Mixed Model Estimation, a Connection to Additive Models,and Beyond...

Contents

Introduction

The goal is to express the tie between generalized additive models and mixed models, and open the door to further modeling expansion. The following is based on the Wood (2006) text on additive models, chapter 6 in particular. It assumes familiarity with standard regression from a matrix perspective and at least passing familiarity with mixed models.

Model Formulation

We can start with a standard linear model (SLiM) expressed as follows:

$$\mathbf{y} = \mathbf{Xb} + \epsilon$$

Here $\mathbf{y}$ is the target variable, $\mathbf{X}$ is a model matrix, $\mathbf{b}$ are the coefficients, and error ϵ. For cleaner presentation (and background coding on my part), note that beyond this point I'll largely refrain from using bold to indicate vectors/matrices, or using subscripts for every ith observation. Let's just assume we are in a typical data situation involving multiple observations, a univariate vector target variable (y), a (design) matrix of predictor variables (X) etc. Hopefully the context and code will make things very clear.

Now consider a data situation in which observations are clustered, and so non-independent. For example, we might have data regarding students within schools, and we wish to account for the fact that observations of students within a particular school are likely correlated. We can do this within a mixed model framework. For a mixed model with a single random effect for some grouping factor (e.g. school), the SLiM extends to:

$$y = Xb + Zg + \epsilon$$

Where Z is a design matrix pertaining to the grouping structure. Consider a factor z representing group/cluster membership, this would convert z to the following:

z	ZA	ZB	ZC
A	1	0	0
A	1	0	0
B	0	1	0

z	ZA	ZB	ZC
B	0	1	0
C	0	0	1
C	0	0	1

The coefficients g are the random effects, assumed $\mathcal{N}(0, \tau^2)$, i.e. normally distributed with zero mean and τ standard deviation. While we are often interested in these specific effects, they do not have to be estimated directly for modeling purposes.

$$y = Xb + Zg + \epsilon$$
$$g \sim \mathcal{N}(0, \psi_\theta)$$
$$\epsilon \sim \mathcal{N}(0, \Lambda\sigma^2)$$

In this depiction, ψ_θ can reflect some more interesting dependencies, but in the simple case of a random intercepts model it can be a single variance estimate τ^2. Λ can be used to model residual covariance but often is just the identity matrix, with the underlying assumption of constant variance σ^2 across observations.

We can combine the random effects and residuals into a single construct reflecting the covariance structure of the observations:

$$e = Zg + \epsilon$$

This makes **e** a multivariate normal vector with mean 0 and covariance (I is the unit matrix):

$$Z\psi_\theta Z^\intercal + I\sigma^2$$

This puts us back to a standard linear model:

$$y = Xb + e$$
$$e \sim \mathcal{N}(0, \Sigma_\theta\sigma^2)$$

where $\Sigma_\theta = \frac{Z\psi_\theta Z^\intercal}{\sigma^2} + I$.

Maximum Likelihood Estimation

Given where we are now, we can proceed to estimate a mixed model via maximum likelihood. For this we'll use the sleepstudy data from the lme4 package. The data has reaction times for 18 individuals over 10 days each (see the help file for the sleepstudy object for more details).

Data

```
data(sleepstudy, package='lme4')
X = model.matrix(~Days, sleepstudy)
Z = model.matrix(~factor(sleepstudy$Subject)-1)
colnames(Z) =  paste0('Subject_', unique(sleepstudy$Subject))  # for cleaner presentation later
rownames(Z) = paste0('Subject_', sleepstudy$Subject)
y = sleepstudy$Reaction
```

ML function

The following is based on the code in Wood (6.2.2), with a couple modifications for consistent nomenclature and presentation. We use optim and a minimizing function, in this case the negative log likelihood, to estimate the parameters of interest, collectively θ, in the code below. The (square root of the) variances will be estimated on the log scale. In Wood, he simply extracts the 'fixed effects' for the intercept and days effects using lm (6.2.3), and we'll do the same.

```
llMixed = function(y, X, Z, theta){
  tau = exp(theta[1])
  sigma = exp(theta[2])
  n = length(y)

  # evaluate covariance matrix for y
  e = tcrossprod(Z)*tau^2 + diag(n)*sigma^2
  L = chol(e)  # L'L = e

  # transform dependent linear model to independent
  y = backsolve(L, y, transpose=TRUE)
  X = backsolve(L, X, transpose=TRUE)
  b = coef(lm(y~X-1))
  LP = X %*% b

  ll = -n/2*log(2*pi) -sum(log(diag(L))) - crossprod(y-LP)/2
  -ll
}
```

Here is an alternative function using a multivariate normal approach that doesn't use the transformation to independent, and might provide additional perspective.

```
llMixedMV = function(y, X, Z, theta){
  tau = exp(theta[1])
  sigma = exp(theta[2])
  n = length(y)

  # evaluate covariance matrix for y
  e = tcrossprod(Z)*tau^2 + diag(n)*sigma^2

  b = coef(lm.fit(X, y))
  mu = X %*% b

  ll = -mvtnorm::dmvnorm(y, mu, e, log=T)
}
```

Results

Now we're ready to use the optim function for estimation. A slight change to tolerance is included to get closer estimates to lme4, which we will compare shortly.

```
paramInit = c(0, 0)
names(paramInit) = c('tau', 'sigma')

modelResults = optim(llMixed, X=X, y=y, Z=Z, par=paramInit, control=list(reltol=1e-10))
```

```
modelResultsMV = optim(llMixedMV, X=X, y=y, Z=Z, par=paramInit, control=list(reltol=1e-10))

rbind(c(exp(modelResults$par), negLogLik = modelResults$value, coef(lm(y~X-1))),
      c(exp(modelResultsMV$par), negLogLik = modelResultsMV$value, coef(lm(y~X-1)))) %>%
  round(2)
```

```
##        tau sigma negLogLik X(Intercept) XDays
## [1,] 36.02  30.9    897.04       251.41 10.47
## [2,] 36.02  30.9    897.04       251.41 10.47
```

As we can see, both formulations produce identical results. We can now compare those results to the lme4 output for the same model, and see that we're getting what we should.

```
library(lme4)
lmeMod = lmer(Reaction ~ Days + (1|Subject), sleepstudy, REML=FALSE)
lmeMod
```

```
## Linear mixed model fit by maximum likelihood  ['lmerMod']
## Formula: Reaction ~ Days + (1 | Subject)
##    Data: sleepstudy
##       AIC       BIC    logLik  deviance  df.resid
## 1802.0786 1814.8505 -897.0393 1794.0786       176
## Random effects:
##  Groups   Name        Std.Dev.
##  Subject  (Intercept) 36.01
##  Residual             30.90
## Number of obs: 180, groups:  Subject, 18
## Fixed Effects:
## (Intercept)         Days
##      251.41        10.47
```

We can also predict the random effects (Wood, 6.2.4), and after doing so again compare the results to the lme4 estimates.

```
tau = exp(modelResults$par)[1]
tausq = tau^2
sigma = exp(modelResults$par)[2]
sigmasq = sigma^2
Sigma = tcrossprod(Z)*tausq/sigmasq + diag(length(y))
ranefEstimated = tausq*t(Z)%*%solve(Sigma) %*% resid(lm(y~X-1))/sigmasq
data.frame(ranefEstimated, lme4 = ranef(lmeMod)$Subject[[1]]) %>% round(2)
```

```
##             ranefEstimated   lme4
## Subject_308          40.64  40.64
## Subject_309         -77.57 -77.57
## Subject_310         -62.88 -62.88
## Subject_330           4.39   4.39
## Subject_331          10.18  10.18
## Subject_332           8.19   8.19
## Subject_333          16.44  16.44
## Subject_334          -2.99  -2.99
```

```
## Subject_335         -45.12 -45.12
## Subject_337          71.92  71.92
## Subject_349         -21.12 -21.12
## Subject_350          14.06  14.06
## Subject_351          -7.83  -7.83
## Subject_352          36.25  36.25
## Subject_369           7.01   7.01
## Subject_370          -6.34  -6.34
## Subject_371          -3.28  -3.28
## Subject_372          18.05  18.05
```

Issues with ML estimation

Situations arise in which using maximum likelihood for mixed models would result in notably biased estimates (e.g. small N, lots of fixed effects), and so it is typically not used. Standard software usually defaults to *restricted* maximum likelihood. However, our purpose here has been served, so we will not dwell further on mixed model estimation.

Link with penalized regression

A link exists between mixed models and a penalized likelihood approach. For a penalized approach with the SLiM, the objective function we want to minimize can be expressed as follows:

$$\|y - X\beta\|^2 + \beta^\intercal\beta$$

The added component to the sum of the squared residuals is the penalty. By adding the sum of the squared coefficients, we end up keeping them from getting too big, and this helps to avoid overfitting. Another interesting aspect of this approach is that it is comparable to using a specific prior on the coefficients in a Bayesian framework.

We can now see mixed models as a penalized technique. If we knew σ and ψ_θ, then the predicted random effects g and estimates for the fixed effects β are those that minimize the following objective function:

$$\frac{1}{\sigma^2}\|y - X\beta - Zg\|^2 + g^\intercal\psi_\theta^{-1}g$$

We'll take this penalized approach explicitly with the generalized additive model below.

Additive model as a mixed model

At this point I'd like to demonstrate some concepts from section 6.6 in Wood. Conceptually, the take home idea is that an additive model, or generalized additive model (GAM), can be seen as a mixed model, which is interesting in and of itself (at least to me), but it also means that GAMs meld nicely with mixed models to form a more general modeling framework. For an introduction to additive models, one can see my document, which is more or less an overview of Wood's text.

Data set up

The data regards motor engine size and wear in 19 Volvos, with the initial assumption that larger capacity engines will wear out less quickly.

```
size = c(1.42,1.58,1.78,1.99,1.99,1.99,2.13,2.13,2.13,2.32,2.32,2.32,2.32,2.32,2.43,2.43,2.78,2.98,2.98)
wear = c(4.0,4.2,2.5,2.6,2.8,2.4,3.2,2.4,2.6,4.8,2.9,3.8,3.0,2.7,3.1,3.3,3.0,2.8,1.7)

x = size - min(size)
x = x / max(x)
d = data.frame(wear, x)
```

Relevant functions

We'll create functions for the cubic spline operation, the creation of a model matrix, the creation of the penalty matrix, and finally the fitting function.

```
# function for cubic spline on [0,1]; requires data and points within domain for knots
rk <- function(x, z) {
  ((z-0.5)^2 - 1/12) * ((x-0.5)^2 - 1/12) / 4 -
    ((abs(x-z)-0.5)^4 - (abs(x-z)-0.5)^2/2 + 7/240) / 24
}

# create the model matrix
splineX <- function(x, knots) {
  q <- length(knots) + 2                  # number of parameters
  n <- length(x)                          # number of observations
  X <- matrix(1, n, q)                    # initialized model matrix
  X[, 2] <- x                             # set second column to x
  X[, 3:q] <- outer(x, knots, FUN = rk)   # remaining to cubic spline
  X
}

# set up the regression spline penalty matrix, given knot sequence knots
Sfunc = function(knots){
  q = length(knots)+2
  S = matrix(0, q, q)                     # initialize
  S[3:q, 3:q] = outer(knots, knots, FUN=rk)
  S
}

# Matrix sqrt function
matSqrt = function(S){
  UDU = eigen(S, symmetric=TRUE)
  U = UDU$vectors
  D = diag(UDU$values)
  B = crossprod(U) %*% sqrt(D)
  B
}

# the fitting function with lambda smoothing parameter
prsFit <- function(y, x, knots, lambda) {
  q = length(knots) + 2                   # dimension of basis
  n = length(x)                           # number of observations
  Xa = rbind(splineX(x, knots),
             matSqrt(Sfunc(knots)) * sqrt(lambda))  # augmented model matrix
  y[(n + 1):(n + q)] = 0                  # augment the data vector
```

```
  lm(y ~ Xa - 1)                              # fit and return penalized regression spline
}
```

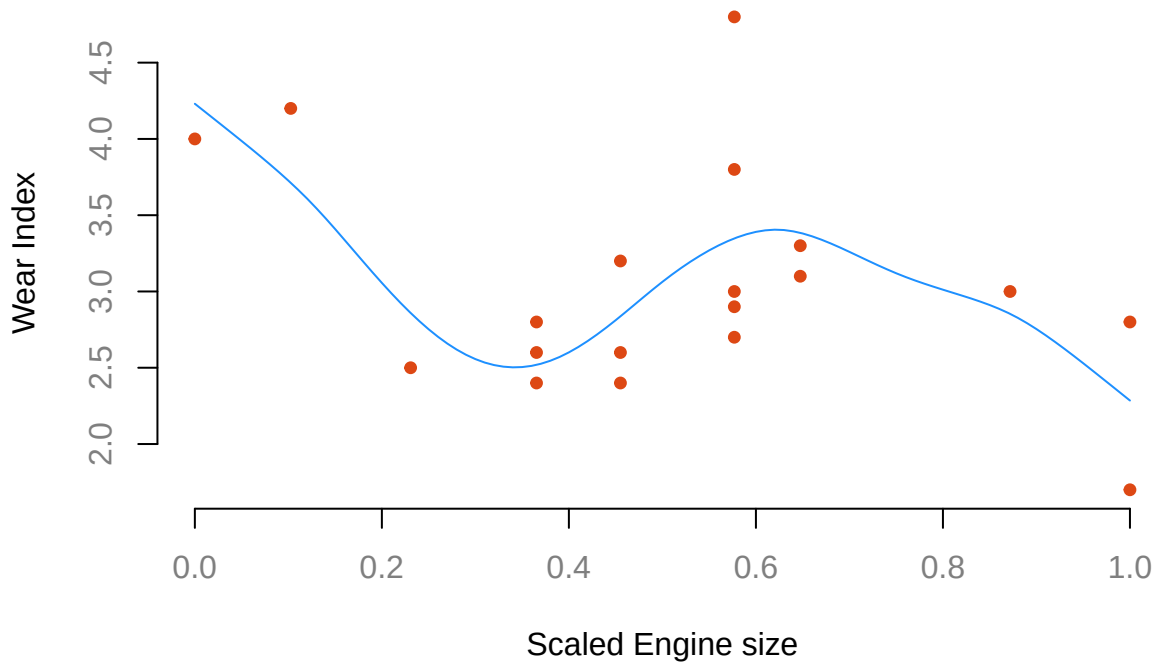
Fit a penalized model

Now we can fit the model and visualize. There does not seem to be a straightforward relationship between engine size and engine wear.

```
x_knots = 1:7/8                               # choose some knots
mod = prsFit(y=wear, x=x, knots=x_knots, lambda=.0001) # fit the penalized spline

x_pred = 0:100/100                            # values for prediction
Xp = splineX(x_pred, x_knots)                 # create design matrix
predictions = Xp %*% coef(mod)

plot(x, wear, xlab='Scaled Engine size', ylab='Wear Index', pch=19,
     col="#dd4814", cex=.75, col.axis='gray50', bty='n')
lines(x_pred, predictions, col='#1e90ff')
```



As a mixed model

One can use the result of eigen decomposition on the penalty matrix to ultimately produce a re-parameterization of the original matrix as fixed and random effects components.

```
S = Sfunc(x_knots)
init = eigen(S)
U = init$vectors
D = diag(init$values)
poseigen = which(diag(D) > 0)
Dpos = D[poseigen, poseigen]            # smallest submatrix containing all positive values
Xf = splineX(x, knots = x_knots)        # spline model matrix
U_F = U[, (ncol(U)-1):ncol(U)]          # partition eigenvector matrix
U_R = U[, 1:(ncol(U)-ncol(U_F))]
X_F = Xf %*% U_F                        # fixed part  with B_F coef to be estimated (not penalized)
X_R = Xf %*% U_R                        # random part with B_R random effects
Z = X_R %*% sqrt(Dpos)
```

The above operations have effectively split the GAM into fixed and random parts:

$$\mathbf{X}_F\beta_F + \mathbf{X}_R\mathbf{b}_R$$
$$\mathbf{b}_R \sim \mathcal{N}(\mathbf{0}, \mathbf{D}_+^{-\mathbf{1}}/\lambda)$$

Here λ is a smoothing parameter, which controls the amount of smoothing. For a penalized spline, the loss function is:

$$\|y - X\beta\|^2 + \lambda\beta^\intercal S\beta,$$

with the second part the added penalty. As $\lambda \to \infty$, we essentially get straight line fit, while a λ of 0 would be the same as an unpenalized fit.

The Z in the code above represents part of the mixed model Z we had before in the standard setting. We can now represent our model as follows:

$$\mathbf{X}_F\beta_F + \mathbf{Z}\mathbf{g}$$
$$\mathbf{g} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}/\lambda)$$

To incorporate a gamm, i.e. a *generalized additive mixed model*, the X_F above would be appended to the 'fixed' effect design matrix, while Z would be added to the random effects component, and estimation would proceed normally as for a mixed model.

The mgcv and associated packages allow us to see this explicitly. Initially we'll just duplicate a standard mixed model using mgcv and gamm4 packages. One can see that the gamm4 is using lme4 and produces the same output.

```
library(mgcv); library(gamm4)
```

```
## This is gamm4 0.2-3
```

```
modGam = gamm4(Reaction ~ Days, random=~(1|Subject), data=sleepstudy)
summary(modGam$mer)
```

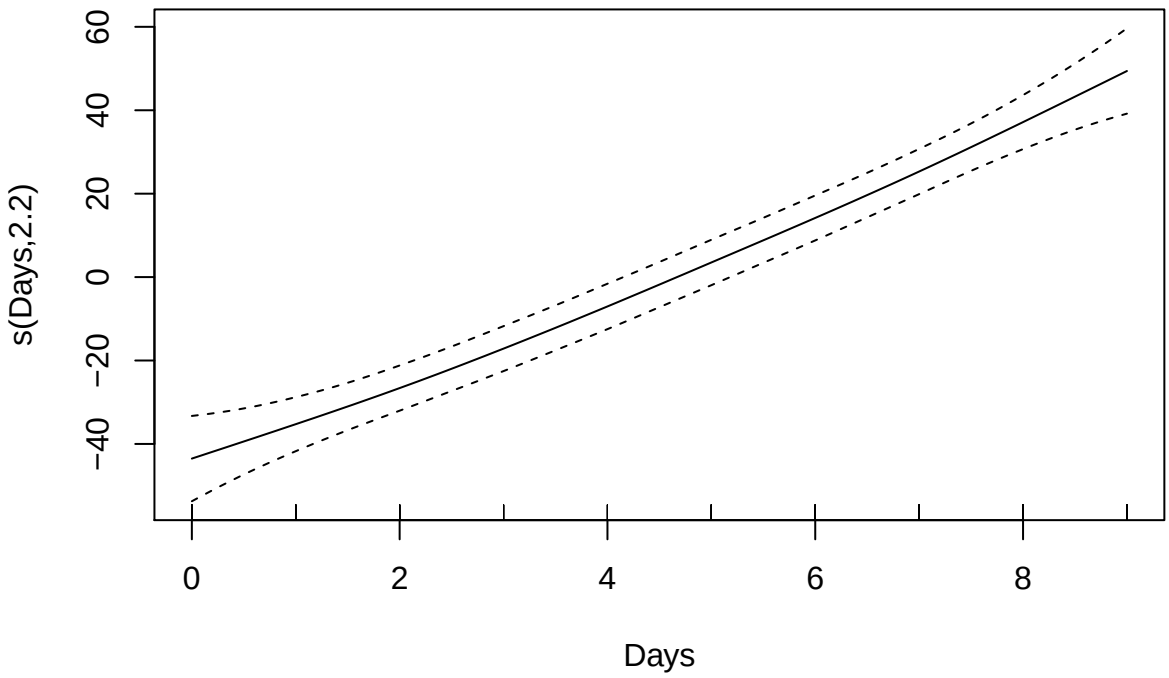
```
## Linear mixed model fit by REML ['lmerMod']
##
## REML criterion at convergence: 1786.5
```

```
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -3.2257 -0.5529  0.0109  0.5188  4.2506
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  Subject  (Intercept) 1378.2   37.12
##  Residual              960.5   30.99
## Number of obs: 180, groups:  Subject, 18
##
## Fixed effects:
##              Estimate Std. Error t value
## X(Intercept) 251.4051     9.7467   25.79
## XDays         10.4673     0.8042   13.02
##
## Correlation of Fixed Effects:
##       X(Int)
## XDays -0.371
```

Now we'll add a cubic spline for the effect of Days, and we can see the smooth term listed as part of the random effects results.

```
modGamS = gamm4(Reaction ~ s(Days, bs='cs'), random=~(1|Subject), data=sleepstudy)
summary(modGamS$mer)
# summary(modGamS$gam)
plot(modGamS$gam)
```

```
## Linear mixed model fit by REML ['lmerMod']
##
## REML criterion at convergence: 1795.3
##
## Scaled residuals:
##     Min      1Q  Median      3Q     Max
## -3.2996 -0.5224  0.0399  0.5340  4.2989
##
## Random effects:
##  Groups   Name        Variance Std.Dev.
##  Subject  (Intercept) 1378.144 37.123
##  Xr       s(Days)        4.455  2.111
##  Residual              960.806 30.997
## Number of obs: 180, groups:  Subject, 18; Xr, 9
##
## Fixed effects:
##   Estimate Std. Error t value
## X   298.51       9.05   32.98
```



Wrap Up

So we've seen that GAMs can be seen as having a fixed and random effect as in mixed models, which means we can use them within the mixed model framework. Another way to look at this is that we have added the capacity to examine nonlinear relationships and other covariance structures to the standard mixed model framework, making a very flexible modeling approach even more so.

It's full of STARs...

However, this goes even further. ***St****ructured* ***A****dditive* ***R****egression models* (STAR) build upon the notion just demonstrated (nicely illustrated in Fahrmeir et al. (2013)). Not only we can combine mixed and additive models, but other model classes as well. This includes interactions and varying coefficient models, spatial effects, gaussian processes/kriging, markov random fields and others. Each model class has a particular design and penalty matrix as we saw in the examples previously, but otherwise can be added to the current model being considered. We can also use other techniques, like boosting to estimate them. Standard regression, glm, gam, etc. are thus special cases of the STAR model. In short, we now have a highly flexible modeling environment within which to tackle the questions we seek to answer with our data.

References

Fahrmeir, Ludwig, Thomas Kneib, Stefan Lang, and Brian Marx. 2013. "Regression."

Wood, Simon. 2006. "Generalized Additive Models."