Maximum likelihood estimation

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Review of ML estimation

ML for HNM

Method of moments

```
aovfit<-anova(lm(y~as.factor(g)) )</pre>
MSG<-aovfit[1,3]
MSE<-aovfit[2,3]
t2<-(MSG-MSE)/n
s2<-MSE
t2; sqrt(t2)
##
## 0.3840768
## 1
## 0.6197393
s2; sqrt(s2)
## [1] 1.787206
## [1] 1.336864
mean(y)
## [1] 16.3064
```

Maximum likelihood estimation

lmer

package:1me4

R Documentation

Fit Linear Mixed-Effects Models

Description:

Fit a linear mixed-effects model (LMM) to data, via REML or maximum likelihood.

Usage:

```
lmer(formula, data = NULL, REML = TRUE, control = lmerControl(),
    start = NULL, verbose = OL, subset, weights, na.action,
    offset, contrasts = NULL, devFunOnly = FALSE)
```

```
library(lme4)
lmer(y~1+(1|g))
## Linear mixed model fit by REML ['lmerMod']
## Formula: y ~ 1 + (1 | g)
## REML criterion at convergence: 177.9876
## Random effects:
## Groups Name
                       Std.Dev.
## g
        (Intercept) 0.6197
## Residual
                        1.3369
## Number of obs: 50, groups: g, 10
## Fixed Effects:
## (Intercept)
##
        16.31
```

A more complicated example

```
nels[1:10,]
##
      school enroll flp public urbanicity hwh
                                                  ses mscore
## 1
        1011
                   5
                                              2 -0.23
                                                      52.11
                       3
                                     urban
                       3
## 2
        1011
                   5
                                     urban
                                              0 0.69
                                                      57.65
## 3
        1011
                                     urban
                                              4 -0.68
                                                      66.44
                                                      44.68
## 4
        1011
                                     urban
                                              5 -0.89
## 5
        1011
                                     urban
                                              3 -1.28
                                                      40.57
                       3
## 6
        1011
                                     urban
                                              5 -0.93
                                                      35.04
## 7
        1011
                       3
                                     urban
                                              1 0.36
                                                      50.71
                       3
## 8
        1011
                                     urban
                                              4 - 0.24
                                                      66.17
                                              8 -1.07
                                                       46.17
## 10
        1011
                                     urban
## 11
        1011
                              1
                                     urban
                                              2 -0.10
                                                      58.76
```

A more complicated example

$$\mathbf{y}_{i,j} = \left(\beta_0 + \textcolor{red}{\beta_{0,j}}\right) + \beta_1 \times \mathsf{flp}_j + \beta_2 \times \mathsf{enroll}_j + \left(\beta_3 + \textcolor{red}{\beta_{3,j}}\right) \times \mathsf{ses}_{i,j} + \epsilon_{i,j}$$

 $\verb|fit<-lmer(mscore"flp+enroll+ses+(ses|school), data=nels, REML=FALSE)|$

```
summary(fit)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscore ~ flp + enroll + ses + (ses | school)
     Data: nels
##
##
       ATC
##
               BIC logLik deviance df.resid
## 92397.7 92457.5 -46190.9 92381.7 12966
##
## Scaled residuals:
## Min 1Q Median 3Q
                                  Max
## -3.9797 -0.6399 0.0180 0.6681 4.5053
##
## Random effects:
## Groups Name
                    Variance Std.Dev. Corr
## school (Intercept) 9.004 3.001
##
           ses 1.600 1.265 0.05
                      67.260 8.201
## Residual
## Number of obs: 12974, groups: school, 684
##
## Fixed effects:
             Estimate Std. Error t value
## (Intercept) 55.429341 0.402910 137.573
## flp
       -2.411521 0.185312 -13.013
            0.007095 0.082024 0.087
## enroll
## ses
            4.116881 0.125381 32.835
##
## Correlation of Fixed Effects:
##
        (Intr) flp enroll
## flp -0.815
## enroll -0.300 -0.193
## ses
        -0.202 0.212 0.007
```

Models and inference

A *statistical model* is a collection of probability distributions for observed data:

$$\mathcal{P} = \{ p(y|\gamma), \gamma \in \Gamma \}$$

- y is the data;
- Γ is the set of parameter values;
- $p(y|\gamma)$ is a probability (density) for each $\gamma \in \Gamma$.

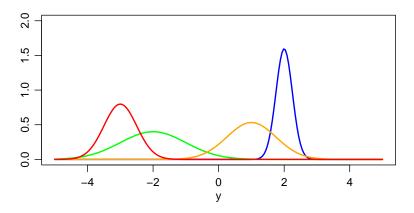
Example: Normal model

For example, the normal model is

$$\{p(y|\theta,\sigma^2) = (2\pi\sigma^2)^{-1/2} \exp\{-(y-\theta)^2/(2\sigma^2)\}, \theta \in \mathbb{R}, \sigma^2 \in \mathbb{R}^+\}.$$

- y is a single scalar data value;
- $\gamma = \{\theta, \sigma^2\}$ is the parameter (or are the parameters);
- $\Gamma = \mathbb{R} \times \mathbb{R}^+$ is the set of possible parameter values;
- $p(y|\theta,\sigma^2)$ is the normal probability density for each θ,σ^2 .

Example: Normal model



Model-based inference

Model-based statistical inference involves

Estimation: Obtain a value $\hat{\gamma} \in \Gamma$ that "best" represents the population.

Inference: Evaluate the plausibility of other γ values.

Inference includes things like: confidence intervals, hypotheses tests.

Likelihood-based statistical inference:

- a type of model based inference;
- estimation and inference are based on the likelihood function.

Joint probability of the data

Independent events: Recall if A and B are independent events,

$$Pr(A \text{ and } B) = Pr(A) \times Pr(B).$$

Independent observations: If y_1 and y_2 are independent observations, then

$$p_{y_1y_2}(y_1, y_2|\gamma) = p(y_1|\gamma) \times p(y_2|\gamma)$$

$$= \prod_{i=1}^2 p(y_i|\gamma).$$

Independent sample: If $y = (y_1, \dots, y_n)$ are independent observations, then

$$p_{\mathbf{y}}(\mathbf{y}|\gamma) = p(y_1|\gamma) \times \cdots \times p(y_n|\gamma)$$
$$= \prod_{i=1}^n p(y_i|\gamma).$$

 $p_{y}(y|\gamma)$, as a function of y, is the *joint probability (density)* of the data.

Example: One sample normal model

$$y_1, \ldots, y_n \sim \text{ i.i.d. } N(\theta, \sigma^2)$$

For this model,

$$p(y_i|\theta,\sigma^2) = (2\pi\sigma^2)^{-1/2} e^{-(y_i-\theta)^2/[2\sigma^2]}$$

$$p(y_1,\ldots,y_n|\theta,\sigma^2) = \prod_{i=1}^n p(y_i|\theta,\sigma^2)$$

$$= (2\pi)^{-n/2} (\sigma^2)^{-n/2} \exp(-\sum (y_i-\theta)^2/[2\sigma^2])$$

Interpretation:

 $p(y|\theta)$ roughly quantifies how probable y is, for a particular (θ, σ^2) .

Likelihood

The *likelihood* is the probability of the data as a function of the parameter:

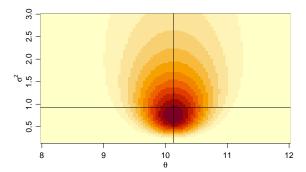
$$L(\theta: \mathbf{y}) = p(\mathbf{y}|\theta)$$

The *maximum likelihood estimator* (*MLE*) is the value of θ that maximizes $L(\theta : y)$:

$$\hat{\theta}_{MLE} = \arg\max_{\theta \in \Theta} L(\theta : \mathbf{y})$$

Likelihood function

```
## some data
y
## [1] 9.373546 10.183643 9.164371 11.595281 10.329508
mean(y)
## [1] 10.12927
var(y)
## [1] 0.9235968
```



Log likelihoods

Likelihoods based on lots of data can give extreme numbers.

Alternatively, we can make inference with the log-likelihood:

If $\hat{\theta}$ maximizes $L(\theta : y)$ then it also maximizes $\log L(\theta : y) = I(\theta : y)$.

$$\log p(\mathbf{y}|\theta,\sigma^2) = -\frac{1}{2} \left(n \log \sigma^2 + \sum_i (y_i - \theta)^2 / \sigma^2 \right) + c$$

Finding the MLE

Recall from calculus that the *tangent* or *derivative* of a function, at a local maximum, will be zero. This tells us how to find the MLE:

$$\hat{\gamma}_{MLE}$$
 satisfies $rac{d}{d\gamma} I(\gamma:m{y})|_{\gamma=\hat{\gamma}}=0$

Let's try this for the normal model. The derivative of the log-likelihood is

$$\frac{d}{d\gamma}I(\gamma:\mathbf{y}) = \binom{n(\bar{y} - \theta)/sigma^2}{(-n/\sigma^2 + \sum_i (y_i - \theta)^2/\sigma^4)/2}$$

The MLE of (θ, σ^2) is then

$$(\hat{\theta}, \hat{\sigma}^2) = \left(\bar{y}, \sum_i (y_i - \bar{y})^2 / n\right).$$

So $\hat{\sigma}^2$ is biased for estimating σ^2 .

Information and precision

The precision of the MLE (how well it estimates the truth) depends on the *information* or second derivative of the log-likelihood.

Information: The observed information about γ is

$$I_n = -\frac{d^2}{d\gamma^2}I(\gamma:\mathbf{y})|_{\hat{\gamma}}$$

In many problems, the inverse of the information gives a variance estimate:

$$\mathsf{Var}[\hat{\gamma}] pprox I_n^{-1}$$
 $\mathsf{sd}(\hat{\gamma}) pprox \mathsf{diag}(I_n^{-1})$

For the normal model,

$$I_n^{-1} = \begin{pmatrix} -n/\hat{\sigma}^2 & 0\\ 0 & -n/[2\hat{\sigma}^4]. \end{pmatrix}$$

So we have

$$\mathsf{Var}[\hat{ heta}] pprox \hat{\sigma}^2/n$$
 $\mathsf{Var}[\hat{\sigma}^2] pprox 2\hat{\sigma}^4/n$

MLE for the hierarchical normal model

$$y_{i,j} = \mu + a_j + \epsilon_{i,j}$$

 $\{\epsilon_{i,j}\} \sim \text{iid } N(0, \sigma^2)$
 $\{a_j\} \sim \text{iid } N(0, \tau^2)$

Parameters to estimate:

Fixed effects: μ

• Variance components: σ^2 , τ^2

Random effects: a₁,..., a_m

Likelihood estimation focuses on estimation of $\theta = (\mu, \sigma^2, \tau^2)$

Alternative methods are required for estimation of a_1, \ldots, a_m .

HNM likelihood

Data:

$$y = (y_{1,1}, \dots, y_{n_j,1}, \dots, y_{1,m}, \dots, y_{n_m,m})$$

$$= (\{y_{1,1}, \dots, y_{n_j,1}\}, \dots, \{y_{1,m}, \dots, y_{n_m,m}\})$$

$$= (y_1, \dots, y_n)$$

Likelihood:

$$I(\mu, \sigma^2, \tau^2 : \mathbf{y}) = p(\mathbf{y}|\mu, \tau^2, \sigma^2)$$

Recall: Under the HNM,

- observations within groups are correlated;
- observations across groups are independent.

$$I(\mu, \sigma^2, \tau^2 : \mathbf{y}) = p(\mathbf{y}|\mu, \tau^2, \sigma^2) = p(\mathbf{y}_1|\mu, \tau^2, \sigma^2) \times \cdots \times p(\mathbf{y}_m|\mu, \tau^2, \sigma^2)$$
$$= \prod_{i=1}^m p(\mathbf{y}_i|\mu, \tau^2, \sigma^2)$$

Likelihood contribution from a single group

$$y_{i,j} = \mu + a_j + \epsilon_{i,j}$$
 $\epsilon_{1,j}, \dots, \epsilon_{n_j,j} \sim \text{iid } N(0, \sigma^2)$ $a_j \sim N(0, \tau^2)$

As we've discussed, the $y_{i,j}$'s are normal with

- $\mathsf{E}[y_{i,j}|\mu] = \mu$
- $Var[y_{i,j}|\mu] = \sigma^2 + \tau^2$
- $Cov[y_{i_1,j}, y_{i_2,j}|\mu] = \tau^2$

In vector form, we can express this as follows:

$$\mathsf{E}[\mathbf{y}_j|\mu] = \begin{pmatrix} \mu \\ \mu \\ \vdots \\ \mu \end{pmatrix} = \mu \mathbf{1} \quad \mathsf{Cov}[\mathbf{y}_j|\mu] = \begin{pmatrix} \sigma^2 + \tau^2 & \tau^2 & \cdots & \tau^2 \\ \tau^2 & \sigma^2 + \tau^2 & \cdots & \tau^2 \\ \vdots & \vdots & & \vdots \\ \tau^2 & \tau^2 & \cdots & \sigma^2 + \tau^2 \end{pmatrix}$$

Multivariate normal distribution

This means that y_i has a multivariate normal distribution.

The density of a general multivariate normal (θ, Σ) distribution is

$$p(\mathbf{y}|\boldsymbol{\theta}, \boldsymbol{\Sigma}) = (2\pi)^{-p/2} |\boldsymbol{\Sigma}|^{-1/2} \exp\{-(\mathbf{y} - \boldsymbol{\theta})^T \boldsymbol{\Sigma}^{-1} (\mathbf{y} - \boldsymbol{\theta})/2\}$$

where

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix} \quad \boldsymbol{\theta} = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_p \end{pmatrix} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_1^2 & \sigma_{1,2} & \cdots & \sigma_{1,p} \\ \sigma_{1,2} & \sigma_2^2 & \cdots & \sigma_{2,p} \\ \vdots & \vdots & & \vdots \\ \sigma_{1,p} & \sigma_{2,p} & \cdots & \sigma_p^2 \end{pmatrix}.$$

```
ldmvnorm<-function(y, theta, Sig)
{
    -.5*(
    length(y)*log(2*pi) +
    log(det(Sig)) +
        t(y-theta)%*%solve(Sig)%*%(y-theta)
        )
}</pre>
```

Computing the log-likelihood

MLEs of (μ, σ^2, τ^2) can be found by maximizing the log likelihood.

Log likelihood:

$$L(\mathbf{y}: \mu, \sigma^2, \tau^2) = p(\mathbf{y}_1, \dots, \mathbf{y}_m | \mu, \sigma^2, \tau^2)$$

$$I(\mathbf{y}: \mu, \sigma^2, \tau^2) = \log p(\mathbf{y}_1, \dots, \mathbf{y}_m | \mu, \sigma^2, \tau^2)$$

$$= \log \prod_{j=1}^{m} p(\mathbf{y}_j | \mu, \sigma^2, \tau^2)$$

$$= \sum_{j=1}^{m} \log p(\mathbf{y}_j | \mu, \sigma^2, \tau^2),$$

where $\log p(\mathbf{y}_i|\mu,\sigma^2,\tau^2)$ is the log of a multivariate normal density.

For the HNM, we replace

- $\boldsymbol{\theta}$ with $\mu \mathbf{1}$
- ullet Σ with the covariance matrix from the previous slide.

Computing the (minus) log-likelihood

```
mll.oneway
## function(mus2t2,y,g)
##
## {
##
     mu<-mus2t2[1]; s2<-mus2t2[2]; t2<-mus2t2[3]
##
##
     11<-0
##
     for(gj in sort(unique(g)))
##
##
##
##
##
       nj<-sum(g==gj)
##
       S<-diag(s2,nj) + matrix(t2,nj,nj)
##
##
       11<-11+1dmvnorm(y[g==gi],mu,S)
##
##
##
##
## -11
##
## }
```

Example: Wheat data

```
mll.oneway( c(16.3, 1.787, 0.31 ), y,g)
##
            [,1]
## [1,] 88.58541
mll.oneway( c(15, 1.787, 0.31 ), y,g)
##
            [,1]
## [1,] 101.3711
mll.oneway( c(16.3, 2, 0.31 ), y,g)
            [,1]
##
## [1,] 88.71672
mll.oneway( c(16.3, 1.787, 0.4), y,g)
##
            [,1]
## [1,] 88.62378
```

Optimization in R

```
fit.ml<-optim(c(15,1,1),mll.oneway,gr=NULL,y=y,g=g,lower=c(-Inf,0,0),method="L-BFGS-B",hessian=TRUE)
fit.ml
## $par
## [1] 16.3063995 1.7872063 0.3099255
##
## $value
## [1] 88.5851
##
## $counts
## function gradient
##
        16
                 16
##
## $convergence
## [1] 0
##
## $message
## [1] "CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH"
##
## $hessian
##
                     [,2]
## [1,] 1,498426e+01 2,186695e-06 1,090683e-05
## [2,] 2,186695e-06 6,710598e+00 2,245294e+00
## [3,] 1.090683e-05 2.245294e+00 1.122654e+01
```

The MLEs are

```
\hat{\mu} = 16.3063995, \hat{\sigma}^2 = 1.7872063, \hat{\tau}^2 = 0.3099255
```

For maximum likelihood estimation in general,

- $\hat{\gamma}_{MLE} \to \theta$ as the sample size goes to infinity (if the model is correct);
- $\hat{\gamma} \stackrel{.}{\sim} \text{normal}(\gamma, \text{Var}[\hat{\gamma}])$, where
- $Var[\hat{\gamma}] \approx I_n^{-1}$ for large sample sizes.

For our hierarchical normal model, this means that approximate 95% confidence intervals for (μ, τ^2, σ^2) can be obtained from the curvature of the log likelihood.

The observed information matrix is the (matrix of) second derivative(s) of the negative log-likelihood function at the MLE (aka the Hessian):

$$I_n(\hat{\gamma}: \mathbf{y}) = \{-\frac{\partial^2 I(\gamma: \mathbf{y})}{\partial \gamma_j \partial \gamma_k}\}|_{\gamma = \hat{\gamma}}$$

The inverse of the information matrix gives an estimate of the variance/covariance of the MLE's:

$$\operatorname{Var}[\hat{\gamma}:y] \approx I_n^{-1}(\hat{\gamma}:y)$$

From this, we can get confidence intervals:

- $\sqrt{(I^{-1})_{jj}}$ gives an approximate standard error for γ_j .
- The MLE plus and minus 2 standard errors gives a rough confidence interval for the parameters.

$$\Pr(\gamma_j \in \hat{\gamma}_j \pm 2 \times \text{se}[\hat{\gamma}_j]) \approx 0.95$$

```
gamma.wheat <- fit.ml $par
gamma.wheat
## [1] 16.3063995 1.7872063 0.3099255
I<-fit.ml$hessian
V.wheat<-solve(I)
V.wheat
##
                [,1] [,2]
                                           [.3]
## [1.] 6.673668e-02 -5.694851e-11 -6.482475e-08
## [2,] -5.694851e-11 1.597051e-01 -3.194081e-02
## [3.] -6.482475e-08 -3.194081e-02 9.546274e-02
sqrt(diag(V.wheat))
## [1] 0.2583344 0.3996312 0.3089705
gamma.wheat-2*sqrt(diag(V.wheat))
## [1] 15.7897307 0.9879440 -0.3080154
gamma.wheat+2*sqrt(diag(V.wheat))
## [1] 16.8230684 2.5864686 0.9278664
```

Comparison to what is known

Fitting via 1me4: Wheat

```
fit.wheat<-lmer(v~1+(1|g),REML=FALSE)
summary(fit.wheat)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: v ~ 1 + (1 | g)
##
      AIC BIC logLik deviance df.resid
##
## 183.2 188.9 -88.6 177.2 47
##
## Scaled residuals:
## Min 1Q Median 3Q Max
## -2.7913 -0.6035 0.1311 0.6520 1.7262
##
## Random effects:
## Groups Name Variance Std.Dev.
## g (Intercept) 0.3099 0.5567
## Residual
                     1.7872 1.3369
## Number of obs: 50, groups: g, 10
##
## Fixed effects:
  Estimate Std. Error t value
##
## (Intercept) 16.3064 0.2583 63.12
gamma.wheat
## [1] 16.3063995 1.7872063 0.3099255
sqrt(diag(V.wheat))
## [1] 0.2583344 0.3996312 0.3089705
```

```
CIs<-confint(fit.wheat)

CIs

## 2.5 % 97.5 %

##.sig01 0.000000 1.228364

##.sigma 1.089911 1.693331

## (Intercept) 15.747322 16.865478

CIs[1:2,]^2

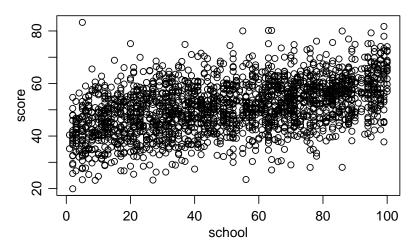
## 2.5 % 97.5 %

##.sig01 0.000000 1.508877

##.sigma 1.187907 2.867369
```

NELS example

100 randomly sampled schools from the NELS dataset



Analysis of all schools

```
fit.ml.nels<-optim(c(50, 1, 1), mll.oneway, gr = NULL, y = nels$mscore, g = nels$school, lower = c(-Inf,
fit.ml.nels
## $par
## [1] 50.93914 73.70881 23.63382
##
## $value
## [1] 46956.63
##
## $counts
## function gradient
##
                  27
##
## $convergence
## [1] 0
##
## $message
## [1] "CONVERGENCE: REL_REDUCTION_OF_F <= FACTR*EPSMCH"
##
## $hessian
##
              [,1] [,2] [,3]
## [1,] 24.35837087 -0.01576882 0.04913818
## [2,] -0.01576882 1.13128044 0.03026526
## [3,] 0.04913818 0.03026526 0.42089960
```

The MLEs are

```
\hat{\mu} = 50.9391407 \; , \; \hat{\sigma}^2 = 73.708808 \; , \; \hat{\tau}^2 = 23.6338229
```

```
gamma.nels<-fit.ml.nels$par
gamma.nels
## [1] 50.93914 73.70881 23.63382
I<-fit.ml.nels$hessian
V.nels<-solve(I)
V.nels
##
                [,1] [,2]
                                           [.3]
## [1.] 0.0410638760 0.0007019913 -0.004844505
## [2,] 0.0007019913 0.8856698641 -0.063767034
## [3,] -0.0048445047 -0.0637670344 2.381014344
sqrt(diag(V.nels))
## [1] 0.2026422 0.9411003 1.5430536
gamma.nels-2*sqrt(diag(V.nels))
## [1] 50.53386 71.82661 20.54772
gamma.nels+2*sqrt(diag(V.nels))
## [1] 51.34443 75.59101 26.71993
```

Fitting via 1me4: Math scores

```
fit.nels<-lmer(mscore~1+(1|school),REML=FALSE,data=nels)
summarv(fit.nels)
## Linear mixed model fit by maximum likelihood ['lmerMod']
## Formula: mscore ~ 1 + (1 | school)
##
     Data: nels
##
##
       ATC
                BIC logLik deviance df.resid
## 93919.3 93941.7 -46956.6 93913.3 12971
##
## Scaled residuals:
              1Q Median 3Q
      Min
                                     Max
## -3.8112 -0.6534 0.0093 0.6732 4.6999
##
## Random effects:
## Groups Name
                       Variance Std.Dev.
## school (Intercept) 23.63 4.861
## Residual
                       73.71 8.585
## Number of obs: 12974, groups: school, 684
##
## Fixed effects:
             Estimate Std. Error t value
## (Intercept) 50.9391 0.2026 251.4
gamma.nels
## [1] 50.93914 73.70881 23.63382
sqrt(diag(V.nels))
## [1] 0.2026422 0.9411003 1.5430536
```

```
CIs<-confint(fit.nels)

CIs

## 2.5 % 97.5 %

## .sig01 4.562275 5.185387

## .sigma 8.479051 8.693913

## (Intercept) 50.541015 51.336528

CIs[1:2,]^2

## 2.5 % 97.5 %

## .sig01 20.81435 26.88823

## .sigma 71.89431 75.58412
```

Our technology so far

ANOVA, method of moments:

- Estimation: $\hat{\mu} = \bar{y}$..., $\hat{\sigma}^2 = MSE$, $\hat{\tau}^2 = (MSG MSE)/n$
- Inference: *F*-test for across-group differences.

Maximum likelihood:

- Estimation: MLEs $(\hat{\mu}, \hat{\sigma}^2, \hat{\tau}^2)$
- Inference: Cls for population parameters via likelihood curvature.

What about estimation and inference for a_i 's or θ_i 's ?