Basic Model

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1. Notations

- n_s is the number of sites
- N_{ts} be the number of species at time t and site s
- d_{si} be the distance between two sites s and site i. Currently I am using the signed(North is positive) distance(unit is degree) of the latitude between each two sites.
- The environmental variables are e_{chi}, e_{sst} and e_{upw}
- Let $y_{ts} = \log N_{(t+1)s}$.

2. The model

The dispersal kernel(for site i) is some constant($K = e^k$) times the following term:

$$N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}},$$

where N_{ti} is the number of species at time t and site i.

So, the raw model is:

$$y = k + \log(\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}) + \beta_1 e_{chi} + \beta_2 e_{sst} + \beta_3 e_{upw} + \epsilon,$$

where $\epsilon \sim N(0, \sigma^2)$. So we have

- three parameters related to the **dispersal**: k, μ_d, σ_d.
- three parameters for the **environmental** variables $\beta_1, \beta_2, \beta_3$.

3. Estimation

Let $\theta = (k, \mu_d, \sigma_d, \beta_1, \beta_2, \beta_3)$, x be our data (N:number of species, d:distance between the sites, e: the environmental variables), $y = f(x, \theta)$ is our model. Then $y \sim N(f(x, \theta), \sigma^2)$

$$L(\theta; y, x) = \prod_{j=1}^{m} \phi(\frac{y_j - f(x_j, \theta)}{\sigma})$$

and

$$l(\theta; y, x) = \log L(\theta; y, x) = \sum_{j=1}^{m} \log \phi(\frac{y_j - f(x_j, \theta)}{\sigma})$$

Note: The model is a nonlinear regression problem. After some calculation about the above log-likelihood function, we can show that: maximum likelihood estimation is equivalent to the nonlinear least square estimation. So we need to minimize the objective function:

$$\sum_{j=1}^{n} (y_j - f(x_j, \theta))^2$$

4. About the Data

As for our data, we have 4 years(year0, year1, year2, year3) data. So y should be

$$y = N_{ts} \quad for \quad [year1(s1,...,s48), year2(s1,...,s48), year3(s1,...,s48)]$$

Predictive variables x contains three parts:

1. species number N,

$$N = N_{ts} \quad for \quad [year0(s1,...,s48), year1(s1,...,s48), year2(s1,...,s48)]$$

2. the distance d, which should be a distance matrix between the sites (s1,...,s48)
3. the environmental variables e_i, which is

$$e_i = e_i \quad for \quad [year0(s1,...,s48), year1(s1,...,s48), year2(s1,...,s48)]$$

5. Code and Results

5.1 EDA

```
library(synchrony)
```

```
## synchrony 0.2.3 loaded.
```

```
data(pisco.data)
head(pisco.data)
```

```
##   latitude longitude       chl      sst upwelling mussel_abund year
## 1 32.71167 -117.2500 0.8897000 16.51596  85.17711       1.0667 2000
## 2 32.82000 -117.2767 0.8095000 16.76317  85.17711      46.7000 2000
## 3 32.84000 -117.2800 0.7844000 16.78249  85.17711      10.6000 2000
## 4 33.44000 -118.4767 0.5192727 16.48601  70.71932       2.8000 2000
## 5 33.45000 -118.4800 0.5192727 16.44148  70.71932       0.9333 2000
## 6 33.46000 -118.5200 0.5017273 16.44452  56.26153       0.4000 2000
```

```
summary(pisco.data)
```

```
##     latitude       longitude           chl                 sst
##  Min.   :32.71   Min.   :-124.7   Min.   : 0.4091   Min.   : 8.598
##  1st Qu.:34.36   1st Qu.:-124.1   1st Qu.: 1.2910   1st Qu.:10.899
##  Median :38.83   Median :-123.4   Median : 3.0401   Median :11.894
##  Mean   :39.55   Mean   :-122.1   Mean   : 4.2056   Mean   :12.643
##  3rd Qu.:44.37   3rd Qu.:-120.0   3rd Qu.: 7.0753   3rd Qu.:14.664
##  Max.   :48.39   Max.   :-117.2   Max.   :15.0320   Max.   :17.290
##    upwelling       mussel_abund         year
```

```
##  Min.   :-57.69   Min.   : 0.000   Min.   :2000
##  1st Qu.:-23.02   1st Qu.: 6.592   1st Qu.:2001
##  Median : 59.26   Median :24.817   Median :2002
##  Mean   : 37.82   Mean   :27.292   Mean   :2002
##  3rd Qu.: 84.36   3rd Qu.:44.008   3rd Qu.:2002
##  Max.   :120.82   Max.   :81.300   Max.   :2003
```

In the above data:

- lat and lon: the location of the stations(48 different stations)
- chl, sst, and upwelling: the environmental variables
- mussel_abund: the variable we want to predict
- year: 2000-2004

Now we extract the target variable, and the predictive variables:

```r
y=subset(pisco.data,year>2000,select=c(mussel_abund)) # species number
y[y[,1]==0,]=min(y[y[,1]!=0,])/2 # replace 0 to half of the minimum positive number
y=log(y) # take log of the species number

N=subset(pisco.data,year<2003,select=c(mussel_abund)) # (past) species number
#D=coord2dist(pisco.data[1:48,1:2],lower.tri = F) # site distance using lat and lon
D=dist(pisco.data[1:48,1],diag = T,upper = T) # site distance using only (signed) lat
D=as.matrix(D)
for(i in 1:48){
    for(j in 1:48){
        if(i>j){
            D[i,j]=-D[i,j]
        }
    }
}
E=subset(pisco.data,year<2003,select=c(chl,sst,upwelling)) # Environment variable
D=as.matrix(D)
D[1:6,1:6]
```

```
##            1           2           3           4            5           6
## 1  0.0000000  0.10833359  0.12833405  0.72833252  0.738334656 0.748332977
## 2 -0.1083336  0.00000000  0.02000046  0.61999893  0.630001068 0.639999390
## 3 -0.1283340 -0.02000046  0.00000000  0.59999847  0.610000610 0.619998932
## 4 -0.7283325 -0.61999893 -0.59999847  0.00000000  0.010002136 0.020000458
## 5 -0.7383347 -0.63000107 -0.61000061 -0.01000214  0.000000000 0.009998322
## 6 -0.7483330 -0.63999939 -0.61999893 -0.02000046 -0.009998322 0.000000000
```

Here, we define the objective function. Since we want to do minimization(not max), the objective function is the either the negative log-likelihood function, or the nonlinear least squre error(they are equivalent in our case). The input arguments are:

- t: all the parameters which need to do minimization, $(k, \mu_d, \sigma_d, \beta_1, \beta_2, \beta_3)$
- y: target variable(log of species number)
- N: past species number
- D: distance matrix among 48 sites
- E: 3 environmental variables

5.2 First Model

$$y = k + \log(\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}) + \beta_1 e_{chi} + \beta_2 e_{sst} + \beta_3 e_{upw} + \epsilon,$$

```
# log-likelihood function
logl2=function(t,y,N,D,E){
  n=dim(y)[1]
  f=rep(0,n) # value of the regression function
  yr=rep(0:2,each=48) # 3 years(0-2) used: 00-03 for X, 01-04 for y
  for(j in 1:n){
    # dispersal kernal (for the 48 sites)
    Ker=exp(-(D[j%%48+((j%%48)==0)*48,]-t[2])^2/(t[3]^2))
    # number of species for 48 sites
    Nj=N[(yr[j]*48+1):((yr[j]+1)*48),]
    # dispersal + three environment terms
    f[j]=t[1]+log(sum(Ker*Nj))+t[4]*E[j,1]+t[5]*E[j,2]+t[6]*E[j,3]
  }

  return(sum((y[,1]-f)^2)) # return the objective function
}


# do the optimization to find the parameters
t0=c(1,0,1,0.1,0.1,0.1)
res2=nlm(logl2,t0,hessian=T,print.level=1,y=y,N=N,D=D,E=E,iterlim=1e4,steptol=1e-5)
```

```
## iteration = 0
## Step:
## [1] 0 0 0 0 0 0
## Parameter:
## [1] 1.0 0.0 1.0 0.1 0.1 0.1
## Function Value
## [1] 16552.29
## Gradient:
## [1]   2640.2677    223.2813   2436.9812   7644.3689  35891.0001 187877.4232
##
## iteration = 61
## Parameter:
## [1]  1.0191051955 -0.0035246753 -0.0106411733  0.0001333653 -0.1045139552
## [6]  0.0015669502
## Function Value
## [1] 106.6706
## Gradient:
## [1] -1.40124793  0.02515411  0.22112269  0.03462215  0.01106416 -0.54526949
##
## Successive iterates within tolerance.
## Current iterate is probably solution.
```

```
t=res2$estimate
print("The estimated parameters are:")
```

```
## [1] "The estimated parameters are:"
```

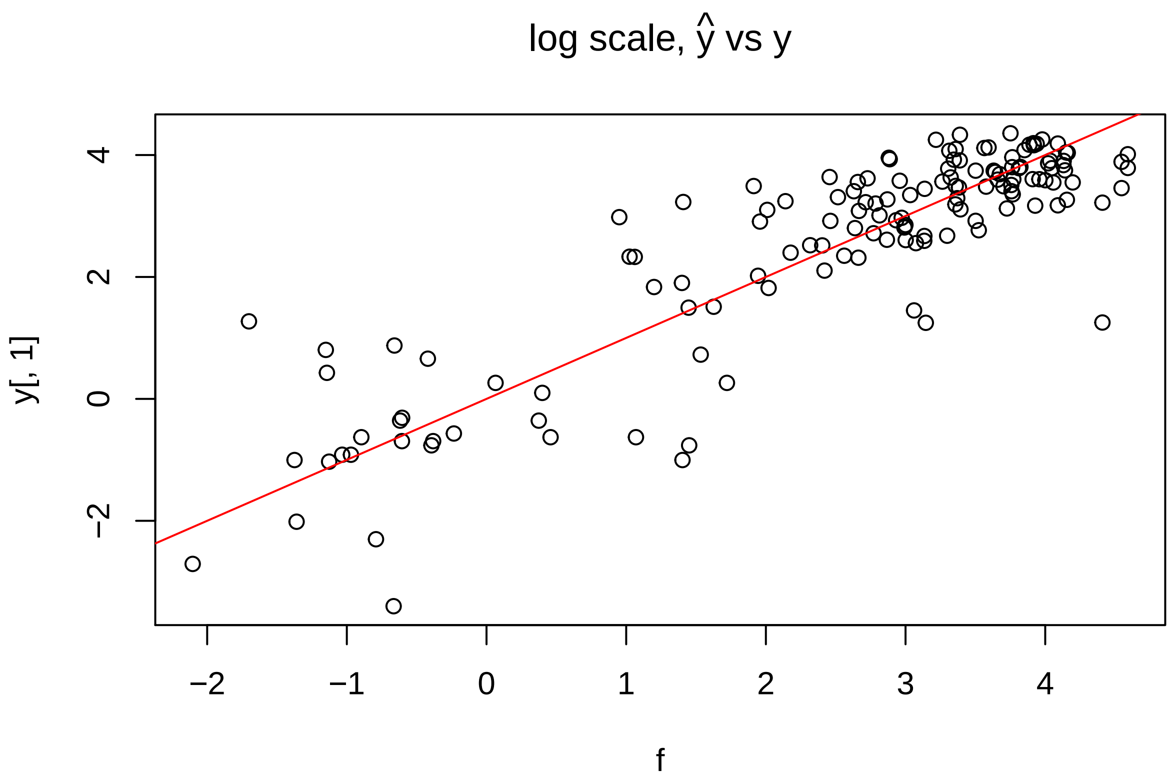
```r
print(t)
```

```
## [1]  1.0191051955 -0.0035246753 -0.0106411733  0.0001333653 -0.1045139552
## [6]  0.0015669502
```

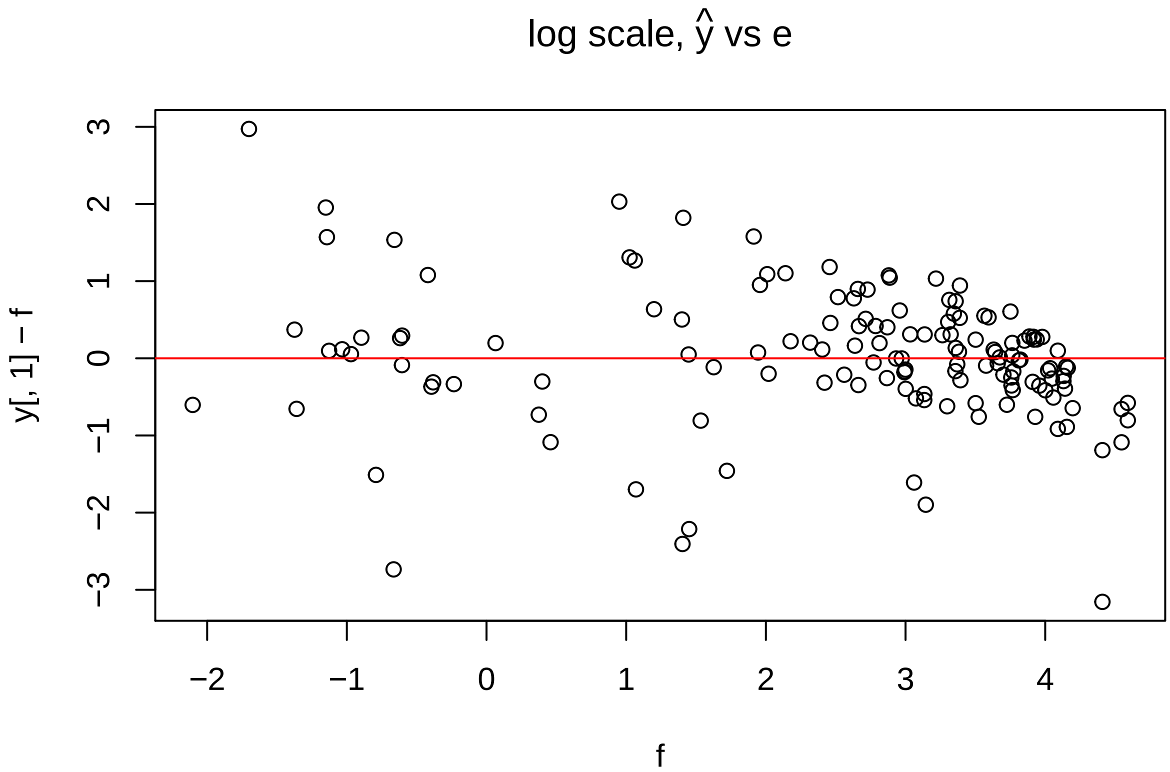
```r
n=dim(y)[1]
  f=rep(0,n) # value of the regression function
  yr=rep(0:2,each=48) # 3 years(0-2) used: 00-03 for X, 01-04 for y
  for(j in 1:n){
    # dispersal kernal (for the 48 sites)
    Ker=exp(-(D[j%%48+((j%%48)==0)*48,]-t[2])^2/(t[3]^2))
    # number of species for 48 sites
    Nj=N[(yr[j]*48+1):((yr[j]+1)*48),]
    # dispersal + three environment terms
    f[j]=t[1]+log(sum(Ker*Nj))+t[4]*E[j,1]+t[5]*E[j,2]+t[6]*E[j,3]
  }
MSE=mean((y[,1]-f)^2)
print(paste("MSE in log scale is: ",MSE))
```

```
## [1] "MSE in log scale is:  0.740768043728402"
```

```r
par(mfrow=c(1,1))
options(repr.plot.width = 10)
options(repr.plot.height = 5)
plot(f,y[,1],main=expression(paste("log scale, ", hat(y)," vs y")))
abline(a=0,b=1,col=2)
```



```r
plot(f,y[,1]-f,main=expression(paste("log scale, ", hat(y)," vs e")))
abline(a=0,b=0,col=2)
```



5.3 95% Confidence Interval for μ_d

Using the fact that MLE is aymptotic normal,

$$\sqrt{n}(\hat{\theta}-\theta) \to N(0, \frac{1}{I_1(\theta)}),$$

i.e. $\hat{\theta} = N(\theta, \frac{1}{I_n(\theta)})$, where $I_n(\theta) = nI_1(\theta)$ is the Fisher Information for n sample points, and one sample point. So the 95% C.I. for θ is

$$\hat{\theta} \pm 1.96\frac{1}{\sqrt{J_n(\hat{\theta})}},$$

where $J_n(\hat{\theta})$ is the observed Fisher Information $J_n(\hat{\theta}) = -l_n''(\theta) = -\sum_{i=1}^{n}(\log f(X_i;\theta))''$

$$\begin{aligned}
l(\theta; y, X) &= \sum_{j=1}^{m} \log\phi(\frac{y_j - f(x_j;\theta)}{\sigma}) \\
&= \sum_{j=1}^{m}[\log(\frac{1}{\sqrt{2\pi}}) - \frac{1}{2}[\frac{y_j - f(x_j;\theta)}{\sigma}]^2 \\
&= m\log(\frac{1}{\sqrt{2\pi}}) - \frac{1}{2\sigma^2}\sum_{j=1}^{m}[y_j - f(x_j;\theta)]^2
\end{aligned}$$

$$\frac{\partial l}{\partial \mu_d} = \frac{1}{\sigma^2}\sum_{j=1}^{m}[y_j - f(x_j;\theta)]\frac{\partial f}{\partial \mu_d}$$

$$\begin{aligned}\frac{\partial^2 l}{\partial \mu_d^2} &= \frac{1}{\sigma^2}\sum_{j=1}^{m}\{[-\frac{\partial f}{\partial \mu_d}]\frac{\partial f}{\partial \mu_d} + [y-f]\frac{\partial^2 f}{\partial \mu_d^2}\} \\ &= \frac{1}{\sigma^2}\sum_{j=1}^{m}[-\frac{\partial f}{\partial \mu_d} - (\frac{\partial f}{\partial \mu_d})^2 + [y-f]\frac{\partial^2 f}{\partial \mu_d^2}]\end{aligned}$$

where,

$$\frac{\partial f}{\partial \mu_d} = \frac{1}{\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}}\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}\frac{2(d_{si}-\mu_d)}{\sigma_d^2}$$

$$\frac{\partial^2 f}{\partial \mu_d^2} = \frac{[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}\frac{2(d_{si}-\mu_d)}{\sigma_d^2}]'[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}] - [\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}]'[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}\frac{2(d_{si}-\mu_d)}{\sigma_d^2}]}{[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}]^2}$$

Here,

$$[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}]' = \sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}\frac{2(d_{si}-\mu_d)}{\sigma_d^2}$$

$$[\sum_{i=1}^{n_s} N_{ti} e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}\frac{2(d_{si}-\mu_d)}{\sigma_d^2}]' = \sum_{i=1}^{n_s} N_{ti}[e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}(\frac{2(d_{si}-\mu_d)}{\sigma_d^2})^2 + e^{-\frac{(d_{si}-\mu_d)^2}{\sigma_d^2}}(-\frac{2}{\sigma_d^2})]$$

```
mu_mle=t[2]
sigma=sd(y[,1]-f)
n=dim(y)[1]
f=rep(0,n) # value of the regression function
fp=rep(0,n)
fpp=rep(0,n)
yr=rep(0:2,each=48) # 3 years(0-2) used: 00-03 for X, 01-04 for y
for(j in 1:n){
    # dispersal kernal (for the 48 sites)
    Ker=exp(-(D[j%%48+((j%%48)==0)*48,]-t[2])^2/(t[3]^2))
    # number of species for 48 sites
    Nj=N[(yr[j]*48+1):((yr[j]+1)*48),]
    # dispersal + three environment terms
    f[j]=t[1]+log(sum(Ker*Nj))+t[4]*E[j,1]+t[5]*E[j,2]+t[6]*E[j,3]
    #--------------------------------------------------------
    dmm=D[j%%48+((j%%48)==0)*48,]-t[2]# d_si - mu_d
    fp[j]=sum(Nj*Ker*2*dmm/t[3]^2)/sum(Ker*Nj) # f'
    Kp=sum(Nj*(Ker*4*dmm^2-Ker*2/t[3]^2)) # derivative of top for f'
    kp=sum(Nj*Ker*2*dmm/t[3]^2) # derivative of bottom for f'
    fpp[j]=(Kp*sum(Ker*Nj)-kp*sum(Nj*Ker*2*dmm/t[3]^2))/sum(Ker*Nj)^2 # f''
}
```

```r
lpp=sum(-fp-fp^2+(y-f)*fp)/sigma^2 #l''(wrt mu_d)
mu_Jn=-lpp # observed Fisher Information
mu_l=1.96/mu_Jn # 95% CI half length
c(t[2]-mu_l, t[2]+mu_l) # 95% CI
```

```
## [1] -0.003526705 -0.003522645
```

6. Comments

- Using $log(N)$ to avoid negative fitting results
- Using signed lat distance to make μ_d having the meaning that the center of the dispersal kernel(moving towards the North ot South of the site). As we can see from the fitting result(second parameter), μ_d is about 0.0035 degree to the South.
- Zero values(in this data set, we do not have too much zeros) are replaced by half of the minimum positive value
- Result may change if the initial value changes(of course, we want the global minimum of the optimization problem).