

ML estimation: TMB continued

FPA2020 Lecture 08: TMB for Random-effect

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```
library(ggplot2)
library(TMB)
```

We shall continue exercises for the use of TMB. In the last lecture, we dealt with just some simple likelihood estimation. Today, we shall cover likelihood analyses with random effects.

1 Analysis (1): IID Normal distribution

1.1 Model description and generation of example data

The assumption is like this. A total n IID observations are obtained from each of K strata (say, $k = 1, 2, \dots, K$) as follows:

$$Y_{k1}, Y_{k2}, \dots, Y_{kn} \sim (iid)N(\mu_k, \sigma^2) \quad (k = 1, 2, \dots, K)$$

Parameter of interest here are μ_k ($k = 1, 2, \dots, K$).

```
set.seed(2020)
Ks <- 20
ns <- 5
# True parameters
# Scenario 1 from U(0,10)
# Scenario 2 from N(5,2^2)
#mu.true <- runif(Ks,0,10)
mu.true <- rnorm(Ks,5,1)
sigma.true <- 2

yobs <- array(NA,c(Ks,ns))
for(k in 1:Ks) yobs[k,] <- rnorm(ns,mu.true[k],sigma.true)

colnames(yobs) <- 1:ns
```

```
cbind(Stratum=1:Ks, round(yobs,2)) %>%
  kable("latex", booktabs=T, caption="Data") %>%
  kable_styling(font_size=9, latex_options=c("hold_position"))
```

Table 1: Data

Stratum	1	2	3	4	5
1	9.73	7.57	6.01	5.23	7.05
2	5.70	7.90	7.17	5.01	5.52
3	2.28	2.41	6.09	8.77	4.68
4	4.45	3.30	4.02	2.75	4.76
5	4.02	1.19	1.60	0.75	-0.16
6	6.23	4.98	5.76	7.04	6.70
7	5.56	7.14	4.59	6.89	6.18
8	5.01	4.40	2.11	3.64	5.93
9	10.58	7.26	3.56	13.16	8.67
10	5.85	6.96	4.71	5.30	5.45
11	5.74	7.44	0.71	3.51	2.34
12	4.50	2.35	4.46	6.00	6.40
13	7.45	6.15	10.82	6.55	4.15
14	9.18	0.85	6.82	8.32	5.67
15	1.81	1.00	5.85	7.37	4.44
16	5.24	7.50	8.16	5.74	5.45
17	3.25	4.72	5.53	7.47	8.20
18	0.10	1.28	5.05	2.49	2.56
19	2.07	5.58	4.72	-0.73	3.31
20	3.41	2.66	2.51	4.81	9.39

The ML estimators for μ 's are exactly given by the sample mean in each stratum.

$$\hat{\mu}_k = \bar{y}_{k\cdot} = \frac{1}{n} \sum_{i=1}^n y_{ki} \quad (k = 1, 2, \dots, K)$$

We shall call this model a “Fixed-effect (FE) model”.

Next we define a “random-effect (RE) model”. We can assume the following latent structure for random effects μ 's as follows:

$$\begin{aligned} Y_{k1}, Y_{k2}, \dots, Y_{kn} | \mu_k &\sim (iid)N(\mu_k, \sigma^2) \\ \mu_1, \mu_2, \dots, \mu_K &\sim (iid)N(\theta, \tau^2). \end{aligned}$$

In this RE model, although an explicit expression for the marginal distribution of the observation can be available, we here leave an integral form of the marginal distribution of the observation Y'_{ik} s as follows:

$$L(\theta, \sigma^2, \tau^2) = \int \cdots \int \prod_k \left[\left\{ \prod_i f(y_{ki} | \mu_k, \sigma^2) \right\} f(\mu_k | \theta, \tau^2) \right] d\mu_1 \cdots d\mu_K.$$

So we will optimize the likelihood function with integration using the Laplace approximation (see Appendix). In this model, a set of variables, $\mu_1, \mu_2, \dots, \mu_K$, plays a role of latent variable vector u .

1.2 TMB coding

```
sink(file="normal_re.cpp")
cat(
#include <TMB.hpp>
template<class Type>
Type objective_function<Type>::operator() ()
```

```
{
DATA_INTEGER(Ks);
DATA_INTEGER(ns);
DATA_MATRIX(yobs);
PARAMETER_VECTOR(mu);
PARAMETER(logSigma);
PARAMETER(theta);
PARAMETER(logTau);
Type sigma = exp(logSigma);
Type tau = exp(logTau);
ADREPORT(sigma);
ADREPORT(tau);

Type f=0.0;

//likelihood from observation yobs (let me use simple coding)
for(int k=0;k<Ks;k++){
    for(int i=0;i<ns;i++){
        f += (-1.0)*dnorm(yobs(k,i),mu(k),sigma,true);
    }
}

//likelihood of random effects
f += (-1.0)*sum(dnorm(mu,theta,tau,true));

return f;
}
", fill=TRUE)
sink()
```

1.3 Compiling “cpp” file and call “Dynamic link”

```
compile("normal_re.cpp")

[1] 0

dyn.load(dylib("normal_re"))
```

1.4 Minimization etc.

- “MakeADFun”: Constructing objective functions with derivatives based on a compiled C++ template
- “nlminb”: Minimization
 - “sdreport”: extract the results

```
data <- list(Ks=Ks, ns=ns, yobs=yobs)
parameters <- list(mu=rep(0,Ks),logSigma=0,theta=0,logTau=0)
model <- MakeADFun(data, parameters, random="mu", DLL="normal_re")
fit <- nlminb(model$par, model$fn, model$gr)
```

```
Optimizing tape... Done
iter: 1 value: 531.5883 mgc: 43.23235 ustep: 1
iter: 2 mgc: 7.993606e-15
iter: 1 mgc: 7.993606e-15
Matching hessian patterns... Done
outer mgc: 387.4819
iter: 1 value: 293.1095 mgc: 0.2544483 ustep: 1
iter: 2 mgc: 7.21645e-16
iter: 1 mgc: 7.21645e-16
outer mgc: 75.56846
iter: 1 value: 305.9279 mgc: 4.733696 ustep: 1
iter: 2 mgc: 3.330669e-15
iter: 1 value: 274.8912 mgc: 1.012086 ustep: 1
iter: 2 mgc: 1.554312e-15
iter: 1 mgc: 1.554312e-15
outer mgc: 36.48937
iter: 1 value: 270.4047 mgc: 0.0777322 ustep: 1
iter: 2 mgc: 6.661338e-16
iter: 1 mgc: 6.661338e-16
outer mgc: 13.26888
iter: 1 value: 265.7147 mgc: 0.4770983 ustep: 1
iter: 2 mgc: 7.771561e-16
iter: 1 mgc: 7.771561e-16
outer mgc: 20.79594
iter: 1 value: 265.0355 mgc: 0.08340726 ustep: 1
iter: 2 mgc: 5.551115e-16
iter: 1 value: 263.0416 mgc: 0.02001583 ustep: 1
iter: 2 mgc: 7.21645e-16
iter: 1 value: 252.0726 mgc: 0.269541 ustep: 1
iter: 2 mgc: 7.910339e-16
iter: 1 mgc: 7.910339e-16
outer mgc: 5.46507
iter: 1 value: 936.2442 mgc: 187.3016 ustep: 1
iter: 2 mgc: 7.21645e-14
iter: 1 value: 246.7648 mgc: 0.4231157 ustep: 1
iter: 2 mgc: 5.551115e-16
iter: 1 mgc: 5.551115e-16
outer mgc: 6.476475
iter: 1 value: 243.6653 mgc: 0.5868904 ustep: 1
iter: 2 mgc: 9.436896e-16
iter: 1 mgc: 9.436896e-16
outer mgc: 6.326165
iter: 1 value: 244.3696 mgc: 0.4258873 ustep: 1
iter: 2 mgc: 5.967449e-16
iter: 1 mgc: 5.967449e-16
outer mgc: 10.85891
iter: 1 value: 243.4602 mgc: 0.2518584 ustep: 1
iter: 2 mgc: 7.077672e-16
iter: 1 mgc: 7.077672e-16
outer mgc: 3.356424
```

```
iter: 1 value: 242.7531 mgc: 0.1629781 ustep: 1
iter: 2 mgc: 1.110223e-15
iter: 1 mgc: 1.110223e-15
outer mgc: 1.90133
iter: 1 value: 242.1932 mgc: 0.2029594 ustep: 1
iter: 2 mgc: 7.771561e-16
iter: 1 mgc: 7.771561e-16
outer mgc: 0.3536151
iter: 1 value: 242.102 mgc: 0.07166562 ustep: 1
iter: 2 mgc: 1.026956e-15
iter: 1 mgc: 1.026956e-15
outer mgc: 0.04056468
iter: 1 value: 242.106 mgc: 0.002495816 ustep: 1
iter: 2 mgc: 7.771561e-16
iter: 1 mgc: 7.771561e-16
outer mgc: 0.005654033
iter: 1 value: 242.1055 mgc: 0.0001412438 ustep: 1
iter: 2 mgc: 6.661338e-16
iter: 1 mgc: 6.661338e-16
outer mgc: 0.0001003698
iter: 1 value: 242.1055 mgc: 4.588619e-06 ustep: 1
iter: 2 mgc: 7.771561e-16
iter: 1 mgc: 7.771561e-16
outer mgc: 1.485505e-06
iter: 1 mgc: 7.771561e-16
rep <- sdreport(model)

iter: 1 mgc: 7.771561e-16
outer mgc: 1.485505e-06
iter: 1 value: 242.1194 mgc: 0.002506295 ustep: 1
iter: 2 mgc: 7.979728e-16
outer mgc: 0.1636533
iter: 1 value: 242.0917 mgc: 0.002511313 ustep: 1
iter: 2 mgc: 7.771561e-16
outer mgc: 0.1639569
iter: 1 value: 242.1055 mgc: 0.0004987753 ustep: 1
iter: 2 mgc: 8.049117e-16
outer mgc: 0.006898426
iter: 1 value: 242.1055 mgc: 0.0004987753 ustep: 1
iter: 2 mgc: 7.771561e-16
outer mgc: 0.006899227
iter: 1 value: 242.1116 mgc: 0.002506295 ustep: 1
iter: 2 mgc: 6.661338e-16
outer mgc: 0.01913545
iter: 1 value: 242.0993 mgc: 0.002511313 ustep: 1
iter: 2 mgc: 6.661338e-16
outer mgc: 0.01912678
outer mgc: 2.114395
```

1.5 Results

You can see a shrinkage effect in the RE model; the estimates under the FE model are shrunk toward the grand mean. This causes a slight bias in the estimation, but it provides better precision as known as “Stein effect”, where a concept of “borrowing the strength” is implemented.

```
mu.est.RE <- as.list(rep, "Est")$mu; round(mu.est.RE,3)

[1] 6.501 5.908 4.931 4.246 2.604 5.826 5.778 4.496 7.558 5.490 4.309 4.859
[13] 6.437 5.844 4.410 6.016 5.613 3.169 3.647 4.729

mu.sd.RE <- as.list(rep, "Std")$mu
mu.est.FE <- apply(yobs,1,mean); round(mu.est.FE,3)

[1] 7.118 6.260 4.847 3.857 1.482 6.142 6.073 4.218 8.646 5.656 3.948 4.743
[13] 7.025 6.167 4.094 6.417 5.834 2.299 2.990 4.555

grand.mean <- mean(yobs)

plot(mu.true, pch="*", ylim=c(0,10), xlab="Stratum", ylab=TeX("Value of $\mu$"))
points(mu.est.RE, col="red", pch=19)
points(mu.est.FE, col="blue", pch=19)
abline(grand.mean,0,lty=2)
for(k in 1:Ks) arrows(k, mu.est.FE[k], k, mu.est.RE[k], length=0.1)
legend(1,3, pch=19, col=c("black","red","blue"),
      legend=c("True","RE","FE"), bty="n")
```

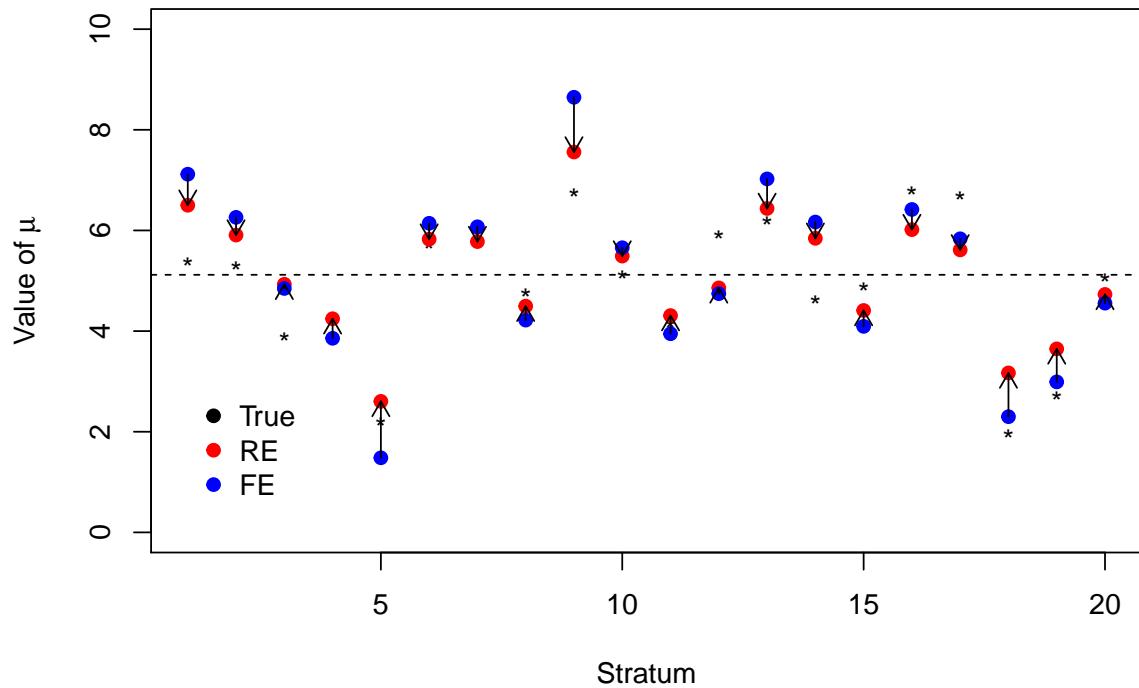


Figure 1: Comparison of estimates between FE and RE models (shrinkage effects).

Appendix: Laplace approximation

Here in general y , u and θ are vectors of the observation, latent variables (random effects) and other parameters, respectively, and let $f(y, u|\theta)$ be a joint distribution as $f(y|u, \theta)$ and $f(u|\theta)$

$$L(\theta) = \int f(y|u, \theta)f(u|\theta)d\mu = \int f(y, u|\theta)du = \int e^{-g(u, \theta)}du$$

where

$$g(u, \theta) = -\log f(y, u|\theta).$$

The Laplace approximation is often used in statistics. The approximation depends on a second-order Taylor expansion of $g(u, \theta)$. Let $\hat{u}(\theta)$ be the vector of u that minimizes $g(u, \theta)$ for fixed θ , that is

$$\hat{u}(\theta) = \arg \min_u g(u, \theta)$$

Then, $L(\theta)$ can be approximated (ignoring factors not depending on θ) as follows:

$$\begin{aligned} L(\theta) &= \int e^{-g(u, \theta)}du \\ &\approx \int \exp \left\{ -g(\hat{u}(\theta), \theta) - \frac{1}{2}(u - \hat{u}(\theta))' H(\theta)(u - \hat{u}(\theta)) \right\} du , \\ &= (2\pi)^{n/2} \det\{H(\theta)\}^{-1/2} \exp\{-g(\hat{u}(\theta), \theta)\} \\ &= L^*(\theta), \end{aligned}$$

where

$$H(\theta) = \frac{\partial^2}{\partial u \partial u'} g(u, \theta)|_{u=\hat{u}(\theta)},$$

and $\det\{H(\theta)\}$ denotes the determinant of $H(\theta)$. Taking the logarithm of $L^*(\theta)$, we get

$$\log L^*(\theta) = Const + \frac{1}{2} \log \det\{H(\theta)\} - g(\hat{u}(\theta), \theta).$$

Once you get

$$\hat{\theta} = \arg \max_u \log L^*(\theta)$$

then you can also get estimates for the latent variables as

$$\hat{u} = \hat{u}(\hat{\theta}).$$

Note that the third term on the right-hand side is the profile log-likelihood of θ . In fact, the equation above can be regarded as an approximate modified profile log-likelihood of θ to reduce the estimation bias (Lindsey 1996, Pawitan 2001).