Unfolding_curves

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Loading libraries and functions

```
library(ggplot2)
library(tidyr)
library(minpack.lm)

nls.fit<-function(data=data){
  y<-nlsLM(unfolding ~ min+ (1-min)/(1+exp((-slope*(Tm-T)))),data=data,
           start=list(slope=.5,Tm=45,min=.3),
           trace=TRUE,control=nls.control(warnOnly = TRUE, tol = 1e-05, maxiter=1000))
  #return(y)
  return(summary(y)$coefficients)
  }


#Function that predicts values given parameter estimates of curves
fud<-function(T=seq(25,50,1),Tm=40,slope=.5,max=1,min=0){
  y<-min+ (max-min)/(1+exp((-slope*(Tm-T))))
  return(y)
  }
```

Comparing aphaeno and pogo

```
#pogo
T<-c(25,30,35,40,43,45,48,50,55,60,65,70)
ten<-c(1.00,0.984,0.974,0.795,0.787,0.726,0.640,0.574,0.482,0.379,0.387,0.392)
ten.dat<-as.data.frame(cbind(T,ten));names(ten.dat)[2]<-"unfolding"
unfold_10min<-nls.fit(ten.dat)
```

```
## It.    0, RSS =   0.177676, Par. =        0.5         45        0.3
## It.    1, RSS =  0.0352449, Par. =    0.28286    45.3116   0.350342
## It.    2, RSS =  0.0106974, Par. =   0.164097    45.8257   0.377331
## It.    3, RSS = 0.00688326, Par. =   0.194593    46.0904   0.374877
## It.    4, RSS = 0.00684283, Par. =   0.191894    46.1629   0.370234
## It.    5, RSS = 0.00684248, Par. =   0.192381    46.1587   0.370452
## It.    6, RSS = 0.00684247, Par. =   0.192295    46.1598   0.370402
## It.    7, RSS = 0.00684247, Par. =    0.19231    46.1596   0.370411
## It.    8, RSS = 0.00684247, Par. =   0.192307    46.1597   0.370409
```

```
#Aphaeno
avon<-c(0.963,1.00,0.940,0.882,0.755,0.627,0.600,0.549,0.502,0.444,0.368,0.379)
aph<-as.data.frame(cbind(T,avon));names(aph)[2]<-"unfolding"
aph.fit<-nls.fit(aph)
```

```
## It.    0, RSS =    0.15087, Par. =       0.5        45       0.3
## It.    1, RSS =   0.016592, Par. =  0.195679   44.4699  0.421938
## It.    2, RSS =   0.011673, Par. =  0.214061   44.8661  0.394201
## It.    3, RSS =  0.0116427, Par. =  0.214667   44.7658   0.39535
## It.    4, RSS =  0.0116418, Par. =  0.215448   44.7589  0.395681
## It.    5, RSS =  0.0116417, Par. =  0.215601   44.7555  0.395783
## It.    6, RSS =  0.0116417, Par. =  0.215646   44.7547  0.395809
## It.    7, RSS =  0.0116417, Par. =  0.215657   44.7545  0.395816
## It.    8, RSS =  0.0116417, Par. =   0.21566   44.7544  0.395818
```

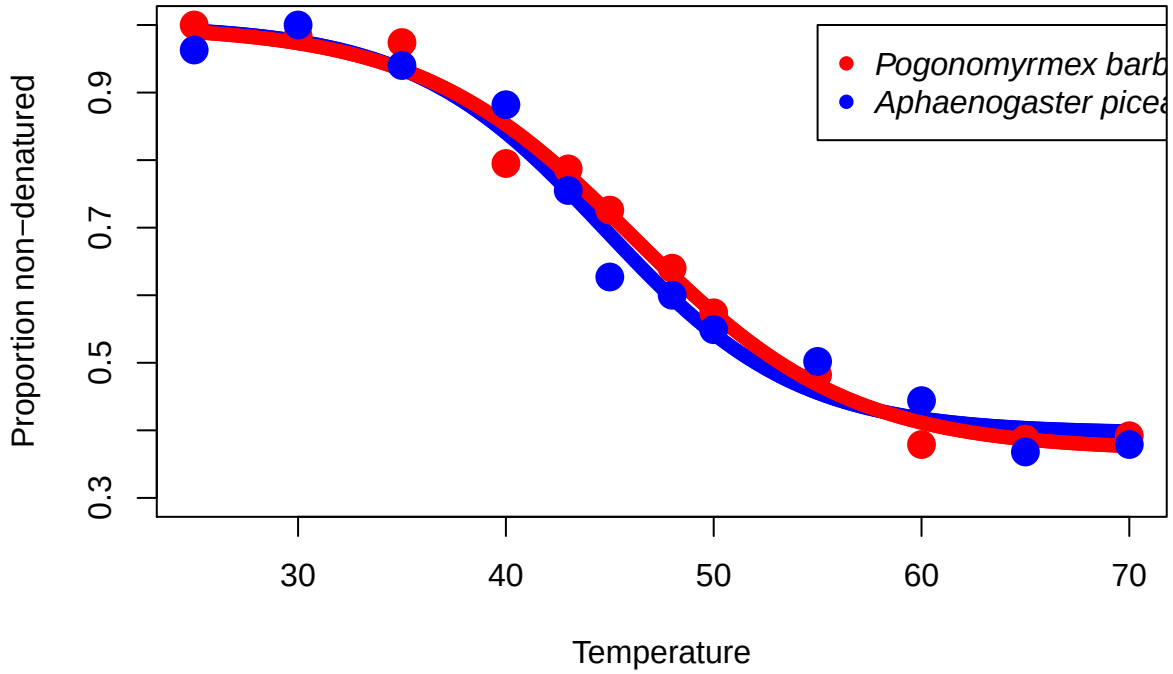
```
#Table of fitted curves
knitr::kable(round(cbind(unfold_10min,aph.fit),3))
```

	Estimate	Std. Error	t value	Pr(>|t|)	Estimate	Std. Error	t value	Pr(>|t|)
slope	0.192	0.021	8.978	0	0.216	0.032	6.735	0
Tm	46.160	0.628	73.484	0	44.754	0.717	62.430	0
min	0.370	0.021	17.755	0	0.396	0.024	16.768	0

```
#difference in TMs
46.16-44.754
```

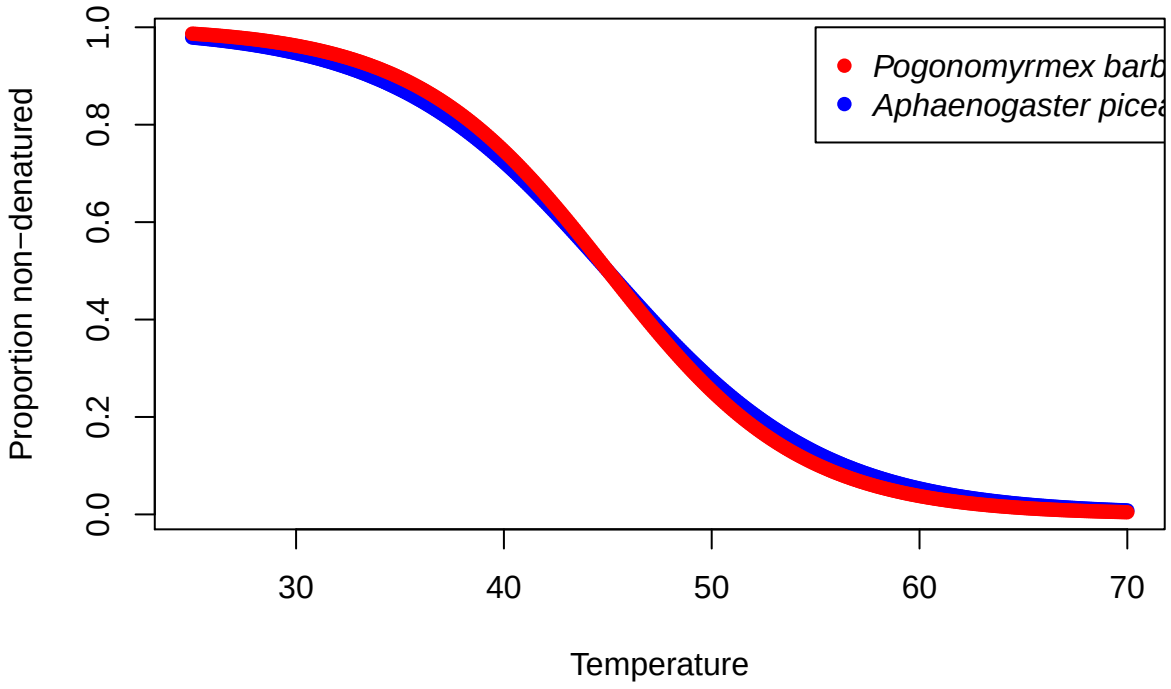
```
## [1] 1.406
```

```
#lets plot these out with all parameters
plot(seq(25,70,.1),fud(T=seq(25,70,.1),max=1,min=0.3958177,Tm=44.7544257,slope=0.2156598),pch=16,col="bl
points(seq(25,70,.1),fud(T=seq(25,70,.1),max=1,min=0.3704093,Tm=46.159662,slope=0.1923073),pch=16,col="
points(ten.dat$T,ten.dat$unfolding,pch=16,col="red",cex=2)
points(aph$T,aph$unfolding,pch=16,col="blue",cex=2)
legend(55,1,c("Pogonomyrmex barbatus","Aphaenogaster picea"),text.font=3,pch=16,col=c("red","blue"))
```



```
#abline(v=c(46.1596629,44.7544257),lty=c(1,3),lwd=3)

##plot by only slope
plot(seq(25,70,.1),fud(T=seq(25,70,.1),slope= 0.192,Tm=45),pch=16,col="blue",ylab="Proportion non-denatu
points(seq(25,70,.1),fud(T=seq(25,70,.1),slope= 0.216,Tm=45),pch=16,col="red")
legend(55,1,c("Pogonomyrmex barbatus","Aphaenogaster picea"),text.font=3,pch=16,col=c("red","blue"))
```



comparing 10 vs 20 min

```
# 10 min inc
#earlier
unfold_10min<-nls.fit(ten.dat)
```

```
## It.    0, RSS =   0.177676, Par. =        0.5         45        0.3
## It.    1, RSS =  0.0352449, Par. =    0.28286    45.3116   0.350342
## It.    2, RSS =  0.0106974, Par. =   0.164097    45.8257   0.377331
## It.    3, RSS = 0.00688326, Par. =   0.194593    46.0904   0.374877
## It.    4, RSS = 0.00684283, Par. =   0.191894    46.1629   0.370234
## It.    5, RSS = 0.00684248, Par. =   0.192381    46.1587   0.370452
## It.    6, RSS = 0.00684247, Par. =   0.192295    46.1598   0.370402
## It.    7, RSS = 0.00684247, Par. =    0.19231    46.1596   0.370411
## It.    8, RSS = 0.00684247, Par. =   0.192307    46.1597   0.370409
```

```
# 20 min incubation
twen<-c(0.977,0.988,1.00,0.822,0.664,0.564,0.479,0.473,0.432,0.350,0.315,0.304)
ty.dat<-as.data.frame(cbind(T,twen));names(ty.dat)[2]<-"unfolding"
unfold_20min<-nls.fit(ty.dat);unfold_20min
```

```
## It.    0, RSS =  0.0814259, Par. =        0.5         45        0.3
## It.    1, RSS =  0.0410429, Par. =   0.168066    43.7697    0.34645
## It.    2, RSS =  0.0156805, Par. =   0.241643    43.3873    0.34359
## It.    3, RSS =  0.0138579, Par. =   0.272779     43.402   0.341841
## It.    4, RSS =  0.0137676, Par. =   0.279046    43.3088   0.344028
## It.    5, RSS =  0.0137596, Par. =   0.281478    43.2893   0.344851
## It.    6, RSS =  0.0137589, Par. =   0.282133    43.2818   0.345118
## It.    7, RSS =  0.0137588, Par. =   0.282345    43.2797   0.345199
## It.    8, RSS =  0.0137588, Par. =   0.282407    43.2791   0.345224
## It.    9, RSS =  0.0137588, Par. =   0.282426    43.2789   0.345231
## It.   10, RSS =  0.0137588, Par. =   0.282432    43.2788   0.345234
```

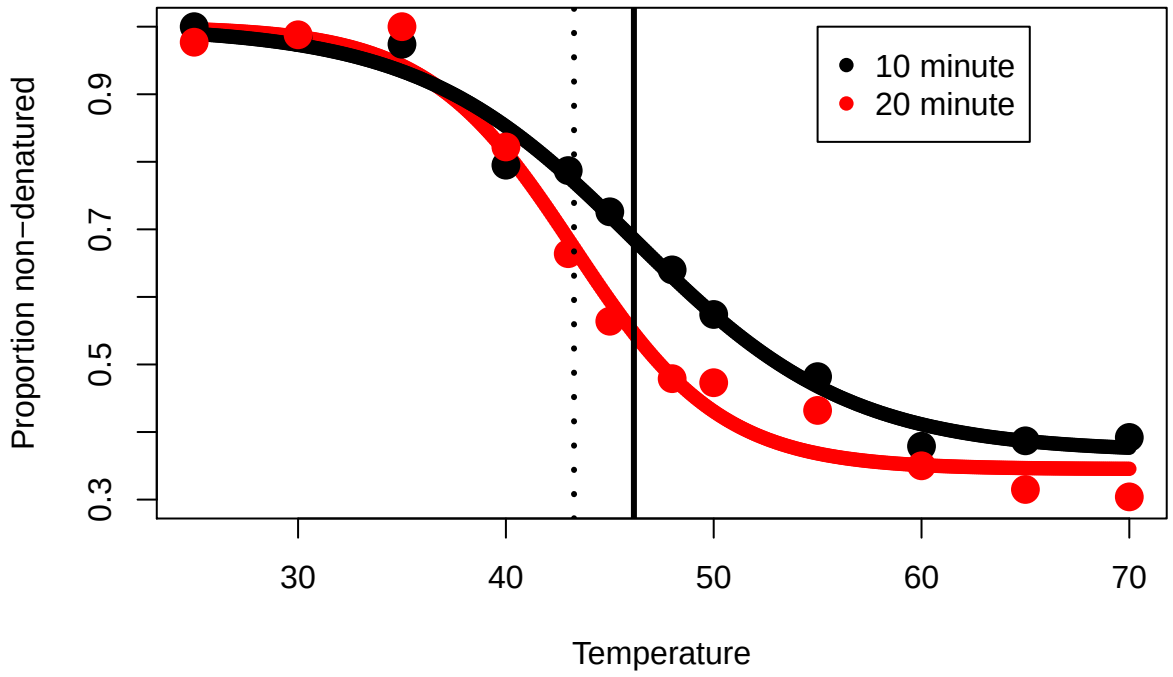
```
##          Estimate Std. Error   t value     Pr(>|t|)
## slope  0.2824321 0.04299893  6.568353 1.029638e-04
## Tm    43.2788185 0.55742928 77.640017 4.936846e-14
## min    0.3452337 0.02148068 16.071821 6.186155e-08
```

```
knitr::kable(round(cbind(unfold_10min,unfold_20min),3))
```

	Estimate	Std. Error	t value	Pr(>|t|)	Estimate	Std. Error	t value	Pr(>|t|)
slope	0.192	0.021	8.978	0	0.282	0.043	6.568	0
Tm	46.160	0.628	73.484	0	43.279	0.557	77.640	0
min	0.370	0.021	17.755	0	0.345	0.021	16.072	0

```
#plots


plot(seq(25,70,.1),fud(T=seq(25,70,.1),max=1,min=0.3452337,Tm=43.2788185,slope=0.2824321),pch=16,col="r
points(seq(25,70,.1),fud(T=seq(25,70,.1),max=1,min=0.3704093,Tm=46.159662,slope=0.1923073),pch=16,col="
points(ten.dat$T,ten.dat$unfolding,pch=16,col="black",cex=2)
points(ty.dat$T,ty.dat$unfolding,pch=16,col="red",cex=2)
abline(v=c(46.1596629,43.2788185),lty=c(1,3),lwd=3)
legend(55,1,c("10 minute","20 minute"),pch=16,col=c("black","red"))
```

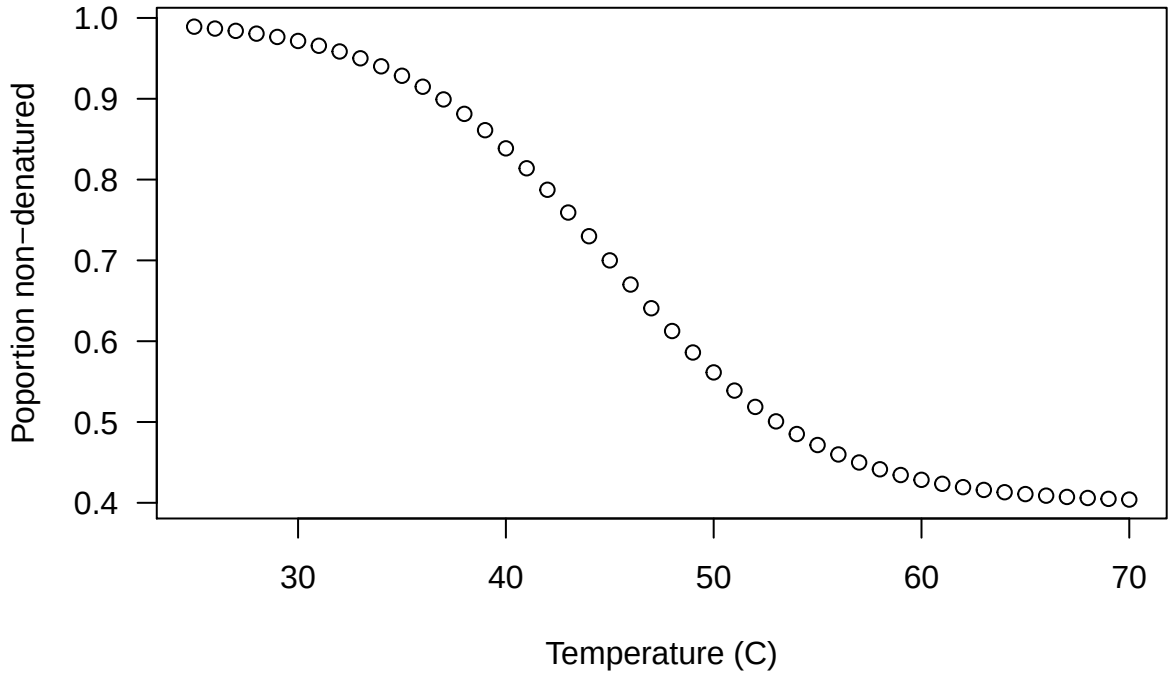


How to sample a reaction norm?

```
unfolding<-fud(T=seq(25,70,1),Tm=45,slope=.2,min=.4)
T<-seq(25,70,1)
com<-cbind(T,unfolding);head(com)
```

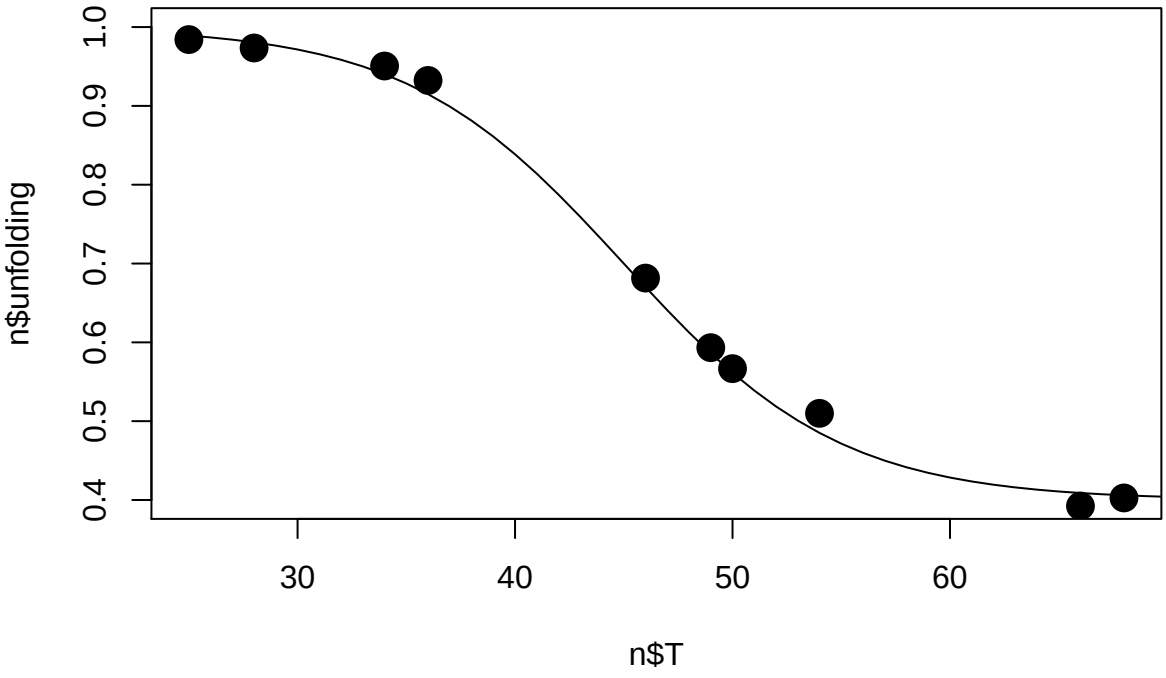
```
##       T unfolding
## [1,] 25 0.9892083
## [2,] 26 0.9868712
## [3,] 27 0.9840418
## [4,] 28 0.9806227
## [5,] 29 0.9765006
## [6,] 30 0.9715445
```

```
plot(T,unfolding,ylab="Poportion non-denatured",xlab="Temperature (C)",las=1)
```




```
#sample random points
n<-as.data.frame(com[sample(nrow(com), 10), ])# randomly sampling
n$unfolding<-n[,2]+rnorm(mean=0,sd=0.02,n=10)# adding error

plot(n$T,n$unfolding,pch=16,col="black",cex=2,ylim=c(.4,1))
lines(T,unfolding)
```




```
tt<-nls.fit(n)
```

```
## It.    0, RSS =   0.170025, Par. =        0.5         45        0.3
```

```
## It.    1, RSS =   0.103582, Par. =   0.411168    45.2577     0.3188
## It.    2, RSS =   0.019024, Par. =    0.26949    45.6514   0.357551
## It.    3, RSS = 0.00125539, Par. =   0.187261    45.4379   0.396895
## It.    4, RSS = 0.000862112, Par. =    0.19808    45.6772   0.392338
## It.    5, RSS = 0.000860807, Par. =   0.198727    45.6604     0.3926
## It.    6, RSS = 0.000860804, Par. =   0.198765    45.6597   0.392628
## It.    7, RSS = 0.000860804, Par. =   0.198767    45.6596   0.392629
```

```
knitr::kable(tt)
```

	Estimate	Std. Error	t value	Pr(>|t|)
slope	0.1987674	0.0095516	20.80993	1e-07
Tm	45.6596053	0.2835719	161.01596	0e+00
min	0.3926294	0.0087033	45.11292	0e+00