STAT 574 Linear and Nonlinear Mixed Models

Lecture 9: Programming

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nlme method from nlme package

syntax:

```
nlme(model, data, fixed, random, groups, start, correlation,
     weights, subset, method, na.action, naPattern, control, verbose)
```

`nlme` method from `nlme` package

model:

- a nonlinear formula or a `nlsList` object.
- if `data` is given, all names should be defined in the data frame.

data:

- an optional data frame containing the variables named in model
- by default, the variables are taken from the environment from which `nlme` is called.

Example

We consider the Soybean dataset in nlme.

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
     fixed=Asym+xmid+scal~1,
     random=Asym~1|Plot, data=Soybean,
     start=c(Asym=19, xmid=55, scal=9))
```

Or use nlsList object:

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
     fixed=Asym+xmid+scal~1,
     random=Asym~1|Plot, data=Soybean)
```

- Note that SSlogis is from stats library.
- SSlogis is a self-starting regression object without a start value.
- Other self-starting regression objects:
  SSasymp, SSasympOff, SSasympOrig, SSbiexp, SSfol, SSfpl,
  SSgompertz, SSlogis, SSmicmen, SSweibull

Example

Call without data:

```
weight = Soybean$weight
Time = Soybean$Time
Plot = Soybean$Plot

nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
     fixed=Asym+xmid+scal~1,
     random=Asym~1|Plot,
     start=c(Asym=19, xmid=55, scal=9))
```

Grouped Data

To use self-starting regression objects, data has to be grouped data.

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
    fixed=Asym+xmid+scal~1,
    random=Asym~1,
    groups=~Plot, data=as.data.frame(Soybean))
```

```
Error in nlsList.formula(model = weight ~ SSlogis(Time, Asym, xmid, scal),
  'data' must be a "groupedData" object if 'formula' does not include grou
```

nlme method from nlme package

fixed:

- a two-sided linear formula of the form `f1+...+fn x1+...+xm`, or a list of twosided formulas of the form `f1 x1+...+xm`
- A `1` on the right hand side of the formula(s) indicates a single fixed effects for the corresponding parameter(s).

random:

- a two-sided formula of the form `r1+...+rn x1+...+xm | g1/.../gQ`
- or a two-sided formula of the form `r1+...+rn x1+..+xm`,
- or a list of two-sided formulas of the form `r1 x1+...+xm`,
- or a `pdMat` object.

groups:

- an optional one-sided formula of the form `g1`(single level of nesting) or `g1/.../gQ`

Example

The following models are the same:

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
     fixed=Asym+xmid+scal~1,
     random=Asym+xmid~1|Plot, data=Soybean)
```

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
     fixed=list(Asym~1, xmid~1, scal~1),
     random=Asym+xmid~1, groups=~Plot, data=Soybean)
```

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
     fixed=Asym+xmid+scal~1,
     random=list(Asym~1, xmid~1),
     groups=~Plot, data=Soybean)
```

Adding group covariates to the model

The Soybean has an addititional component Year, which are Plot-specific variables. We can call a NLME model with covariates as

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
     fixed=Asym+xmid+scal~Year,
     random=Asym~1|Plot,
     data=Soybean,
     start=c(19, 0, 0, 55, 0, 0, 9, 0, 0))
```

```
Nonlinear mixed-effects model fit by maximum likelihood
  Model: weight ~ Asym/(1 + exp((xmid - Time)/scal))
  Data: Soybean
  Log-likelihood: -744.1072
  Fixed: Asym + xmid + scal ~ Year
Asym.(Intercept)    Asym.Year1989    Asym.Year1990 xmid.(Intercept)    xmid.Year1989    xmid.Year199(
      22.8886238       -7.5909875       -3.5418714       57.5063970       -3.0099322       -3.572876(
scal.(Intercept)    scal.Year1989    scal.Year1990
       9.3029953       -1.5650331       -0.1703382
```

- We need an initial value of 9 elements because Year is categorical with 3 values.

Adding group covariates to the model

Note that we CANNOT use self-starting regression objects:

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
     fixed=Asym+xmid+scal~Year,
     random=Asym+xmid~1|Plot, data=Soybean)
```

```
Nonlinear mixed-effects model fit by maximum likelihood
  Model: weight ~ SSlogis(Time, Asym, xmid, scal)
  Data: Soybean
  Log-likelihood: -751.7345
  Fixed: list(Asym ~ 1, xmid ~ 1, scal ~ 1)
     Asym      xmid      scal
18.972162 54.870774  8.591342
```

- The `fixed` is overridden by the self-starting regression object.
- because it provides the `start` value.

Adding group covariates to the model

In order to use the self-starting regression object. We need to **update** the model after the initial fit.

```
initial.fit = nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
                   fixed=Asym+xmid+scal~1,
                   random=Asym+xmid~1|Plot, data=Soybean)
fix.coef = fixef(initial.fit)
update(initial.fit, fixed=Asym+xmid+scal~Year,
       start=c(fix.coef[1], 0, 0,
               fix.coef[2], 0, 0,
               fix.coef[3], 0, 0))
```

Grouped Data

The `Year` should be the identical within each `Plot`.

```
> head(Soybean)
Grouped Data: weight ~ Time | Plot
    Plot Variety Year Time weight
1 1988F1       F 1988   14  0.106
2 1988F1       F 1988   21  0.261
3 1988F1       F 1988   28  0.666
4 1988F1       F 1988   35  2.110
5 1988F1       F 1988   42  3.560
6 1988F1       F 1988   49  6.230
```

- But a general data frame cannot ensure that!!

Additional Covariance Structures

The `random` can be a `pdMat` object. Samples are

- `pdSymm`: general positive-definite matrix, with no additional structure
- `pdLogChol`: general positive-definite matrix, with no additional structure, using a log-Cholesky parameterization
- `pdDiag`: diagonal
- `pdIdent`: multiple of an identity
- `pdCompSymm`: compound symmetry structure (constant diagonal and constant off-diagonal elements)
- `pdBlocked`: block-diagonal matrix, with diagonal blocks of any "atomic" pdMat class

Example

Default setting:

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
    fixed=Asym+xmid+scal~1,
    random=Asym+xmid~1|Plot,
    data=Soybean,
    start=c(19, 55, 9))
```

```
Random effects:
 Formula: list(Asym ~ 1, xmid ~ 1)
 Level: Plot
 Structure: General positive-definite, Log-Cholesky parametrization
         StdDev   Corr
Asym     4.346361 Asym
xmid     2.730445 0.569
Residual 1.188992
```

Example

Diagonal setting:

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
    fixed=Asym+xmid+scal~1,
    random=pdDiag(Asym+xmid~1),
    groups=~Plot,
    data=Soybean,
    start=c(19, 55, 9))
```

```
Random effects:
 Formula: list(Asym ~ 1, xmid ~ 1)
 Level: Plot
 Structure: Diagonal
            Asym     xmid Residual
StdDev: 4.078015 2.524942 1.192395
```

Example

Blocked setting:

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
    fixed=Asym+xmid+scal~1,
    random=pdBlocked(list(Asym~1,xmid~1)),
    groups=~Plot,
    data=Soybean,
    start=c(19, 55, 9))
```

```
Random effects:
 Composite Structure: Blocked

 Block 1: Asym
 Formula: Asym ~ 1 | Plot
            Asym
StdDev: 4.077911

 Block 2: xmid
 Formula: xmid ~ 1 | Plot
             xmid Residual
StdDev: 2.524931 1.192399
```

Example

Identity setting:

```
nlme(model=weight~Asym/(1+exp((xmid-Time)/scal)),
    fixed=Asym+xmid+scal~1,
    random=pdIdent(Asym+xmid~1),
    groups=~Plot,
    data=Soybean,
    start=c(19, 55, 9))
```

```
Random effects:
Formula: list(Asym ~ 1, xmid ~ 1)
Level: Plot
Structure: Multiple of an Identity
            Asym     xmid Residual
StdDev: 3.561028 3.561028 1.185689
```

`nlme` method from `nlme` package

correlation:

- Specifies with-in group (conditional) correlation of data.
- Some choices:
  - `NULL`: no correlation (default).
  - `corAR1`, `corARMA`, `corCAR1`: time series correlation.
  - `corExp`, `corGaus`, `corLin`, `corRatio`, `corSpher`: spatial correlation.
  - `corCompSymm`, `corSymm`: symmetric correlation.

weights:

- Specifies with-in group heteroscedasticity structure.

method:

- Fitting method. "REML" or "ML". Default is "ML".

nlme method from nlme package

control:

- Specify algorithmic controls.

```
nlme(model=weight~SSlogis(Time, Asym, xmid, scal),
    fixed=Asym+xmid+scal~1,
    random=Asym~1|Plot, data=Soybean,
    control=nlmeControl(MaxIter=5))
```

Example: Linear Growth Curve Model

```
coef0 = coef(lm(weight~Time, data=Soybean))
nlme(weight~a+b*Time,
    fixed=a+b~Year,
    random=a+b~Year|Plot,
    data=Soybean,
    start=c(coef0[1], 0, 0,
            coef0[2], 0, 0))
```

- The code above is slow due to misspecficiation of the model.