOHdataset1, {'Data','PublicationNo', 'VarName48','Reference','Remarks','',
% Active plane, Crystallite size, pore radius and pore volume are removed
% due to too many missing values

inputs = double(inputs1{:,:});

InputsFilled = fillmissing(inputs, "constant", 0);

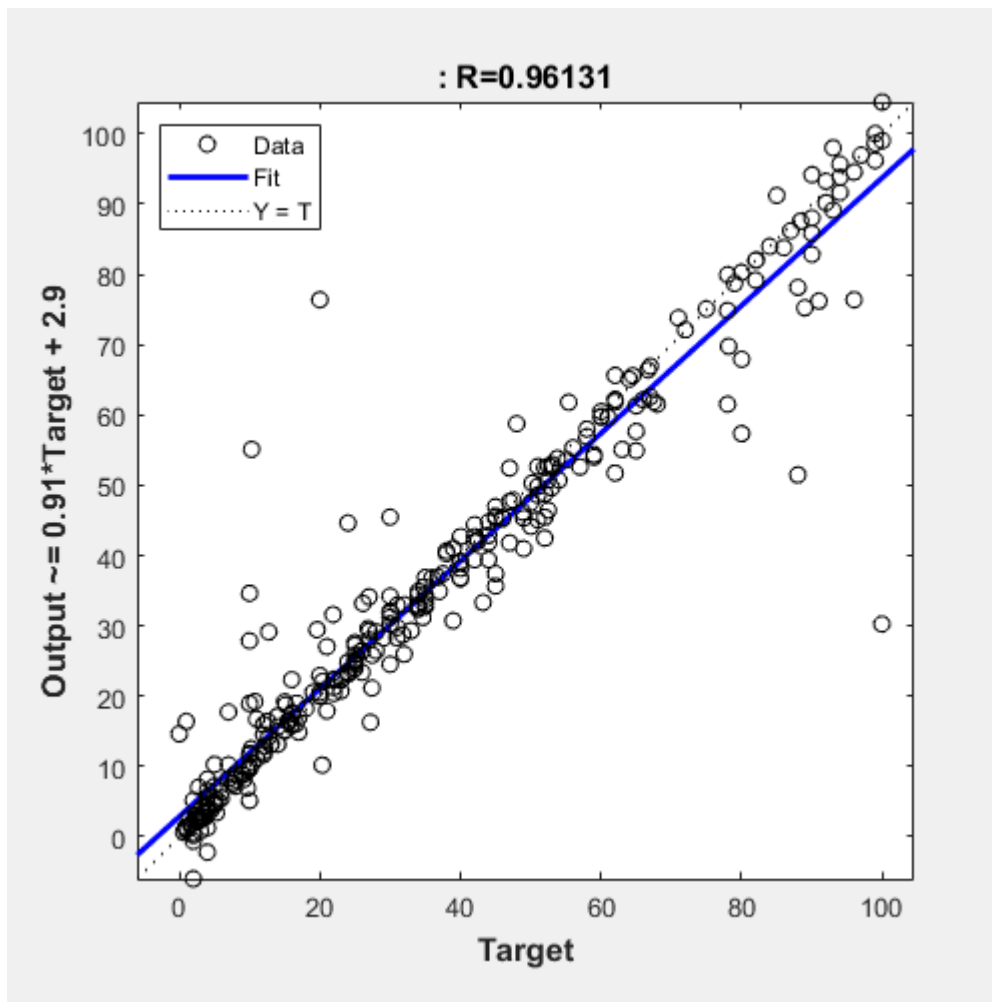
InputsandTarget = [InputsFilled, BOHdataset1.Conversion];
targets = BOHdataset1.Conversion;
transposedInput = transpose(InputsFilled);

```

```

y = BOHnet(transposedInput);
ty = transpose(y);
plotregression(targets, ty)

```



```

e = gsubtract(targets,y);
totalPerformance = perform(BOHnet,targets,ty)

```

```
totalPerformance = 59.5659
```

```
totalRMSE = sqrt(totalPerformance)
```

```
totalRMSE = 7.7179
```

Variable: Noble Metals

```

inputNM = inputs1;

inputNM.Au = zeros([318 1]); inputNM.Pd = zeros([318 1]);
inputNM = double(inputNM{:,:});

inputNM = fillmissing(inputNM, "constant", 0);
transposedInputNM = transpose(inputNM);

```

```

xNM = transposedInputNM;

yNM = BOHnet(xNM);
tyNM = transpose(yNM);
%e = gsubtract(t,yNM);
performance = perform(BOHnet,targets,tyNM)

```

```
performance = 1.1529e+03
```

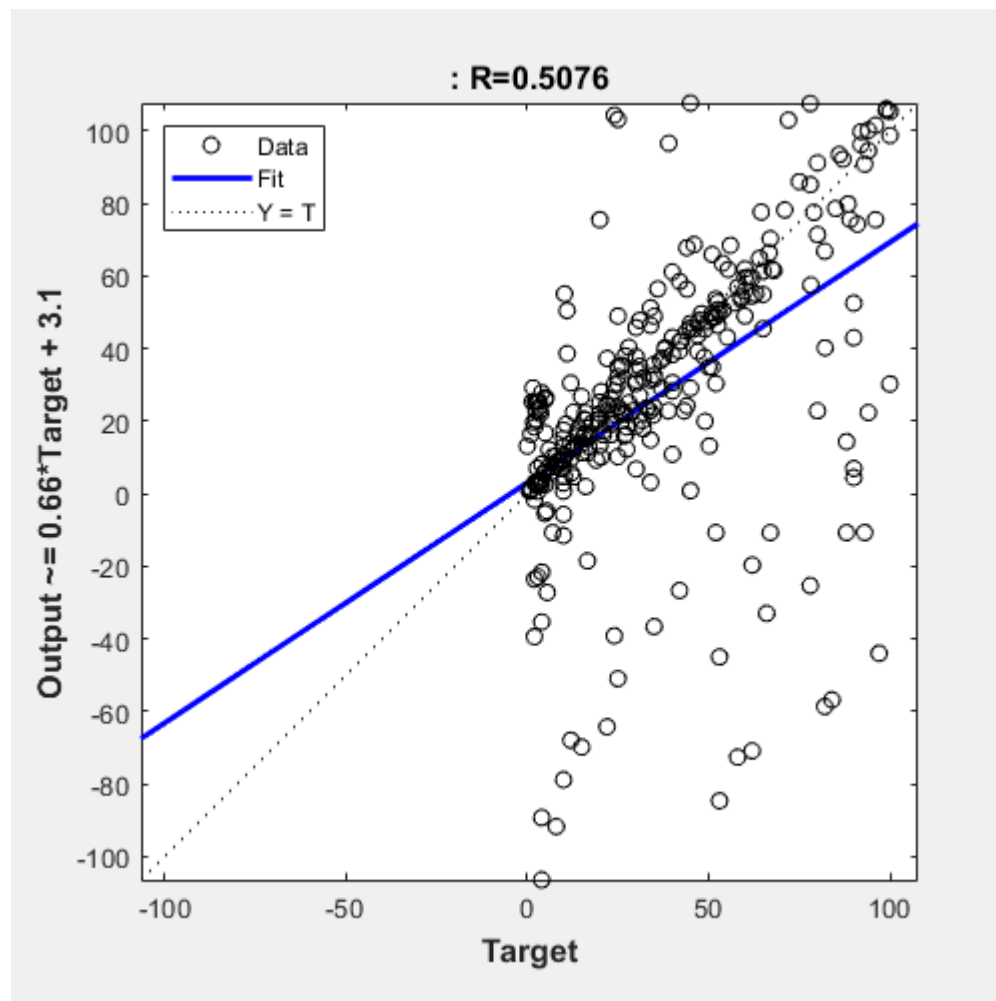
```
totalRMSENM = sqrt(performance)
```

```
totalRMSENM = 33.9541
```

```
RImpNM = (totalRMSENM - totalRMSE)
```

```
RImpNM = 26.2362
```

```
plotregression(targets, tyNM)
```



Variable : Promoters

```
inputPr = inputs1;
```

```

inputPr.Sm = double(inputPr.Sm);
inputPr.Ca = double(inputPr.Ca);
inputPr.Ba = double(inputPr.Ba);
inputPr.Mg = double(inputPr.Mg);

inputPr.Zr = zeros([318 1]); inputPr.Bi = zeros([318 1]); C3N4 = zeros([318 1]); inputPr.Mn = zeros([318 1]);
inputPr.V = zeros([318 1]); inputPr.Co = zeros([318 1]); inputPr.Cu = zeros([318 1]); inputPr.A = zeros([318 1]);
inputPr.Sm = zeros([318 1]); inputPr.Ba = zeros([318 1]); inputPr.Ca = zeros([318 1]); inputPr.Mg = zeros([318 1]);
inputPr = double(inputPr{:,:});
inputPr = fillmissing(inputPr, "constant", 0);

transposedInputPr = transpose(inputPr);

xPr = transposedInputPr;

yPr = BOHnet(xPr);
tyPr = transpose(yPr);
%e = gsubtract(t,yPr);
performance = perform(BOHnet,targets,tyPr)

performance = 303.5785

totalRMSEPr = sqrt(performance)

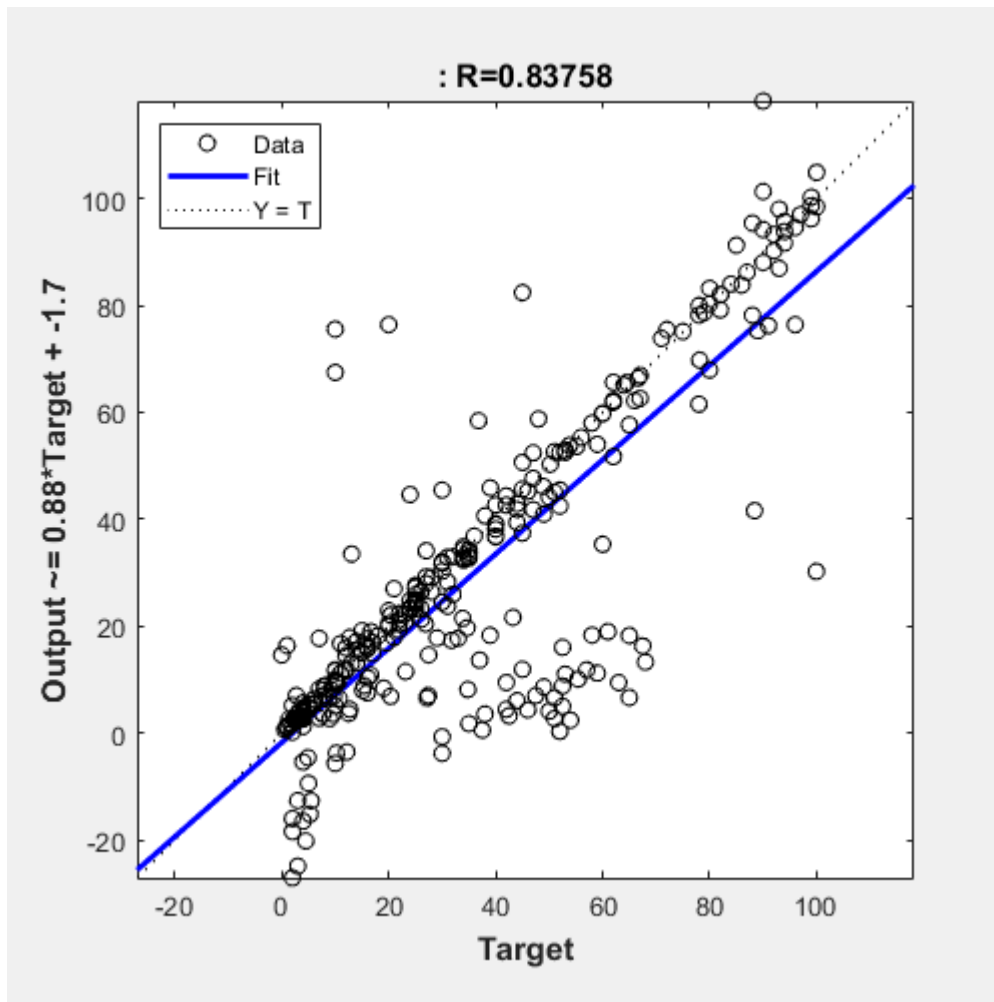
totalRMSEPr = 17.4235

RImpPr = (totalRMSEPr - totalRMSE)

RImpPr = 9.7056

plotregression(targets, tyPr)

```



Variable: CeO2 Type

```
inputCT = inputs1;
inputCT.DCeO2Type1 = zeros([318 1]) ; inputCT.DCeO2Type2 = zeros([318 1]); inputCT.DCeO2Type3 = zeros([318 1]);

inputCT;
inputCT = double(inputCT{:,:});

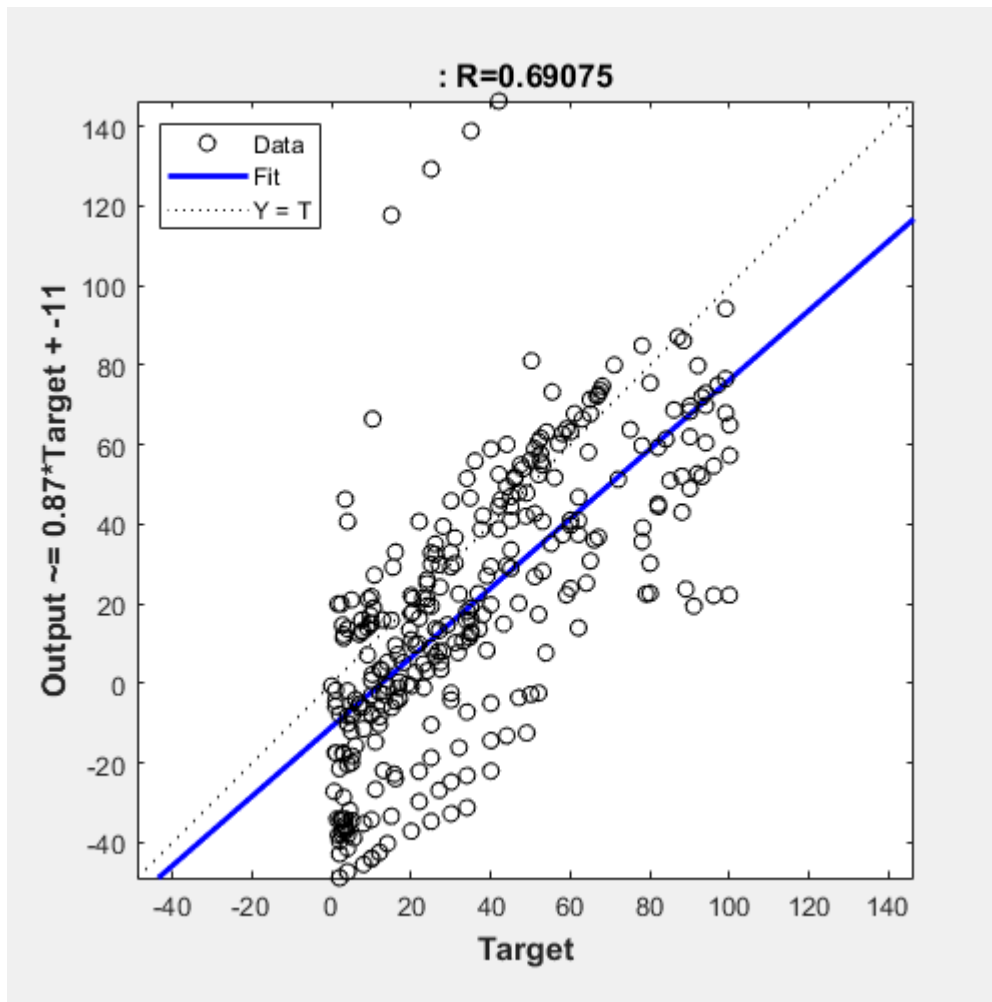
inputCT = fillmissing(inputCT, "constant", 0);
transposedInputCT = transpose(inputCT);

xCT = transposedInputCT;

yCT = BOHnet(xCT);
tyCT = transpose(yCT);
%e = gsubtract(t,yCT);
performance = perform(BOHnet,targets,tyCT);
totalRMSECT = sqrt(performance);
RImpCT = (totalRMSECT - totalRMSE)
```

RImpCT = 22.2880

```
plotregression(targets, tyCT)
```



Variable: Solvents

```
inputSv = inputs1;
inputSv.DSolvent1 = zeros([318 1]); inputSv.DSolvent2 = zeros([318 1]); inputSv.DSolvent3 = zeros([318 1]);
inputSv.DSolvent5 = zeros([318 1]); inputSv.DSolvent6 = zeros([318 1]); inputSv.DSolvent7 = zeros([318 1]);
inputSv.DSolvent9 = zeros([318 1]); inputSv.DSolvent10 = zeros([318 1]);

inputSv = double(inputSv{:,:});

inputSv = fillmissing(inputSv, "constant", 0);
transposedInputSv = transpose(inputSv);
xSv = transposedInputSv;

ySv = BOHnet(xSv);
tySv = transpose(ySv);
%e = gsubtract(t,ySv);
performance = perform(net,targets,tySv)
```

```
performance = 1.0473e+03
```

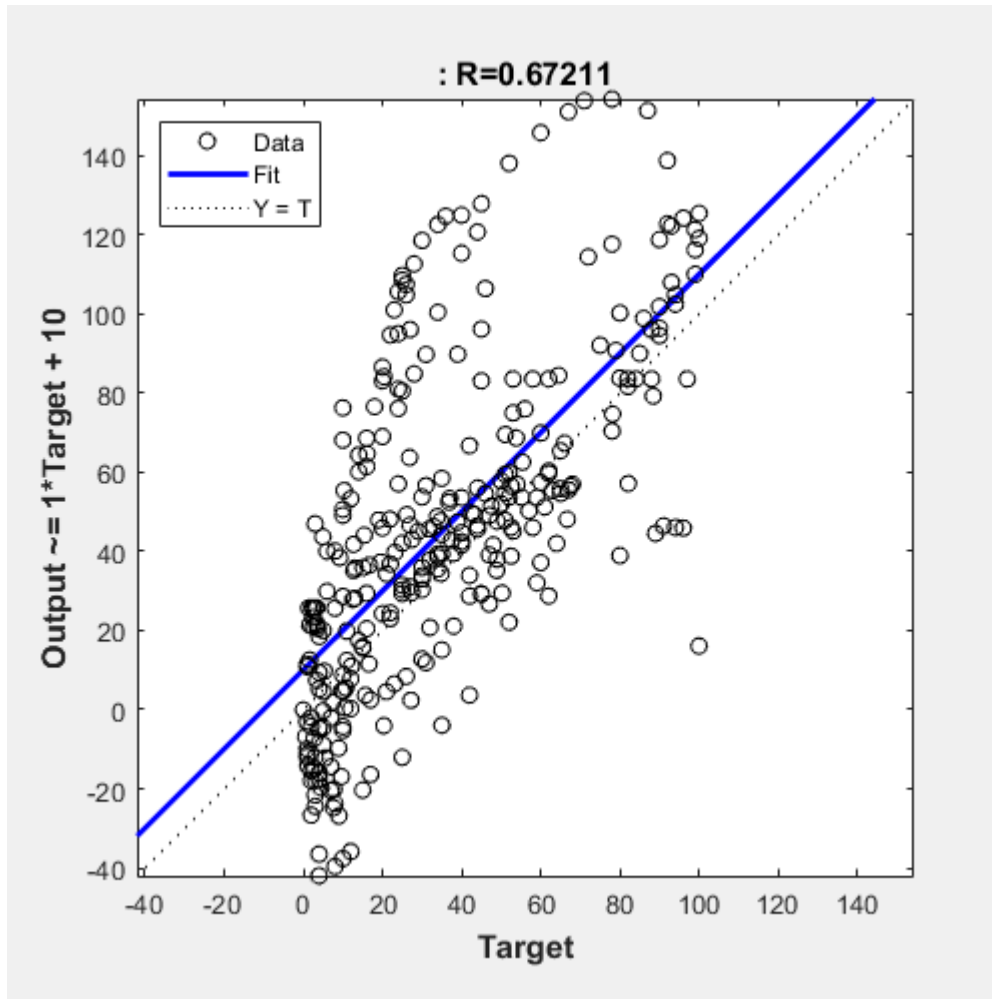
```
totalRMSEsv = sqrt(performance)
```

```
totalRMSEsv = 32.3626
```

```
RImpSv = (totalRMSEsv - totalRMSE)
```

```
RImpSv = 24.6447
```

```
plotregression(targets, tySv)
```



Variable: Volume of Solution

```
inputSA = inputs1;  
inputSA.SolutionAmount = zeros([318 1]) ;  
  
inputSA;  
inputSA = double(inputSA{:,:});  
  
inputSA = fillmissing(inputSA, "constant", 0);  
transposedInputSA = transpose(inputSA);  
  
xSA = transposedInputSA;
```

```

ySA = BOHnet(xSA);
tySA = transpose(ySA);
%e = gsubtract(t,ySA);
performance = perform(BOHnet,targets,tySA)

```

```

performance = 364.2138

```

```

totalRMSESA = sqrt(performance)

```

```

totalRMSESA = 19.0844

```

```

RImpSA = (totalRMSESA-totalRMSE)

```

```

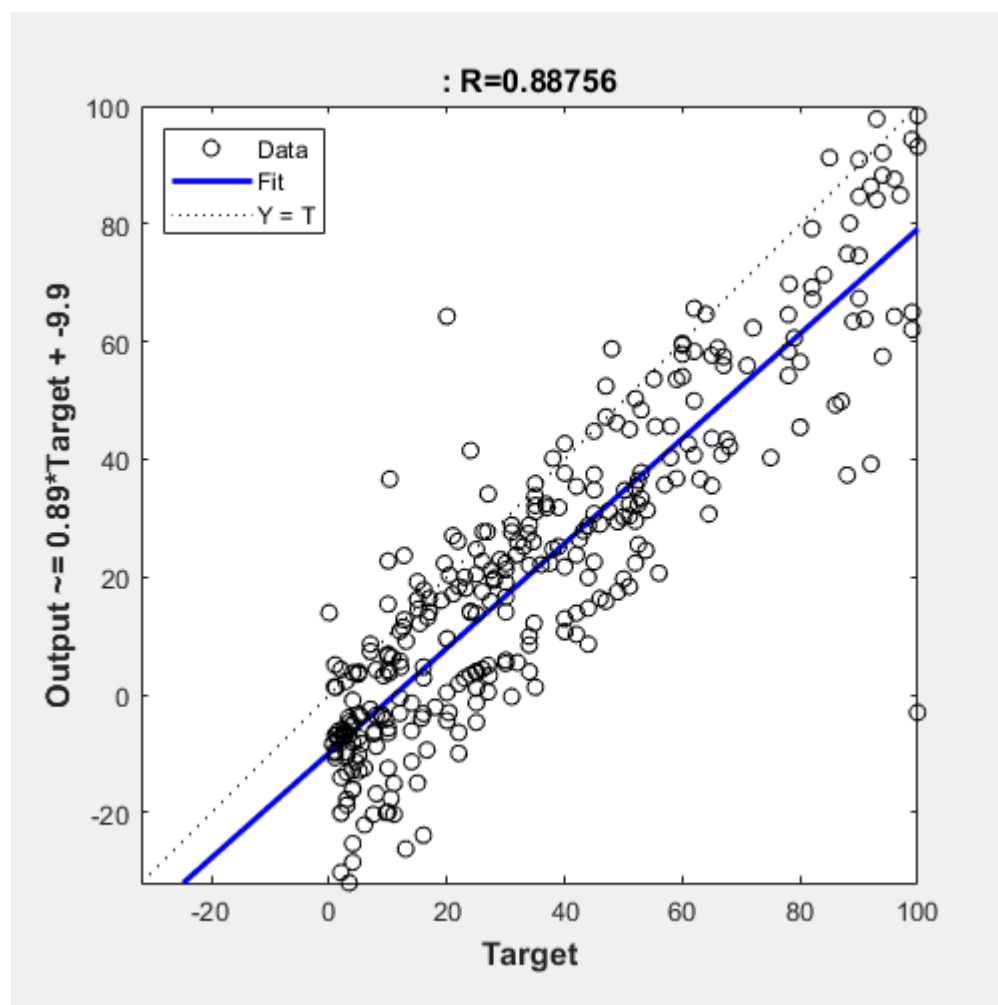
RImpSA = 11.3665

```

```

plotregression(targets, tySA)

```



Variable: Concentration of Benzyl Alcohol

```

inputCB = inputs1;
inputCB.ConcBOHmol = zeros([318 1]);
inputCB = double(inputCB{:,:});

```



```
inputCB = fillmissing(inputCB, "constant", 0);
transposedInputCB = transpose(inputCB);
xCB = transposedInputCB;
```

```
yCB = BOHnet(xCB);
tyCB = transpose(yCB);
%e = gsubtract(t,ySv);
performance = perform(net,targets,tyCB)
```

```
performance = 184.0146
```

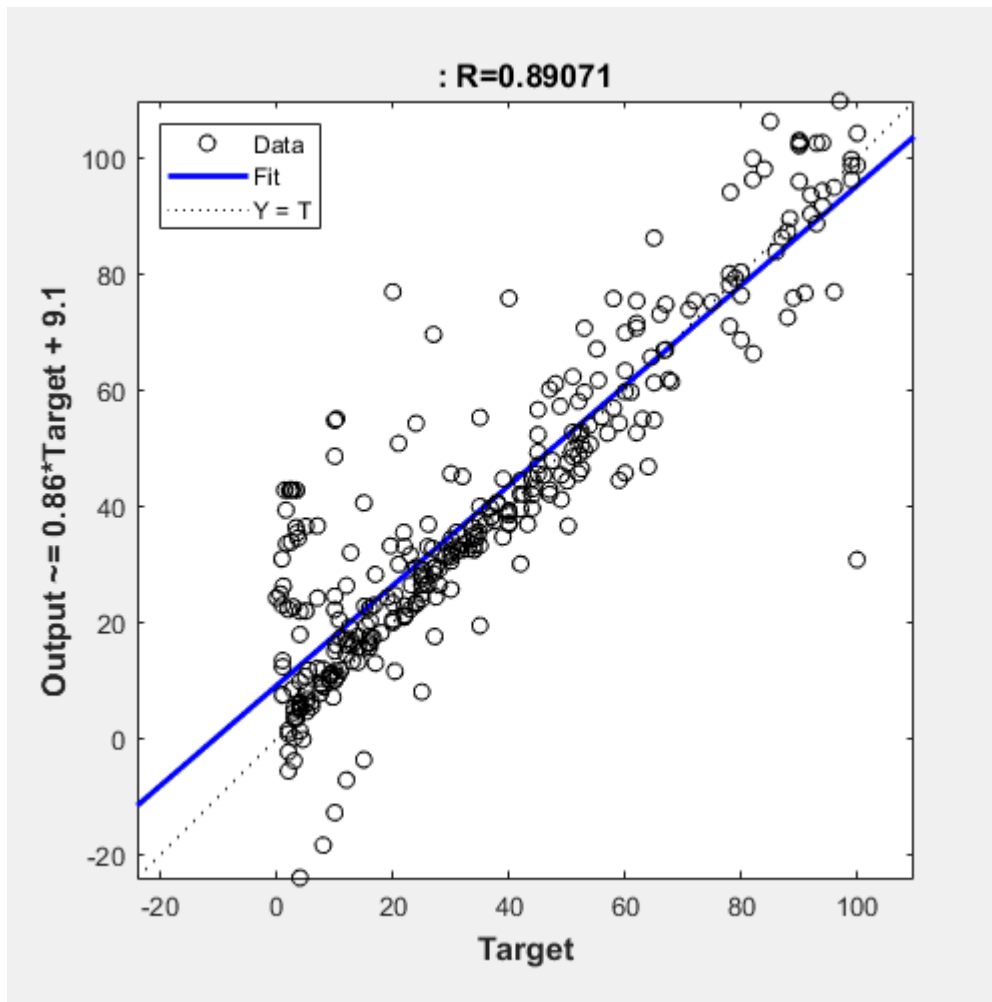
```
totalRMSECB = sqrt(performance)
```

```
totalRMSECB = 13.5652
```

```
RImpCB = (totalRMSECB - totalRMSE)
```

```
RImpCB = 5.8473
```

```
plotregression(targets, tyCB)
```



Variable: Reaction Time

```

inputRt = inputs1;
inputRt.ReactionTimeh = zeros([318 1]);
inputRt = double(inputRt{:,:});

inputRt = fillmissing(inputRt, "constant", 0);
transposedInputRt = transpose(inputRt);
xRt = transposedInputRt;

yRt = BOHnet(xRt);
tyRt = transpose(yRt);
%e = gsubtract(t,yRt);
performance = perform(net,targets,tyRt)

```

```
performance = 1.4261e+03
```

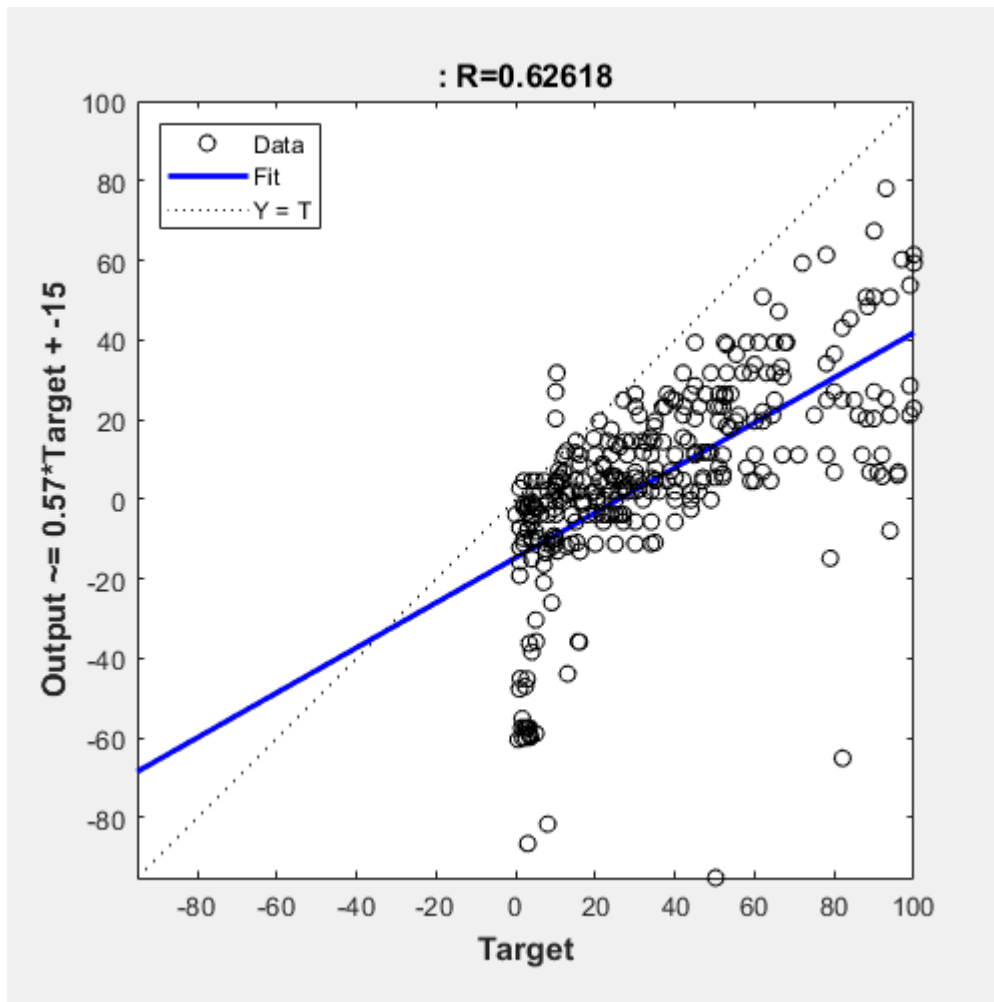
```
totalRMSERt = sqrt(performance)
```

```
totalRMSERt = 37.7633
```

```
RImpRt = (totalRMSERt - totalRMSE)
```

```
RImpRt = 30.0454
```

```
plotregression(targets, tyRt)
```



Variable: Catalyst Amount

```
inputCA = inputs1;
inputCA.CatalystAmountg = zeros([318 1]) ;

inputCA;
inputCA = double(inputCA{:,:});

inputCA = fillmissing(inputCA, "constant", 0);
transposedInputCA = transpose(inputCA);

xCA = transposedInputCA;

yCA = BOHnet(xCA);
tyCA = transpose(yCA);
%e = gsubtract(t,yCA);
performance = perform(BOHnet,targets,tyCA)
```

```
performance = 312.0647
```

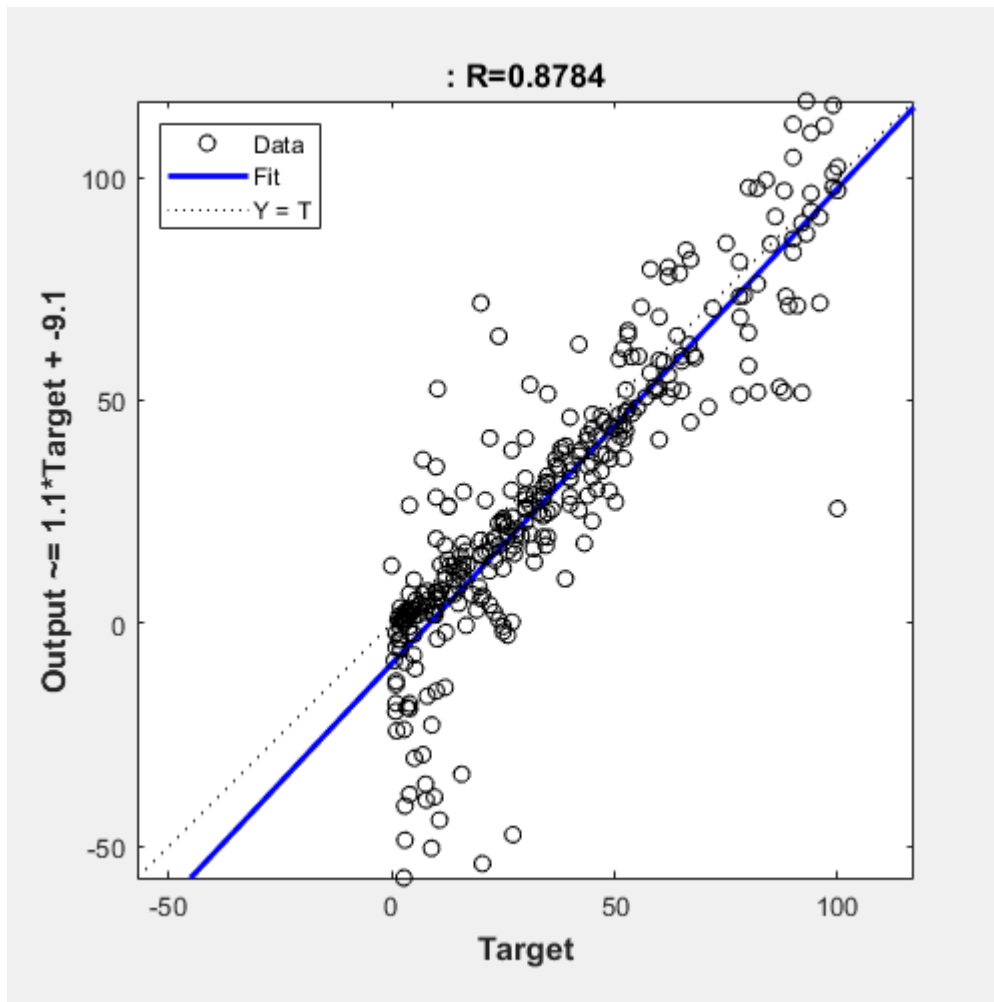
```
totalRMSECA = sqrt(performance)
```

```
totalRMSECA = 17.6654
```

```
RImpCA = (totalRMSECA-totalRMSE)
```

```
RImpCA = 9.9475
```

```
plotregression(targets, tyCA)
```



Variable: Reaction Temperature

```
inputRT = inputs1;  
inputRT.TemperatureK = zeros([318 1]);  
inputRT = double(inputRT{:,:});  
  
inputRT = fillmissing(inputRT, "constant", 0);  
transposedInputRT = transpose(inputRT);  
xRT = transposedInputRT;  
  
yRT = BOHnet(xRT);  
tyRT = transpose(yRT);  
%e = gsubtract(t,ySv);  
performance = perform(net,targets,tyRT)
```

```
performance = 2.8135e+04
```

```
totalRMSERT = sqrt(performance)
```

```
totalRMSERT = 167.7355
```

```
RImpRT = (totalRMSERT - totalRMSE)
```

```
RImpRT = 160.0176
```

```
plotregression(targets, tyRT)
```

