

Pressure1

```
> # pressure1.R
>
> pressure <- read.table("N:/courses/stat8230/Fall11/pressure.dat", header = T)
> plot(pressure$temp,pressure$pres,xlab="Temperature",ylab="Pressure")
> pressure2 <- pressure[2:14, ]
> th10 <- 4.14
> lm1 <- lm(l(1/log(pres/4.14)) ~ l(1/temp), data = pressure2)
> th20 <- 1/coef(lm1)[1]
> th30 <- coef(lm1)[2] * th20
> th10
[1] 4.14
> th20
(Intercept)
 18.07346
> th30
l(1/temp)
 240.0301
> PresMod <- deriv(~ th1 * exp((th2 * x)/(th3 + x)), c("th1", "th2", "th3"),
+   function(x, th1, th2, th3) { })
> nls(pres~PresMod(temp,th1,th2,th3),data=pressure,
+   start=c(th1=4.14,th2=18.07,th3=240.03))
Nonlinear regression model
  model: pres ~ PresMod(temp, th1, th2, th3)
  data: pressure
   th1  th2  th3
5.267 19.722 294.995
residual sum-of-squares: 1718

Number of iterations to convergence: 3
Achieved convergence tolerance: 9.695e-06
> PresModInit <- function(mCall, LHS, data)
+ {
+   xy <- sortedXyData(mCall[["x"]], LHS, data)
+   th1 <- xy[1, "y"]
+   lmx <- 1/(xy[xy[, "x"] != 0, "x"])
+   lmy <- 1/log(xy[xy[, "x"] != 0, "y"]/th1)
+   coefs <- coef(lm(lmy ~ lmx))
+   th2 <- 1/coefs[1]
+   th3 <- coefs[2] * th2
+   value <- c(th1, th2, th3)
+   names(value) <- mCall[c("th1", "th2", "th3")]
+   value
+ }
> SSPresMod <- selfStart(PresMod, initial = PresModInit,
+   parameters=c("th1", "th2", "th3"))
> getInitial(pres ~ SSPresMod(temp, th1, th2, th3), data = pressure)
  th1  th2  th3
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```

4.14000 18.07346 240.03007
> m1pressure.nls <- nls(pres ~ SSPresMod(temp, th1, th2, th3), data = pressure,
+ trace=T)
19137.55 : 4.14000 18.07346 240.03007
2328.742 : 5.150948 19.384466 285.321030
1719.827 : 5.270145 19.719408 294.924061
1718.211 : 5.267344 19.721933 294.995358
1718.211 : 5.267307 19.721839 294.992925
> summary(m1pressure.nls)

```

Formula: pres ~ SSPresMod(temp, th1, th2, th3)

Parameters:

```

Estimate Std. Error t value Pr(>|t|)
th1  5.267    2.275   2.316 0.04088 *
th2 19.722    4.706   4.191 0.00151 **
th3 294.993  127.218   2.319 0.04066 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

Residual standard error: 12.5 on 11 degrees of freedom

Number of iterations to convergence: 4

Achieved convergence tolerance: 3.609e-07

```

> m1coef<-coef(m1pressure.nls)
> x0<-seq(from=0.1,to=105,by=.1)
> y1<-PresMod(x0,m1coef[1],m1coef[2],m1coef[3])
> lines(x0,y1,lty=1)
> title(main="Pressure vs Steam and NLS Fitted Curve - Good Starting Values")
> m2pressure.nls <- nls(pres ~ PresMod(temp,th1,th2,th3),data=pressure,
+ start=c(th1=10,th2=100,th3=10),trace=T)
3.544460e+81 : 10 100 10
1.433430e+55 : 6.359357e-13 1.000000e+02 1.000000e+01
1.308725e+30 : -1.921539e-25 1.000000e+02 1.000000e+01
1.941651e+13 : 7.403863e-34 1.000000e+02 1.000000e+01
2.632062e+12 : 7.402606e-34 9.900860e+01 1.011884e+01
92722551278 : 1.964200e-33 9.637810e+01 1.044180e+01
2543836 : 2.600513e-32 8.326012e+01 1.215914e+01
Error in nls(pres ~ PresMod(temp, th1, th2, th3), data = pressure, start = c(th1 = 10, :
singular gradient
>
>
>
> plot(pressure$temp,pressure$pres,xlab="Temperature",ylab="Pressure")
> lines(x0,PresMod(x0,10,100,10))
> title(main="Plot of (bad) starting values (10,100,10)")
>

```

```
> plot(pressure$temp,pressure$pres,xlab="Temperature",ylab="Pressure")
> lines(x0,PresMod(x0,.1,.1,.1))
> title(main="Plot of (bad) starting values (.1,.1,.1)")
>
> plot(pressure$temp,pressure$pres,xlab="Temperature",ylab="Pressure")
> lines(x0,PresMod(x0,13.8904,3.882e10,9.651e11),lty=2)
> title(main="Plot of two fitted models obtained from good and bad starting values")
> y1<-PresMod(x0,m1coef[1],m1coef[2],m1coef[3])
> lines(x0,y1,lty=3)
> legend(locator(1),lty=c(2,3),legend=c("SAS fit from bad starting values","Fit from good starting
values"))
>
```