

# Assessing the precision of estimates of variance components

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Estimates and standard errors

Summarizing mixed-effects model fits

A simple (but real) example

A brief overview of the theory and computation for mixed models

Profiled deviance as a function of  $\theta$

Summary

## Describing the precision of parameters estimates

- ▶ In many ways the purpose of statistical analysis can be considered as quantifying the variability in data and determining how the variability affects the inferences that we draw from it.
- ▶ Good statistical practice suggests, therefore, that we not only provide our “best guess”, the point estimate of a parameter, but also describe its precision (e.g. interval estimation).
- ▶ Some of the time (but not nearly as frequently as widely believed) we also want to check whether a particular parameter value is consistent with the data (i.e.. hypothesis tests and p-values).
- ▶ In olden days it was necessary to do some rather coarse approximations such as summarizing precision by the standard error of the estimate or calculating a test statistic and comparing it to a tabulated value to derive a 0/1 response of “significant (or not) at the 5% level”.

## Modern practice

- ▶ Our ability to do statistical computing has changed from the “olden days”. Current hardware and software would have been unimaginable when I began my career as a statistician. We can work with huge data sets having complex structure and fit sophisticated models to them quite easily.
- ▶ Regrettably, we still frequently quote the results of this sophisticated modeling as point estimates, standard errors and p-values.
- ▶ Understandably, the client (and the referees reading the client’s paper) would like to have simple, easily understood summaries so they can assess the analysis at a glance. However, the desire for simple summaries of complex analyses is not, by itself, enough to these summaries meaningful.
- ▶ We must not only provide sophisticated software for statisticians and other researchers; we must also change their thinking about summaries.

## Summaries of mixed-effects models

- ▶ Commercial software for fitting mixed-effects models (SAS PROC MIXED, SPSS, MLwin, HLM, Stata) provides estimates of fixed-effects parameters, standard errors, degrees of freedom and p-values. They also provide estimates of variance components and standard errors of these estimates.
- ▶ The mixed-effects packages for R that I have written (nlme with José Pinheiro and lme4 with Martin Mächler) do not provide standard errors of variance components. lme4 doesn't even provide p-values for the fixed effects.
- ▶ This is a source of widespread anxiety. Many view it as an indication of incompetence on the part of the developers ("Why can't lmer provide the p-values that I can easily get from SAS?")
- ▶ The 2007 book by West, Welch and Galecki shows how to use all of these software packages to fit mixed-effects models on 5 different examples. Every time they provide comparative tables they must add a footnote that lme doesn't provide standard errors of variance components.

## The Dyestuff data set

- ▶ The Dyestuff, Penicillin and Pastes data sets all come from the classic book *Statistical Methods in Research and Production*, edited by O.L. Davies and first published in 1947.
- ▶ The Dyestuff data are a balanced one-way classification of the Yield of dyestuff from samples produced from six Batches of an intermediate product. See ?Dyestuff.

```
> str(Dyestuff)
```

```
'data.frame': 30 obs. of 2 variables:
 $ Batch: Factor w/ 6 levels "A","B","C","D",...: 1 1 1 1 1 2 2 2 2 2 ..
 $ Yield: num 1545 1440 1440 1520 1580 ...
```

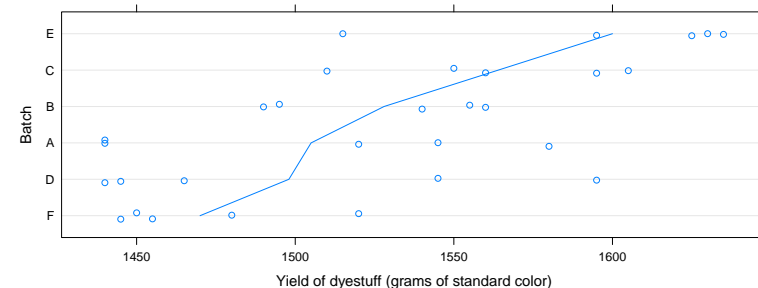
```
> summary(Dyestuff)
```

```
Batch      Yield
A:5   Min.    :1440
B:5   1st Qu.:1469
C:5   Median :1530
D:5   Mean    :1528
E:5   3rd Qu.:1575
F:5   Max.    :1635
```

## What does a standard error tell us?

- ▶ Typically we use a standard error of a parameter estimate to assess precision (e.g. a 95% confidence interval on  $\mu$  is roughly  $\bar{x} \pm 2 \frac{s}{\sqrt{n}}$ ) or to form a test statistic (e.g. a test of  $H_0 : \mu = 0$  versus  $H_a : \mu \neq 0$  based on the statistic  $\frac{\bar{x}}{s/\sqrt{n}}$ ).
- ▶ Such intervals or test statistics are meaningful when the distribution of the estimator is more-or-less symmetric.
- ▶ We would not, for example, quote a standard error of  $\widehat{\sigma^2}$  because we know that the distribution of this estimator, even in the simplest case (the mythical i.i.d. sample from a Gaussian distribution), is not at all symmetric. We use quantiles of the  $\chi^2$  distribution to create a confidence interval.
- ▶ Why, then, should we believe that when we create a much more complex model the distribution of estimators of variance components will magically become sufficiently symmetric for standard errors to be meaningful?

## Dyestuff data plot



- ▶ The line joins the mean yields of the six batches, which have been reordered by increasing mean yield.
- ▶ The vertical positions are jittered slightly to reduce overplotting. The lowest yield for batch A was observed on two distinct preparations from that batch.

## A mixed-effects model for the dyestuff yield

```
> fm1 <- lmer(Yield ~ 1 + (1 | Batch), Dyestuff)
> print(fm1)
```

```
Linear mixed model fit by REML
Formula: Yield ~ 1 + (1 | Batch)
Data: Dyestuff
AIC   BIC logLik deviance REMLdev
325.7 329.9 -159.8   327.4   319.7
Random effects:
Groups   Name      Variance Std.Dev.
Batch    (Intercept) 1764.0   42.00
Residual                2451.3   49.51
Number of obs: 30, groups: Batch, 6
Fixed effects:
              Estimate Std. Error t value
(Intercept)  1527.50     19.38    78.81
```

- ▶ Fitted model fm1 has one fixed-effect parameter, the mean yield, and one random-effects term, generating a simple, scalar random effect for each level of Batch.

## Re-fitting the model for ML estimates

```
> (fm1M <- update(fm1, REML = FALSE))
```

```
Linear mixed model fit by maximum likelihood
Formula: Yield ~ 1 + (1 | Batch)
Data: Dyestuff
AIC   BIC logLik deviance REMLdev
333.3 337.5 -163.7   327.3   319.7
Random effects:
Groups   Name      Variance Std.Dev.
Batch    (Intercept) 1388.4   37.261
Residual                2451.2   49.510
Number of obs: 30, groups: Batch, 6
Fixed effects:
              Estimate Std. Error t value
(Intercept)  1527.50     17.69    86.33
```

(The extra parentheses around the assignment cause the value to be printed. Generally the results of assignments are not printed.)

## REML estimates versus ML estimates

- ▶ The default parameter estimation criterion for linear mixed models is restricted (or “residual”) maximum likelihood (REML).
- ▶ Maximum likelihood (ML) estimates (sometimes called “full maximum likelihood”) can be requested by specifying `REML = FALSE` in the call to `lmer`.
- ▶ Generally REML estimates of variance components are preferred. ML estimates are known to be biased. Although REML estimates are not guaranteed to be unbiased, they are usually less biased than ML estimates.
- ▶ Roughly, the difference between REML and ML estimates of variance components is comparable to estimating  $\sigma^2$  in a fixed-effects regression by  $SSR/(n - p)$  versus  $SSR/n$ , where  $SSR$  is the residual sum of squares.
- ▶ For a balanced, one-way classification like the Dyestuff data, the REML and ML estimates of the fixed-effects are identical.

## Evaluating the deviance function

- ▶ The *profiled deviance* function for such a model can be expressed as a function of 1 parameter only, the ratio of the random effects’ standard deviation to the residual standard deviation.
- ▶ A very brief explanation is based on the  $n$ -dimensional response random variation,  $\mathbf{Y}$ , whose value,  $\mathbf{y}$ , is observed, and the  $q$ -dimensional, unobserved random effects variable,  $\mathbf{B}$ , with distributions

$$(\mathbf{Y}|\mathbf{B} = \mathbf{b}) \sim \mathcal{N}(\mathbf{Z}\mathbf{b} + \mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}_n), \quad \mathbf{B} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma}_\theta),$$

- ▶ For our example,  $n = 30$ ,  $q = 6$ ,  $\mathbf{X}$  is a  $30 \times 1$  matrix of 1s,  $\mathbf{Z}$  is the  $30 \times 6$  matrix of indicators of the levels of Batch and  $\boldsymbol{\Sigma}$  is  $\sigma_b^2 \mathbf{I}_6$ .
- ▶ We never really form  $\boldsymbol{\Sigma}_\theta$ ; we always work with the *relative covariance factor*,  $\boldsymbol{\Lambda}_\theta$ , defined so that

$$\boldsymbol{\Sigma}_\theta = \sigma^2 \boldsymbol{\Lambda}_\theta \boldsymbol{\Lambda}_\theta^\top$$

so  $\theta = \frac{\sigma_b}{\sigma}$  and  $\boldsymbol{\Lambda}_\theta = \theta \mathbf{I}_6$ .

## Orthogonal or “unit” random effects

- ▶ We will define a  $q$ -dimensional “spherical” or “unit” random-effects vector,  $\mathbf{U}$ , such that

$$\mathbf{U} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}_q), \mathbf{B} = \mathbf{\Lambda}_\theta \mathbf{U} \Rightarrow \text{Var}(\mathbf{B}) = \sigma^2 \mathbf{\Lambda}_\theta \mathbf{\Lambda}_\theta^\top = \mathbf{\Sigma}_\theta.$$

- ▶ The linear predictor expression becomes

$$\mathbf{Z}\mathbf{b} + \mathbf{X}\boldsymbol{\beta} = \mathbf{Z}\mathbf{\Lambda}_\theta \mathbf{u} + \mathbf{X}\boldsymbol{\beta} = \mathbf{U}_\theta \mathbf{u} + \mathbf{X}\boldsymbol{\beta}$$

where  $\mathbf{U}_\theta = \mathbf{Z}\mathbf{\Lambda}_\theta$ .

- ▶ The key to evaluating the log-likelihood is the Cholesky factorization

$$\mathbf{L}_\theta \mathbf{L}_\theta^\top = \mathbf{P} (\mathbf{U}_\theta^\top \mathbf{U}_\theta + \mathbf{I}_q) \mathbf{P}^\top$$

( $\mathbf{P}$  is a fixed permutation that has practical importance but can be ignored in theoretical derivations). The sparse, lower-triangular  $\mathbf{L}_\theta$  can be evaluated and updated for new  $\theta$  even when  $q$  is in the millions and the model involves random effects for different factors.

## Profiling the deviance with respect to $\beta$

- ▶ Because the deviance depends on  $\beta$  only through  $r^2(\theta, \beta)$  we can obtain the conditional estimate,  $\hat{\beta}_\theta$ , by extending the PLS problem to

$$r^2(\theta) = \min_{\mathbf{u}, \beta} \left[ \|\mathbf{y} - \mathbf{X}\beta - \mathbf{U}_\theta \mathbf{u}\|^2 + \|\mathbf{u}\|^2 \right]$$

with the solution satisfying the equations

$$\begin{bmatrix} \mathbf{U}_\theta^\top \mathbf{U}_\theta + \mathbf{I}_q & \mathbf{U}_\theta^\top \mathbf{X} \\ \mathbf{X}^\top \mathbf{U}_\theta & \mathbf{X}^\top \mathbf{X} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{u}}_\theta \\ \hat{\beta}_\theta \end{bmatrix} = \begin{bmatrix} \mathbf{U}_\theta^\top \mathbf{y} \\ \mathbf{X}^\top \mathbf{y} \end{bmatrix}$$

- ▶ The profiled deviance, which is a function of  $\theta$  only, is

$$-2\tilde{\ell}(\theta) = \log(|\mathbf{L}_\theta|^2) + n \left[ 1 + \log \left( \frac{2\pi r^2(\theta)}{n} \right) \right]$$

## The profiled deviance

- ▶ The Cholesky factor,  $\mathbf{L}_\theta$ , allows evaluation of the conditional mode  $\tilde{\mathbf{u}}_{\theta, \beta}$  (also the conditional mean for linear mixed models) from

$$(\mathbf{U}_\theta^\top \mathbf{U}_\theta + \mathbf{I}_q) \tilde{\mathbf{u}}_{\theta, \beta} = \mathbf{P}^\top \mathbf{L}_\theta \mathbf{L}_\theta^\top \mathbf{P} \tilde{\mathbf{u}}_{\theta, \beta} = \mathbf{U}_\theta^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$$

Let  $r^2(\theta, \beta) = \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta} - \mathbf{U}_\theta \tilde{\mathbf{u}}_{\theta, \beta}\|^2 + \|\tilde{\mathbf{u}}_{\theta, \beta}\|^2$ .

- ▶  $\ell(\theta, \beta, \sigma^2 | \mathbf{y}) = \log L(\theta, \beta, \sigma^2 | \mathbf{y})$  can be written

$$-2\ell(\theta, \beta, \sigma^2 | \mathbf{y}) = n \log(2\pi\sigma^2) + \frac{r^2(\theta, \beta)}{\sigma^2} + \log(|\mathbf{L}_\theta|^2)$$

- ▶ The conditional estimate of  $\sigma^2$  is

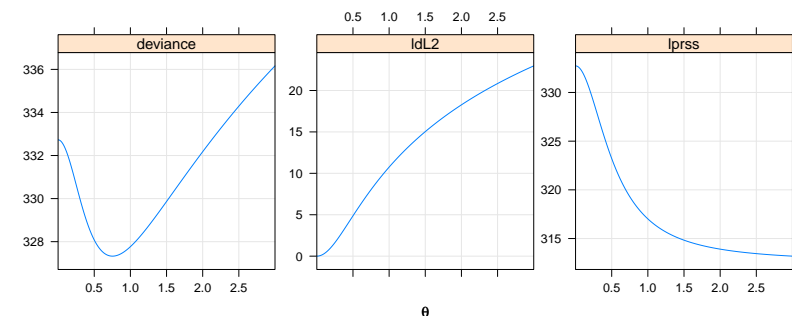
$$\widehat{\sigma^2}(\theta, \beta) = \frac{r^2(\theta, \beta)}{n}$$

producing the *profiled deviance*

$$-2\tilde{\ell}(\theta, \beta | \mathbf{y}) = \log(|\mathbf{L}_\theta|^2) + n \left[ 1 + \log \left( \frac{2\pi r^2(\theta, \beta)}{n} \right) \right]$$

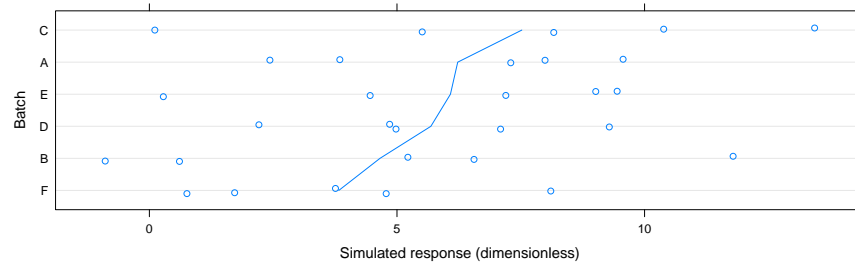
## Profiled deviance and its components

- ▶ For this simple model we can evaluate and plot the deviance for a range of  $\theta$  values. We also evaluate  $\log(|\mathbf{L}_\theta|^2)$  (1dL2) and  $n \left[ 1 + \log \left( \frac{2\pi r^2(\theta)}{n} \right) \right]$  (1prss).
- ▶ 1prss measures fidelity to the data. It is bounded above and below.  $\log(|\mathbf{L}_\theta|^2)$  measures complexity of the model. It is bounded below but not above.

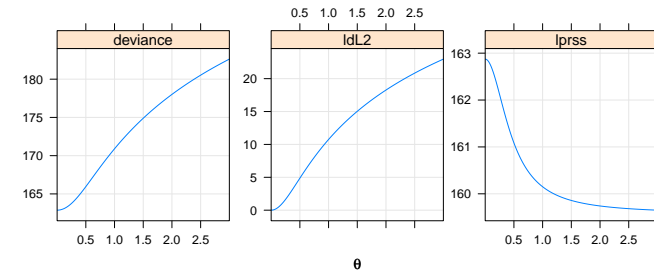


## The MLE (or REML estimate) of $\sigma_b^2$ can be 0

- For some model/data set combinations the estimate of  $\sigma_b^2$  is zero. This occurs when the decrease in  $\text{lprss}$  as  $\theta \uparrow$  is not sufficient to counteract the increase in the penalty. The Dyestuff2 data from Box and Tiao (1973) show this.

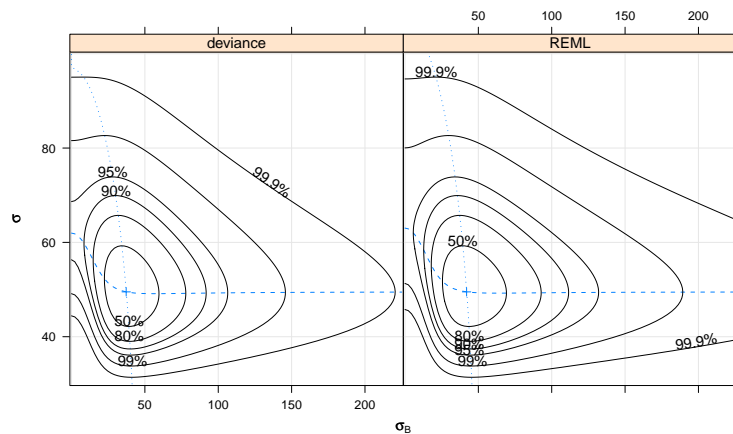


## Components of the profiled deviance for Dyestuff2

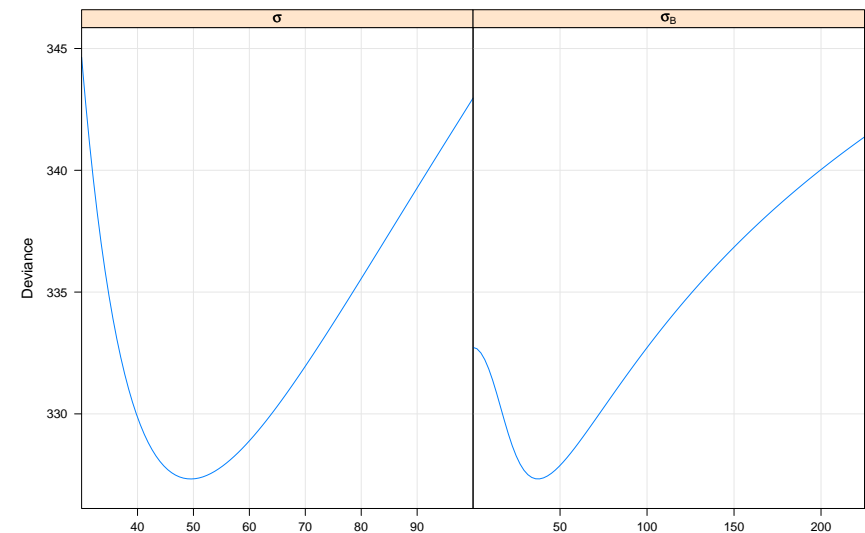


- For this data set the difference in the upper and lower bounds on  $\text{lprss}$  is not sufficient to counteract the increase in complexity of the model, as measured by  $\log(|\mathbf{L}_\theta|^2)$ .
- Software should gracefully handle cases of  $\sigma_b^2 = 0$  or, more generally,  $\mathbf{\Lambda}_\theta$  being singular. This is not done well in the commercial software.
- One of the big differences between inferences for  $\sigma_b^2$  and those for  $\sigma^2$  is considering what to do about values of zero.

## Profiled deviance and REML criterion for $\sigma_b$ and $\sigma$

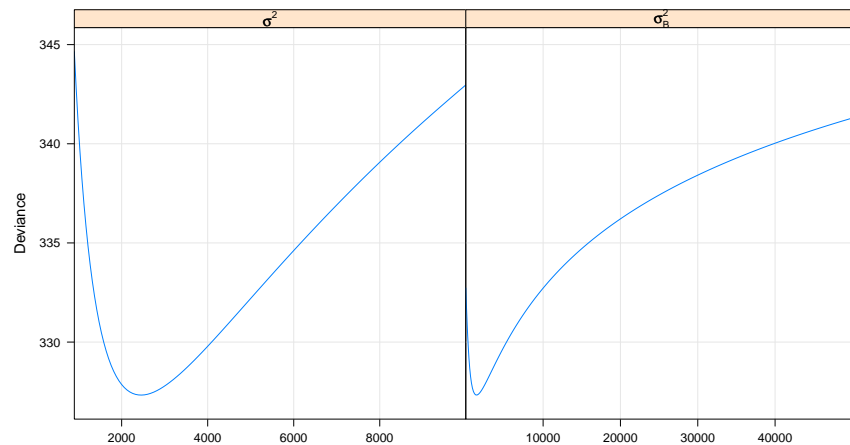


## Profiling with respect to each parameter separately



## Profiled deviance of the variance components

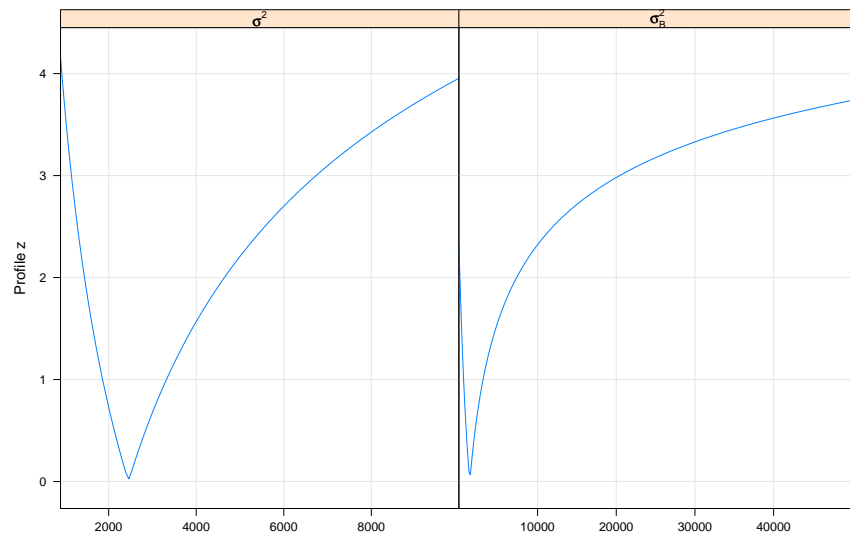
- Recall that we have been working on the scale of the standard deviations,  $\sigma_b$  and  $\sigma$ . On the scale of the variance, things look worse.



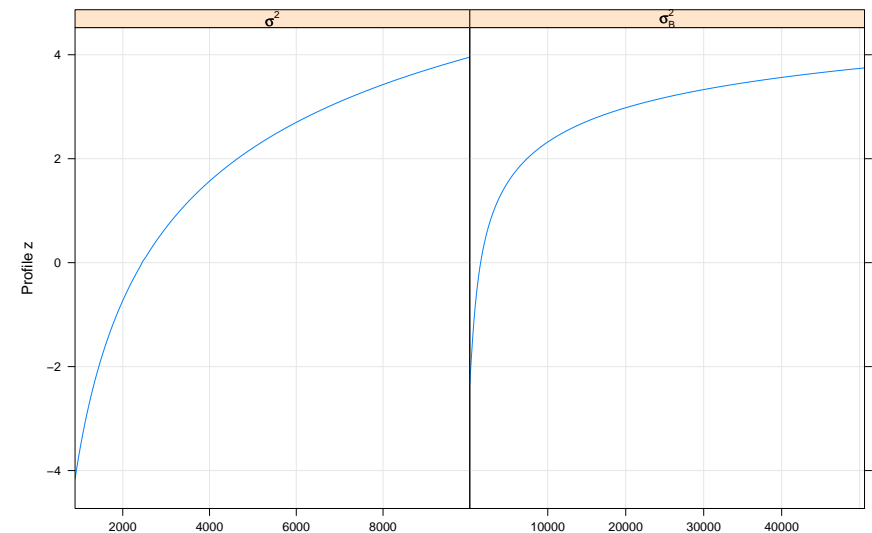
## Square root of change in the profiled deviance

- The difference of the profiled deviance at a value of  $\sigma$  or  $\sigma_b$  is the likelihood ratio test statistic for that parameter value.
- If the use of a standard error, and the implied symmetric intervals, is appropriate then this function should be quadratic in the parameter and its square root should be like an absolute value function.
- The assumption that the change in the deviance has a  $\chi_1^2$  distribution is equivalent to saying that  $\sqrt{\text{LRT}}$  is the absolute value of a standard normal.
- If we use the *signed square root* transformation where we assign a sign of  $-$  to parameters to the left of the estimate, we should get a straight line on a standard normal scale.

## Plot of square root of LRT statistic



## Signed square root plot of LRT statistic



## Summary

- ▶ Summaries based on parameter estimates and standard errors are appropriate when the distribution of the estimator can be assumed to be reasonably symmetric.
- ▶ Estimators of variances do not tend to have a symmetric distribution. If anything the scale of the log-variance (which is a multiple of the log-standard deviation) would be the more appropriate scale on which to assume symmetry.
- ▶ Estimators of variance components are more problematic because they can take on the value of zero.
- ▶ Profiling the deviance and plotting the result can help to visualize the precision of the estimates.