# robustlmm: Robust Estimating Equations and Examples

#### Manuel Koller

Seminar für Statistik, ETH Zürich and Institute of Social and Preventive Medicine, University of Bern

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This vignette attempts to give some background on the robust estimation method implemented in "rlmer". Moreover, two example analyses are included that aim to facilitate the first time user to start working with this package. The text presented here is basically a summary of Koller (2013). In said reference, a detailed derivation of the methods underlying "rlmer" can be found.

The model and some notation is introduced in Section 1. The robust estimating equations are given in Section 2. Then two examples are analyzed in Sections 3 and 4. Both datasets are also analyzed in Bates (2011). For the convenience of the reader, the description of the datasets found there has been included here. Finally, in Section 5 we provide tables of tuning constants and the definition of the *smoothed Huber*  $\psi$ -function.

## 1 The Model

Following Bates (2011), we work with the formulation of mixed effects models in terms of spherical random effects,

$$y = X\beta + ZU_b(\theta) b^* + U_e \varepsilon^*,$$

$$b^* \sim \mathcal{N}(\mathbf{0}, \sigma^2 I_q), \quad \varepsilon^* \sim \mathcal{N}(\mathbf{0}, \sigma^2 I_n), \quad b^* \perp \varepsilon^*,$$
(1)

where q is the number of random effects (the length of  $b^*$ ) and n is the number of observations (length of y). The vector  $\theta$  parameterizes the lower triangular part  $U_b(\theta)$  of the Cholesky decomposition of the covariance matrix of the random effects  $V_b(\theta)$ , i.e.,  $V_b(\theta) = U_b(\theta) U_b(\theta)^{\intercal}$ . We assume the random effects to be ordered in a way such that correlated random effects are grouped toghether. The covariance matrix  $V_b(\theta)$  is therefore block diagonal. We use the index i for observations, j for random effects and k for blocks of random effects. For notatinal simplicity, we assume that there is only one type of blocks. Generalizing the estimating equations given below is straightforward and left to the reader.

## 2 Robust Estimating Equations

#### 2.1 Fixed and Random Effects

Let k(j) be a function that maps random effect j to the corresponding block k, then the squared Mahalanobis distances of the estimated random effects are

$$d = (d(b_{k(j)}/\sigma))_{j=1,...,q}$$
, where  $d(b_k) = b_k^{*\intercal}b_k^*$ .

Then we may define the robustness weight for the jth random effect as  $w_b(d_j)$ . We use standard (location and linear regression) robustness weights:

$$w_b(d) = \begin{cases} \psi_b(\sqrt{d})/\sqrt{d} & \text{if } d \neq 0, \\ \psi_b'(0) & \text{if } d = 0. \end{cases}$$

It is convenient to represent the robustness weights as (diagonal) weighting matrix,

$$\mathbf{W}_{b}\left(\boldsymbol{d}\right) = \mathbf{Diag}\left(w_{b}\left(d_{k(j)}\right)\right)_{j=1,\dots,q}.$$

The robust estimating equations are then

$$\boldsymbol{X}^{\mathsf{T}}\boldsymbol{U}_{e}^{-\mathsf{T}}\boldsymbol{\psi}_{e}(\widehat{\boldsymbol{\varepsilon}}^{*}/\sigma) = 0 ,$$

$$\boldsymbol{U}_{b}^{\mathsf{T}}\boldsymbol{Z}^{\mathsf{T}}\boldsymbol{U}_{e}^{-\mathsf{T}}\boldsymbol{\psi}_{e}(\widehat{\boldsymbol{\varepsilon}}^{*}/\sigma) - \boldsymbol{\Lambda}_{b}\mathbf{W}_{b}\left(\widehat{\boldsymbol{d}}\right)\widehat{\boldsymbol{b}}^{*}/\sigma = 0 ,$$
(2)

where  $\Lambda_b = \mathbf{Diag}(\lambda_e/\lambda_{b,j})_{j=1,\dots,q}$  is a diagonal matrix with elements depending on the block size  $s_{k(j)}$ ,  $\lambda_e = \mathbb{E}_0\left[\psi_e'(\varepsilon^*)\right]$  and  $\lambda_{b,j} = \widetilde{\lambda}\left(s_{k(j)}\right)$ ,

$$\widetilde{\lambda}(s) = \mathbb{E}_0 \left[ \frac{\partial}{\partial b_1^*} \left( w_b(\boldsymbol{b}^{*\intercal} \boldsymbol{b}^*) \, \boldsymbol{b}_1^* \right) \right] \quad \boldsymbol{b}^* \sim \boldsymbol{\mathcal{N}}(\boldsymbol{0}, \boldsymbol{I}_s) \ .$$

#### 2.2 Scale

We apply the Design Adaptive Scale approach following Koller and Stahel (2011). We get

$$\sum_{i=1}^{n} \tau_{e,i}^{2} w_{e}^{(\sigma)} \left( \frac{\widehat{\varepsilon}_{i}^{*}}{\tau_{e,i} \widehat{\sigma}} \right) \left[ \left( \frac{\widehat{\varepsilon}_{i}^{*}}{\tau_{e,i} \widehat{\sigma}} \right)^{2} - \kappa_{e}^{(\sigma)} \right] = 0 , \qquad (3)$$

where the superscript  $\cdot^{(\sigma)}$  is used to distinguish the weighting functions used for the scale and covariance parameters from the ones for the fixed effects. Just as in the linear regression case, we define  $\tau_{e,i}$  as the value that zeroes the expectation of the *i*-th summand in (3). The expectation is

$$\mathbb{E}\left[w_e^{(\sigma)} \left(\frac{\widehat{\varepsilon}_i^*}{\tau_{e,i}\widehat{\sigma}}\right) \left(\frac{\widehat{\varepsilon}_i^*}{\tau_{e,i}\widehat{\sigma}}\right)^2 - \kappa_e^{(\sigma)} w_e^{(\sigma)} \left(\frac{\widehat{\varepsilon}_i^*}{\tau_{e,i}\widehat{\sigma}}\right)\right] = 0, \qquad (4)$$

where the distribution of the residuals is approximated using a linear expansion of  $\hat{\beta}$  and  $\hat{b}^*$  around their true values (Koller, 2013, Appendix C), and  $\kappa_e^{(\sigma)}$  is

$$\kappa_e^{(\sigma)} = \mathbb{E}_0 \left[ w_e^{(\sigma)}(\varepsilon) \, \varepsilon^2 \right] / \mathbb{E}_0 \left[ w_e^{(\sigma)}(\varepsilon) \right].$$

The weighting functions used for the scale estimates are the squared robustness weights used for the estimation of the fixed and random effects,  $w_e^{(\sigma)}(x) = (\psi_e^{(\sigma)}(x)/x)^2$ ,  $w_e^{(\sigma)}(0) = \psi_e^{(\sigma)}(0)$ , for convex  $\rho$ -functions. For redescending  $\rho$ -functions, it is not necessary to use the squared robustness weights, using the same weights as for the fixed and random effects still gives robust estimates (assuming  $\psi(x)x$  is bounded). When using the squared weights, it is crucial to use a different set of tuning parameters for estimating the scale and covariance parameters. Tables of tuning parameters can be found in Section 5.

#### 2.3 Covariance Parameters

For the covariance parameters, we have to treat the diagonal and the non-diagonal  $U_b$  case separately.

#### 2.3.1 Diagonal Case

In the case of diagonal  $U_b(\theta)$ , the estimation of  $\hat{\theta}$  is essentially a scale estimation problem on  $\hat{b}^*$ . It can be robustified just like the estimating equation for  $\hat{\sigma}$  (3). The robust estimating equations are

$$\sum_{j=1}^{q} \tau_{b,j}^2 w_b^{(\sigma)} \left( \frac{\hat{b}_j^*}{\tau_{b,i} \hat{\sigma}} \right) \left[ \left( \frac{\hat{b}_j^*}{\tau_{b,j} \hat{\sigma}} \right)^2 - \kappa_b^{(\sigma)} \right] = 0 , \qquad (5)$$

with  $\tau_{b,i}$  such that

$$\mathbb{E}\left[w_b^{(\sigma)}\left(\frac{\widehat{b}_i^*}{\tau_{b,i}\widehat{\sigma}}\right)\left[\left(\frac{\widehat{b}_i^*}{\tau_{b,i}\widehat{\sigma}}\right)^2 - \kappa_b^{(\sigma)}\right]\right] = 0,$$

and normalizing constant

$$\kappa_b^{(\sigma)} = \mathbb{E}_0 \left[ w_b^{(\sigma)}(b^*) b^{*2} \right] / \mathbb{E}_0 \left[ w_b^{(\sigma)}(b^*) \right].$$

#### 2.3.2 Non-diagonal Case

For non-diagonal  $U_b\left(\theta\right)$  we have to take care of the block structure. The normalizing constant  $\tau_{b,i}^2$  has to be replaced by a matrix  $T_{b,k}$  which is defined for each block k. Analogue to the estimator for the covariance matrix and location problem, we have to use two different weight functions, one for the size of the matrix  $w_b^{(\tau)}$  and another one for the shape  $w_b^{(\eta)}$ . For details, we refer to Stahel (1987) and Hampel et al. (1986, Chapter 5). As is done in the cited references, we introduce a third weight function  $w_b^{(\delta)}$  to simplify notation. For block types with dimension s > 1, let

$$w_b^{(\delta)}(d) = \left(dw_b^{(\eta)}(d) - \left(d - s\kappa_b^{(\tau)}\right)w_b^{(\tau)}\left(d - s\kappa_b^{(\tau)}\right)\right)/s,$$

where  $\kappa_h^{(\tau)}$  is defined such that

$$\mathbb{E}\left[\left(u - s\kappa_b^{(\tau)}\right) w_b^{(\tau)} \left(u - s\kappa_b^{(\tau)}\right)\right] = 0 \quad \text{for } u \sim \chi_s^2.$$

Remark. The optimal B-robust estimator derived in Stahel (1987) is given by  $w_b^{(\tau)}(d) = \min(1/b_\tau, 1/d)$  and  $w_b^{(\eta)}(d) = \min(1/b_\eta, 1/d)$ . Other weight functions may be chosen, as long as  $\psi(d) = dw(d)$  is a  $\psi$ -function. For  $w_b^{(\tau)}$  and  $w_b^{(\eta)}$  given above, this would be the Huber  $\psi$ -function. For low dimensions s one may choose  $w_b^{(\tau)} = w_b^{(\eta)}$ . In higher dimensions, the efficiency loss for the estimated size is negligible. Hence one may choose a smaller tuning parameter for  $w_b^{(\eta)}$ . For s = 2, and Huber or smoothed Huber  $\psi$ -functions (see Section 5), one may use the squared tuning parameter of  $\rho_e^{(\sigma)}$  for  $w_b^{(\tau)}$  to get approximately the same efficiency for  $\hat{\theta}$  as for  $\hat{\sigma}$ . Tables of tuning parameters for higher dimensions for the Huber and the lqq  $\psi$ -functions can be found in Section 5.

The robust estimating equation in the non-diagonal case can then be defined as follows. For  $l=1,\ldots,r,$ 

$$\sum_{k=1}^{K} \left[ w_b^{(\eta)} \left( d \left( \mathbf{T}_{b,k}^{-1/2} \widehat{\boldsymbol{b}}_k^* / \widehat{\sigma} \right) \right) \widehat{\boldsymbol{b}}_k^{*\dagger} \mathbf{Q}_{l,k}(\widehat{\boldsymbol{\theta}}) \widehat{\boldsymbol{b}}_k^* / \widehat{\sigma}^2 - w_b^{(\delta)} \left( d \left( \mathbf{T}_{b,k}^{-1/2} \widehat{\boldsymbol{b}}_k^* / \widehat{\sigma} \right) \right) \operatorname{tr} \left( \mathbf{T}_{b,k} \mathbf{Q}_{l,k}(\widehat{\boldsymbol{\theta}}) \right) \right] = 0 ,$$
(6)

where  $Q_{l,k}(\widehat{\boldsymbol{\theta}})$  is the  $s \times s$  submatrix of  $Q_l(\widehat{\boldsymbol{\theta}})$  which acts on block k and  $T_{b,k}^{-1/2}$  is the inverse of any square root of the  $s \times s$  matrix  $T_{b,k}$ . As in the diagonal case, we define the matrix  $T_{b,k}$  such

that each summand has expectation zero. For  $l = 1, \ldots, r$ ,

$$\mathbb{E}\left[w_b^{(\eta)}\left(d\left(\boldsymbol{T}_{b,k}^{-1/2}\widehat{\boldsymbol{b}}_k^*/\sigma\right)\right)\widehat{\boldsymbol{b}}_k^{*\dagger}\boldsymbol{Q}_{l,k}(\widehat{\boldsymbol{\theta}})\widehat{\boldsymbol{b}}_k^*/\sigma^2\right.$$
$$\left.-w_b^{(\delta)}\left(d\left(\boldsymbol{T}_{b,k}^{-1/2}\widehat{\boldsymbol{b}}_k^*/\sigma\right)\right)\operatorname{tr}\left(\boldsymbol{T}_{b,k}\boldsymbol{Q}_{l,k}(\widehat{\boldsymbol{\theta}})\right)\right]=0.$$

Remarks. The symmetric matrix  $T_{b,k}$  is fully defined for unstructured covariance matrices only, where r = s(s+1)/2. For other covariance matrix structures we can replace  $T_{b,k}$  by the variance of the linear approximation of  $b^*$ .

Since in the classical case, the linear approximations for  $\hat{\boldsymbol{b}}^*$  and  $\hat{\boldsymbol{\varepsilon}}^*$  are exact, the estimating equation (6) reduces to the REML estimating equations. A similar argument is valid for the estimating equation for  $\hat{\sigma}$  (3).

## 3 Penicillin Example

The dataset, shown in Figure 1, was originally published by Davies and Goldsmith (1972). They describe it as data coming from an investigation to

assess the variability between samples of penicillin by the *B. subtilis* method. In this test method a bulk-inoculated nutrient agar medium is poured into a Petri dish of approximately 90 mm. diameter, known as a plate. When the medium has set, six small hollow cylinders or pots (about 4 mm. in diameter) are cemented onto the surface at equally spaced intervals. A few drops of the penicillin solutions to be compared are placed in the respective cylinders, and the whole plate is placed in an incubator for a given time. Penicillin diffuses from the pots into the agar, and this produces a clear circular zone of inhibition of growth of the organisms, which can be readily measured. The diameter of the zone is related in a known way to the concentration of penicillin in the solution.

The datasets contains the measurements of 6 samples and 24 plates.

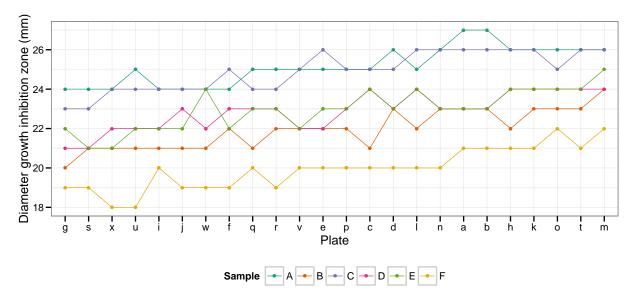


Figure 1: Diameters of growth inhibition zones of 6 samples applied to each of 24 agar plates to assess penicillin concentration in the *B. subtilis* method. The lines join the observations of the same sample. The plates have been reordered by their means.

The raw data for the Penicillin example is shown in Figure 1. In R , the data is provided as part of the R package "lme4". It is a data.frame with three columns:

# > str(Penicillin) 'data.frame': 144 obs. of 3 variables: \$ diameter: num 27 23 26 23 23 21 27 23 ...

\$ plate : Factor w/ 24 levels "g","s","x","u",...: 18 18 18 18 18 18 19 19 ...
\$ sample : Factor w/ 6 levels "A","B","C","D",...: 1 2 3 4 5 6 1 2 ...

The column "diameter" is the response and the two factors "plate" and "sample" indicate where the observation was measured. As Bates (2011), we fit a linear mixed effects model with an intercept and two random effects for the two factors.

We fit the classical linear mixed effects model using the function "lmer" of the R package "lme4". The random effects are specified in brackets. The pipe symbol "—" is used to split the factors and covariables from the grouping variable. In this case, we only have a random intercept "1" that varies by group "plate" and "sample", respectively.

```
> st(classical <- lmer(diameter ~ 1 + (1|plate) + (1|sample),
+ Penicillin))

user system elapsed
0.088 0.003 0.092</pre>
```

The "st" function is just a shortcut to "system.time", a function that measures the time required to evaluate the expression given as argument.

The robust mixed effects model is fit using the function "rlmer". The call is quite similar to "lmer"'s call. By default, it uses the smoothed Huber  $\psi$ -function with tuning parameter k=1.345 and s=10. Since we are mainly interested in the estimates of the variance components, we adjust the tuning parameter for the  $\psi^{(\sigma)}$  functions to k=2.28 and specify that squared weights are used. This makes sure that the variance components are estimated with an efficiency of about 95%. One can do this with one call to the function "psi2propII". Afterwards, we have a look at the summary of the fitted object

```
> st(robust <- rlmer(diameter ~ 1 + (1|plate) + (1|sample), Penicillin,
                     rho.sigma.e = psi2propII(smoothPsi, k = 2.28),
                     rho.sigma.b = psi2propII(smoothPsi, k = 2.28)))
   user
        system elapsed
  8.331
          0.062
                  8.398
> summary(robust)
Robust linear mixed model fit by DAStau
Formula: diameter ~ 1 + (1 | plate) + (1 | sample)
   Data: Penicillin
Scaled residuals:
     Min
           10
                   Median
                                 30
                                         Max
-2.21589 -0.80171 -0.06409 0.45911 2.86571
Random effects:
Groups
                      Variance Std.Dev.
          (Intercept) 0.7582
plate
          (Intercept) 3.8865
                               1.9714
Residual
                      0.2997
                               0.5475
Number of obs: 144, groups: plate, 24; sample, 6
Fixed effects:
            Estimate Std. Error t value
(Intercept) 23.0419
                         0.8466
Robustness weights for the residuals:
 116 weights are ~= 1. The remaining 28 ones are summarized as
```

```
Min. 1st Qu. Median
                          Mean 3rd Qu.
  0.469
         0.760
                 0.893
                          0.855
                                 0.954
                                         0.999
Robustness weights for the random effects:
 25 weights are ~= 1. The remaining 5 ones are
   1 2 3 24
                          30
0.836 0.836 0.938 0.802 0.858
Rho functions used for fitting:
  Residuals:
    eff: smoothed Huber (k = 1.345, s = 10)
    sig: smoothed Huber, Proposal II (k = 2.28, s = 10)
  Random Effects, variance component 1 (plate):
   eff: smoothed Huber (k = 1.345, s = 10)
    vcp: smoothed Huber, Proposal II (k = 2.28, s = 10)
  Random Effects, variance component 2 (sample):
    eff: smoothed Huber (k = 1.345, s = 10)
    vcp: smoothed Huber, Proposal II (k = 2.28, s = 10)
```

The first half of the summary shows information about the model that was fitted and displays the parameter estimates including standard errors for the fixed effects. After that, a summary of the robustness weights is shown. In this case, we can see that some of the observations have been downweighted, but practically none of the random effects. Finally there is a table that gives details about which  $\psi$ -functions were used to fit the model.

Remark. Note that the column "Std.Dev." contains the estimated standard deviances, i.e., just the square roots of the estimated variances. A common mistake is to interpret them as the standard errors of the variance component estimates. The same table is shown for the summary of an lme4 object and to ease the transition from "lmer" to "rlmer", we use the same convention here.

Alternatively, one might be interested in a model that does not downweight the random effects of "sample" – for example because there might be structural outliers and one is interested in the variability including these. To enable this, "rlmer" accepts list input for the arguments "rho.b" and "rho.sigma.b". The list entries correspond to the  $\psi$ -functions used for the variance components as shown in the summary output. The call to fit a model that does uses the classical estimates for the "sample" variance components is as follows.

	classical	robust	robust2
Coefficients (Std. Error)			
(Intercept)	23 (0.809)	23 (0.847)	$23 \ (0.807)$
Variance components			
(Intercept)   plate	0.847	0.871	0.871
$(Intercept) \mid sample$	1.932	1.971	1.921
σ	0.55	0.547	0.547
REML	331		

Table 1: Comparison table of the fitted models for the Penicillin example.

The results of the three fits are summarized in Table 1. The differences are minimal. Interestingly, the estimated variance for "sample" is a little smaller for "robust" than for "robust". The common residual analysis plots, Tukey-Anscombe and qq-normal, are shown in Figure 2 for the "robust" object. The points that got a lower robustness weight are indicated by a darker

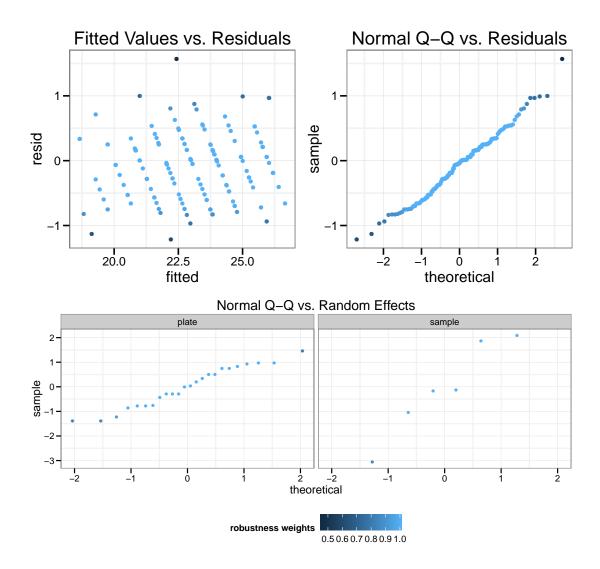


Figure 2: Residual analysis plots for the "robust" object of the Penicillin example.

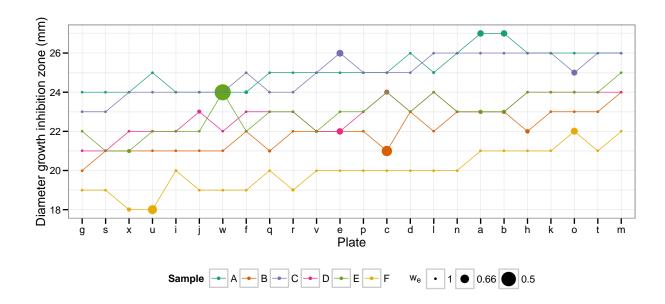


Figure 3: Diameters of growth inhibition zones of 6 samples applied to each of 24 agar plates to assess penicillin concentration in the *B. subtilis* method. The lines join the observations of the same sample. The plates have been reordered by their means. The sizes of the data points show the robustness weights.

color. The rest of the observations seem to follow the central model quite nicely. In Figure 3 we again show a plot of the data, this time highlighting the observations that got a low robustness weight.

# 4 Sleepstudy Example

This dataset is a subset of data gathered by Belenky et al. (2003) for a study of the effects of sleep deprivation time. The 18 subjects were chosen from a population of long distance drivers that were allowed to sleep for only three hours each night. Each subject's reaction time was measured several times on each day of the trial. The measurements were made over a course of 10 days. The data are shown in Figure 4.

The data frame consists of three columns:

As in Bates (2011), we will fit a random intercept and slope model. This is an extension of a linear regression model with Reaction as response and Days as predictor. In this model, the coefficients for each subject are split into a population average (fixed) and a subject specific (random) part.

The calls to "lmer" and "rlmer" are quite similar. This time, we omit the optional "1" for the intercept in both the fixed and the random part. The random effect specification (Days|Subject) is interpreted as (1+Days|Subject). Specified in this way, the fitted model also includes a correlation term. To get uncorrelated random effects, one would have to use two terms, namely (1|Subject) + (0+Days|Subject). The 0 tells the method not to include an intercept term. Since the random effects now have a non-diagonal covariance matrix  $U_b(\theta)$ , we have to use another tuning constant for "rho.sigma.b". It corresponds roughly to the square of the one used in the diagonal case.

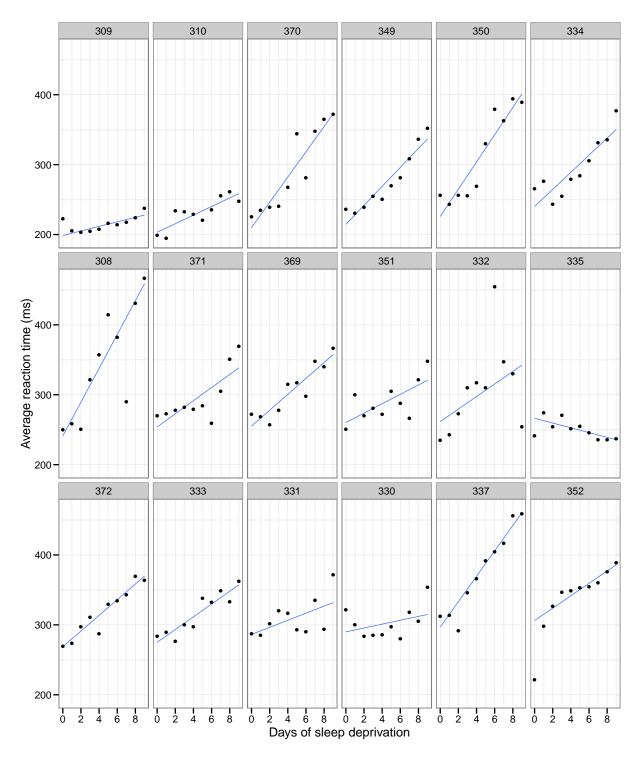


Figure 4: The average reaction time of subjects versus days of sleep deprivation. Each subject is shown in a separate facet. The lines show the robust linear regression fit to the subject's data. The subjects have been ordered by increasing intercept. The robust fits were computed using the method lmrob of the R package robustbase (Rousseeuw et al., 2012) using setting="KS2011".

```
> st(classical <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy))</pre>
  user system elapsed
  0.071
        0.000 0.078
> st(robust <-
    rlmer(Reaction ~ Days + (Days|Subject), sleepstudy,
          rho.sigma.e = psi2propII(smoothPsi, k = 2.28);
          rho.sigma.b = chgDefaults(smoothPsi, k = 5.11, s=10)))
   user system elapsed
         1.479 1112.664
1110.791
> summary(robust)
Robust linear mixed model fit by DAStau
Formula: Reaction ~ Days + (Days | Subject)
  Data: sleepstudy
Scaled residuals:
   Min 1Q Median
                           3Q
-5.1920 -0.6973 -0.1172 0.5406 6.4518
Random effects:
 Groups Name
                    Variance Std.Dev. Corr
Subject (Intercept) 784.05 28.001
                    41.68 6.456
                                      -0.04
        Days
                    404.16 20.104
Residual
Number of obs: 180, groups: Subject, 18
Fixed effects:
           Estimate Std. Error t value
(Intercept) 252.090 7.397 34.08
            10.827
                       1.662 6.52
Correlation of Fixed Effects:
    (Intr)
Days -0.137
Robustness weights for the residuals:
 147 weights are ~= 1. The remaining 33 ones are summarized as
  Min. 1st Qu. Median Mean 3rd Qu.
  0.997
Robustness weights for the random effects:
 24 weights are \tilde{\ }= 1. The remaining 12 ones are summarized as
  Min. 1st Qu. Median Mean 3rd Qu.
                                       Max
  0.631 0.692 0.723 0.735 0.742
                                       0.901
Rho functions used for fitting:
  Residuals:
   eff: smoothed Huber (k = 1.345, s = 10)
   sig: smoothed Huber, Proposal II (k = 2.28, s = 10)
  Random Effects, variance component 1 (Subject):
   eff: smoothed Huber (k = 1.345, s = 10)
   vcp: smoothed Huber (k = 5.11, s = 10)
```

The residual analysis plots are shown in Figure 5. There are some points that are outside the bulk of the residuals and accordingly get quite a low robustness weight. The qq-plot of the random effects shows some structure, but admittedly, the sample size of 18 is quite low.

The fitted values for classical and the robust fits as well as the robust per-subject fit are shown in Figure 6. While most of the subjects follow the general population fit quite closely,

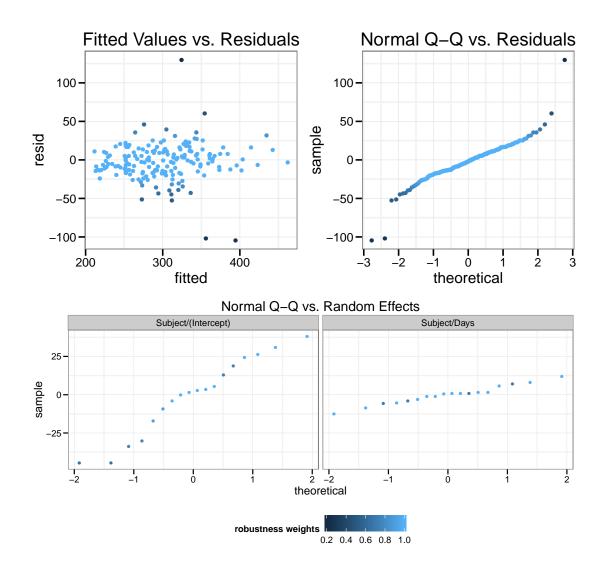


Figure 5: Residual analysis plots for robust fit "robust" of the Sleepstudy example.

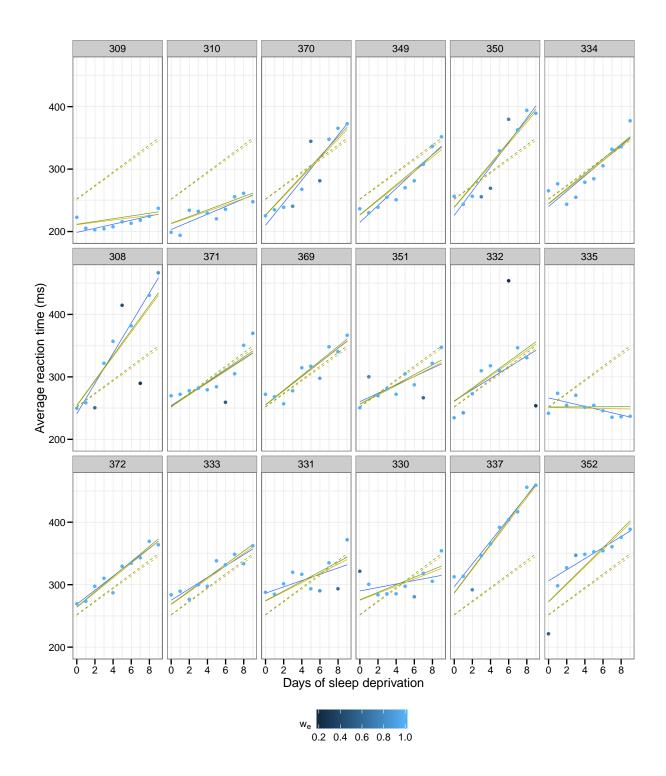


Figure 6: The average reaction time of subjects versus days of sleep deprivation. Each subject is shown in a separate facet. The blue lines show the robust linear regression fit to the subject's data. The yellow lines show the fitted values of the classical mixed effects model including random effects. The green lines show the corresponding robust linear mixed effects fit. The dashed lines show the population wide fit, robust and classical methods almost coincide. The subjects have been ordered by increasing intercept. The robust linear regression fits were computed using the method lmrob of the R package robustbase (Rousseeuw et al., 2012) using setting="KS2011".

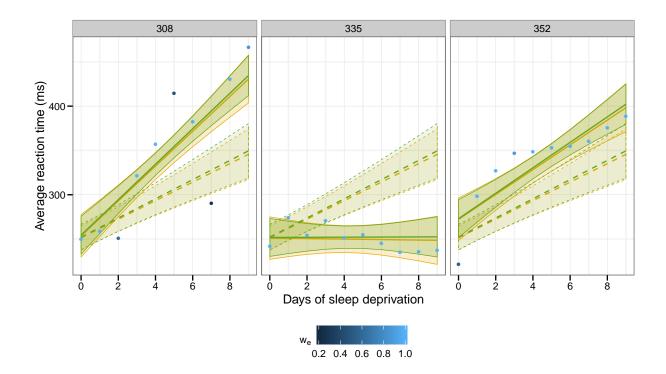


Figure 7: The average reaction time of selected subjects versus days of sleep deprivation. Additional to the features shown also in Figure 6, we show the pointwise 95% confidence intervals for the fitted values. For better visibility, we omit the linear regression fit and show only the three subjects with the most pronounced differences between classical and robust fits.

others, such as subject 335, show even a negative trend. Nevertheless, the robustness weights for the random effects do not show any clear outliers. The lowest robustness weight is assigned to subject 309 while subject 335 is given a weight of 0.69. The three subjects with the most notable difference between classical and robust fit are shown again in Figure 7. The differences in Subject 308 are most pronounced. The predicted slope of the classical fit is pulled downwards, causing the observations to lie outside or just at the border of the estimated confidence intervals. The confidence intervals for the population level estimates of the robust and classical fit are very similar. Compared to the total number of observations, there are only a very little observations with a low robustness weight. They are most probably not able to increase the variance components estimates.

We may check this statement by fitting the same model with redescending  $\psi$ -functions. As initial estimate, we use the values of the above robust fit. With "rlmer", one can do this conveniently by using the "update" function and specifying redescending  $\psi$ -functions. The object that is being updated will be used as initial fit.

```
> st(redesc <-
+     update(robust, rho.e = chgDefaults(lqqPsi, cc=c(1.47, 0.98, 1.5)),
+          rho.sigma.e = chgDefaults(lqqPsi, cc=c(2.19, 1.46, 1.5)),
+          rho.b = chgDefaults(lqqPsi, cc=c(1.47, 0.98, 1.5)),
+          rho.sigma.b = chgDefaults(lqqPsi, cc=c(5.95, 3.97, 1.5))))
    user     system elapsed
2663.114     3.607 2667.865
> summary(redesc)
Robust linear mixed model fit by DAStau
Formula: Reaction ~ Days + (Days | Subject)
    Data: sleepstudy
```

```
Scaled residuals:
   Min 1Q Median
                            3Q
-5.2055 -0.6839 -0.1008 0.5605 6.5074
Random effects:
                     Variance Std.Dev. Corr
Groups Name
Subject (Intercept) 809.17 28.446
                     43.66
                              6.607
                                       -0.07
Residual
                     399.39
                             19.985
Number of obs: 180, groups: Subject, 18
Fixed effects:
           Estimate Std. Error t value
                     7.528 33.45
(Intercept) 251.775
                         1.704
                                  6.35
            10.822
Correlation of Fixed Effects:
    (Intr)
Days -0.160
Robustness weights for the residuals:
 137 weights are ~= 1. The remaining 43 ones are summarized as
  Min. 1st Qu. Median Mean 3rd Qu.
0.0127 0.7400 0.9010 0.8010 0.9680 0.9980
Robustness weights for the random effects:
 14 weights are \tilde{\ }= 1. The remaining 22 ones are summarized as
  Min. 1st Qu. Median
                         Mean 3rd Qu.
                                          Max.
  0.690 0.778 0.929
                         0.879
                                0.977
                                         0.995
Rho functions used for fitting:
  Residuals:
    eff: lqq (cc1 = 1.47, cc2 = 0.98, cc3 = 1.5)
    sig: lqq (cc1 = 2.19, cc2 = 1.46, cc3 = 1.5)
  Random Effects, variance component 1 (Subject):
    eff: lqq (cc1 = 1.47, cc2 = 0.98, cc3 = 1.5)
    vcp: lqq (cc1 = 5.95, cc2 = 3.97, cc3 = 1.5)
```

	classical	robust	redesc
Coefficients (Std. Error)			
(Intercept)	251.4(6.82)	$252.1\ (7.40)$	251.8(7.53)
Days	10.5 (1.55)	10.8 (1.66)	10.8(1.70)
Variance components			
$(Intercept) \mid Subject$	24.74	28.00	28.45
Days   Subject	5.92	6.46	6.61
Correlations			
$(Intercept) \times Days \mid Subject$	0.0656	-0.0369	-0.0695
σ	25.6	20.1	20
REML	1744		

Table 2: Comparison table of the fitted models for the Sleepstudy example.

A comparison table of the three fits is shown in Table 2. The two robust fits are quire similar. The variance attributed to the between subjects effects is a little lower for the fit using redescending  $\psi$ -functions, while the two estimates of the residual standard errors are almost identical. We therefore conclude that the few observations with a small robustness weight were not able to unduly increase the estimates residual standard error. While the estimated residual standard errors for both robust fits are smaller than for the classical fit, the estimated standard errors of the fixed effects estimates are a little increased (the estimated standard error for the classical fit is 6.82 for the intercept and 1.55 for "Days").

The robust fits return a negative estimate of the correlation between the random intercept and slopes. When choosing smaller tuning parameters for the functions "rho.b" and "rho.sigma.b", the correlation is estimated even lower. A scatterplot of the estimated random effects is shown in Figure 8. With help from the coloring of the points, one can see a hint of a negative correlation between the two random effects (suppressing the points below and above the falling diagonal). This is picked up by the estimator. For smaller tuning parameters, the weight function decreases more quickly and the off-diagonal points get a lower weight, finally this leads to a negative estimate of the correlation.

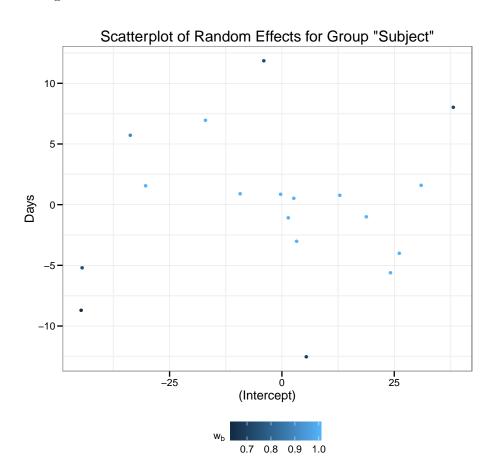


Figure 8: Scatterplot of the estimated random effects for the "redesc" fit for the Sleepstudy example using redescending lqq  $\psi$ -functions.

## 5 $\psi$ -functions and Tables of Tuning Constants

The smoothed Huber  $\psi$ -function is defined as

$$\psi(x,k,s) = \begin{cases} x & |x| \le c\\ \operatorname{sign}(x) \left(k - \frac{1}{(|x| - d)^s}\right) & \text{otherwise} \end{cases}, \tag{7}$$

where  $c = k - s^{\frac{-s}{s+1}}$  and  $d = c - s^{\frac{1}{s+1}}$ . We have always used s = 10 for our simulations. With this value, the asymptotic properties of the regular Huber function and the smoothed Huber function are almost identical. We can therefore safely use the same tuning parameter k for both  $\psi$ -functions. A comparison of the two  $\psi$ -functions is shown in Figure 9. Useful tables of tuning constants for this and the lqq  $\psi$ -function are given in Tables 3 to 6.

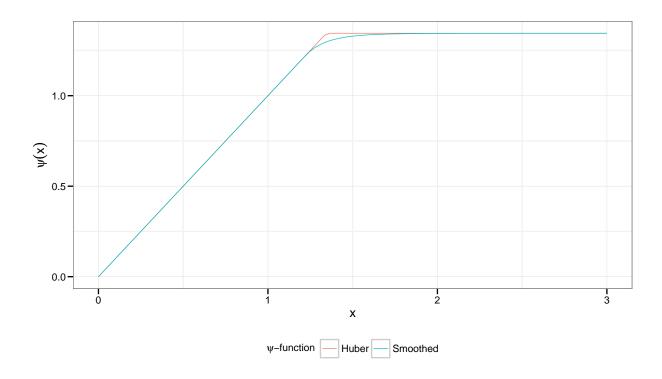


Figure 9: Comparison of the Huber and the smoothed Huber  $\psi$ -function for k=1.345 and s=10.

efficiency	$k \text{ for } \hat{\mu}$	$k \text{ for } \hat{\sigma}_{(3)}$	$k \text{ for } \hat{\sigma}_{(3)}, \text{ Prop. II}$
0.80	0.53	0.50	1.49
0.85	0.73	0.71	1.69
0.90	0.98	1.08	1.94
0.95	1.345	1.66	2.28

Table 3: Tuning parameters k for scale estimates such that they reach the same asymptotic efficiency as the location estimate. For the Huber  $\psi$ -function.

	dimension $s$					
	2	3	4	5	6	7
$\overline{b_{\eta}}$	5.66	6.41	7.14	7.87	8.58	9.28
$b_{ au}$	5.15	5.55	5.91	6.25	6.55	6.84
$b_{\mu}$	1.5	1.63	1.73	1.81	1.87	1.9

Table 4: Tuning parameters for the optimal *B*-estimator to yield 95% efficiency, non-diagonal case. For the Huber  $\psi$ -function.

efficiency	$cc$ for $\hat{\mu}$	$cc \text{ for } \hat{\sigma}_{(3)}$
0.80	(0.946, 0.631)	(1.414, 0.942)
0.85	(1.058, 0.705)	(1.57, 1.05)
0.90	(1.214, 0.809)	(1.79, 1.19)
0.95	(1.474, 0.982)	(2.19,1.46)

Table 5: Tuning parameters for lqq  $\psi$ -function for the location and scale estimates such that they reach the given asymptotic efficiency. The third parameter is always taken to be 1.5.

	dimension $s$				
	2	3	4	5	6
$\overline{cc_{\eta}}$	(6.44, 4.29)	(7.23, 4.82)	(8.01, 5.34)	(8.77, 5.85)	(9.52, 6.35)
$cc_{ au}$	(5.95, 3.97)	(6.41, 4.27)	(6.82, 4.55)	(7.2,4.8)	(7.55, 5.03)
$cc_{\mu}$	(1.63, 1.09)	(1.77, 1.18)	(1.88, 1.26)	(1.99, 1.32)	(2.08, 1.39)

Table 6: Tuning parameters for the lqq weight function to yield 95% efficiency, non-diagonal case. The third parameter is always taken to be 1.5.

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