

Unfolding_curves

Antdrew D. Nguyen

2016-April-26

```
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=.5),
  #return(y)
  return(summary(y)$coefficients)
}
```

```
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)
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)

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

```
ty.dat<-as.data.frame(cbind(T,twen));names(ty.dat)[2]<-"unfolding"
unfold_20min<-nls.fit(ty.dat)
```

## 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

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

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