

Unfolding_curves

Antdrew D. Nguyen

2016-April-26

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
```

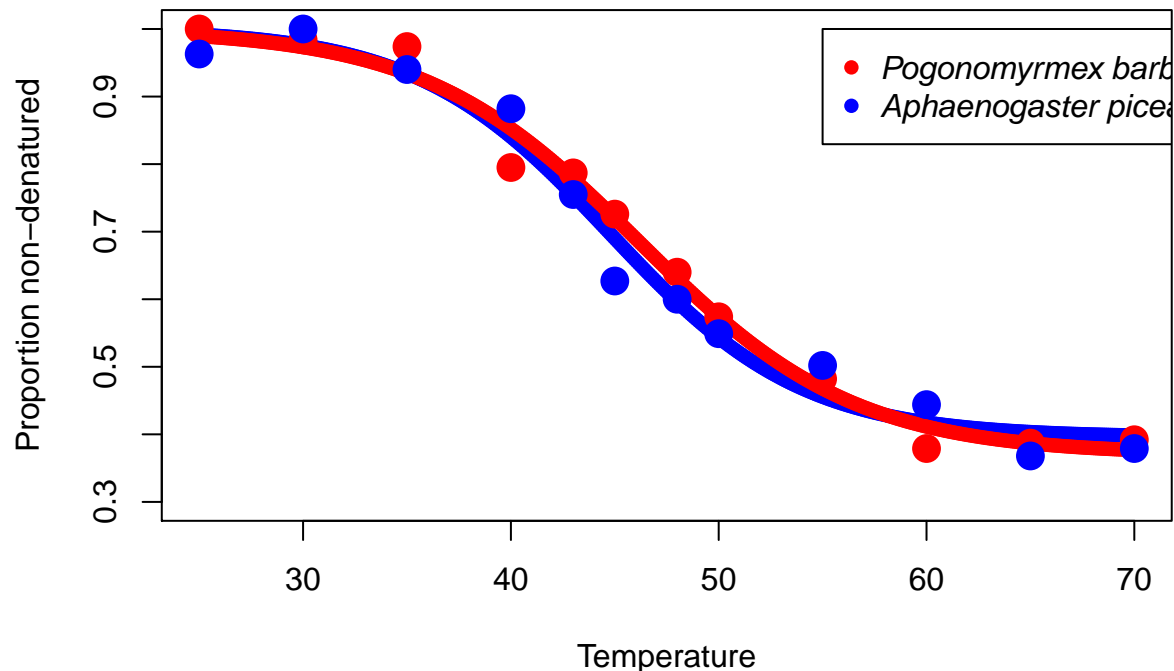
```
#Table of fitted curves
knitr::kable(round(cbind(unfold_10min,aph.fit),3))
```

	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="blue",lty=1)
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="red",lty=1)
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"))
```



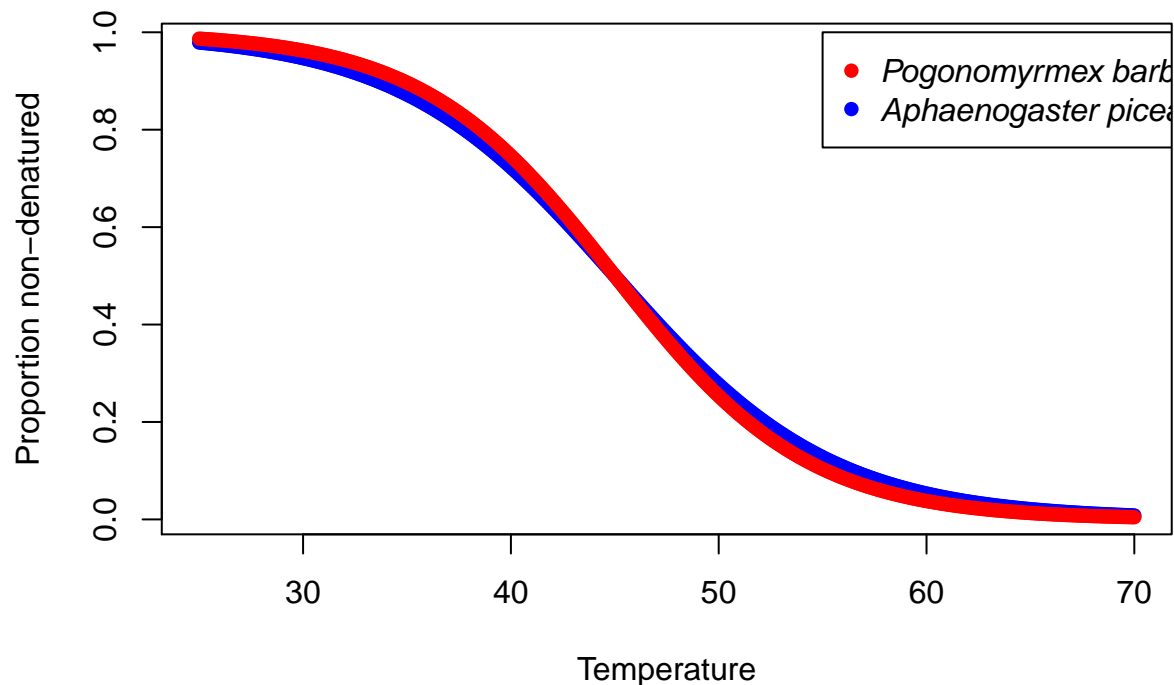
```
#abline(v=c(46.1596629,44.7544257),lty=c(1,3),lwd=3)
```

```
##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-denatured",
```

```
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",lty=1)
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="r",lty=1)
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"))
```

