Journal of Statistical Software

MMMMMM YYYY, Volume VV, Issue II. *http://www.jstatsoft.org/*

Comparing Optimization Algorithms in the Fitting of Linear Mixed Models: Evaluating Speed and Accuracy using lme4 in R and lmm in Julia

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Abstract

The **Timings** package allows for the comparison of several optimizers, in both R and Julia, used in the fitting of various linear mixed models. In R the optimizers are called by lmer from the **lme4** package (version 1.1-8). In Julia the optimizers are called by lmm from **MixedModels** package. From the **Timings** package, conclusions regarding an optimizers relative speed, accuracy and general effectiveness of different optimizers paired with different types of models (ranging from simple to complex) can easily be drawn and interpretted.

There are differences in the model formulations in **lme4** and in **MixedModels**. The numerical representation of the model in **lme4** and the method of evaluating the optimizers, described in this paper, is the same for all models. In **MixedModels** there are specialized representations for some model forms, such as models with a single grouping factor for the random effects. Some of the specialized representations allow for evaluation of the gradient of the objects, which can enhance convergence (but, interestingly, sometimes can impede convergence).

Keywords: optimizers, mixed models, linear mixed models, lme4, lmm, R, Julia.

1. Introduction

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2. Methods

To provide consistency we have copied all the data sets used in the timings to the **Timings** package itself. We have done all timings on the same computer. This computer has a relatively recent Intel processor and we used the Intel Math Kernel Library (MKL) with Julia. We attempted to use Revolution R Open (RRO) as the R implementation as it can be configured with **MKL**. However, we ran into version problems with this so we used the standard Ubuntu version of R linked against OpenBLAS, which is also multi-threaded.

Variables were renamed in the pattern:

- **Y** the response
- **A**, **B**, ... categorical covariates
- **G**,**H**, **I**, ... grouping factors for random effects
- **U**, **V**, ... (skipping **Y**) continuous covariates

The timing results are saved in JSON (JavaScript Object Notation) files in the directory accessible as

```
> system.file("JSON",package="Timings")
```

within **R**. The directory name will end with `./Timings/inst/JSON/` in the package source directory, for example the result of cloning the github repository. There is one `.json` file for each data set. Each such file contains results on timings of one or more models.

The **Timings** package for R provides a `retime` function that takes the name of one of these JSON files and, optionally, the name of a file with the updated timings. Similarly there are some source files for **Julia** retimings.

```
> include("../julia/retime.jl")
> retime("../JSON/Alfalfa.json","/tmp/Alfalfa.json")
> retime("../JSON/Alfalfa.json","/tmp/Alfalfa.json")
```

INCLUDE SUMMARY TABLE USING res.rda

The timing was repeated so that compilation time is not included in the results. This repetition is only needed once per session.

A careful examination of these results shows that the main differences in the **Julia** timings (the **R** timings are merely reported, not evaluated) are that the `LN_BOBYQA` and `LD_MMA` optimizers

are much faster in the second run. This is because much of the code needs to be compiled the first time that a derivative-free optimizer and a derivative-based optimizer are used.

The names of the optimizers used with `lmm` are those from the **NLopt** package for Julia. Names that begin with `LD_` are gradient-based methods. Names that begin with `LN_` are derivative-free methods. There is one other derivative-free method, `LN_PRAXIS`, available in the **NLopt** package but, for some reason, it can hang on very simple problems like this. Frequently we omit it.

The optimizers used with `lmer` include the `Nelder_Mead` optimizer built into the **lme4** package, the `bobyqa` optimizer from the **minqa** package, the derivative-free optimizers from the **nloptr** package and several optimizers from the **optimx** pacakge.

The `optimx:bobyqa` optimizer is just a wrapper around `bobyqa` (bounded optimization by quadratic approximation) from the **minqa** package and should provide results similar to those from the `bobyqa` optimizer. For some reason the number of function evaluations is not reported for the version in **optimx**.

The optimizers from **nloptr** (i.e. those whose names begin with `NLOPT_LN_`) use the same underlying code as do the similarly named optimizers in the **NLopt** package for Julia. The number of iterations to convergence should be similar for the same underlying code, although not nessarily exactly the same because the evaluation of the objective in R and in Julia may produce slightly different answers. Also the convergence criteria in the Julia version are more strict than those in the R version

Also shown are the value of the criterion (negative twice the log-likelihood, lower is better) achieved, the elapsed time and the number of function and gradient evaluations. The `nopt` value is the number of parameters in the optimization problem. `mtype` is the model type in the Julia code. There are special methods for solving the penalized least squares (PLS) problem, and for evaluating the objective and its gradient when there is only one grouping factor for the random effects. The model type is called `PLSOne`.

The `Alfalfa` example is a particularly easy one and all of the optimizerws converge to an objective value close to -10.81023 in less than 0.6 seconds.

3. Results

For the `Alfalfa` data there is not much of a burden in refitting the model with all the **Julia** optimizers just to get the table shown above. But other examples can take an hour or more to converge and we don't really need to refit them every time. The `tabulate.jl` file contains a function `optdir` to create a `DataFrame` from the results of all the model fits.

```
> include("../julia/tabulate.jl")
> res = optdir("../JSON");
```

The `time` column is the time in seconds to converge. The `reltime` column is the time relative to the `LN_BOBYQA` optimizer in the **MixedModels** package for Julia.

For Julia the time column is the time in seconds to converge. The reltime column is the time relative to the $\mathrm{LN}_BOBYQAoptimizerintheMixedModelspackagefor$Julia.

	opt	dsname	n	p	np	excess	time	reltime
1	LD_CCSAQ	Alfalfa	72	12	1	0.00	0.00	1.13
2	LD_CCSAQ	AvgDailyGain	32	8	1	0.00	0.00	0.82
3	LD_CCSAQ	AvgDailyGain	32	5	1	0.00	0.00	0.93
4	LD_CCSAQ	BIB	24	8	1	0.00	0.00	0.79
5	LD_CCSAQ	Bond	21	3	1	0.00	0.00	1.03
6	LD_CCSAQ	bs10	1104	4	20	0.00	1.10	4.44
7	LD_CCSAQ	bs10	1104	4	8	39.99	0.04	0.56
8	LD_CCSAQ	cake	270	18	1	0.00	0.00	1.37
9	LD_CCSAQ	Cultivation	24	6	1	0.00	0.00	0.99
10	LD_CCSAQ	Demand	77	5	2	3.22	0.01	0.81
11	LD_CCSAQ	dialectNL	225866	4	6	0.00	6.99	3.99
12	LD_CCSAQ	Dyestuff2	30	1	1	0.00	0.00	0.68
13	LD_CCSAQ	Dyestuff	30	1	1	0.00	0.00	1.02
14	LD_CCSAQ	ergoStool	36	4	1	0.00	0.00	1.10
15	LD_CCSAQ	Exam	4059	5	1	0.00	0.01	1.19
16	LD_CCSAQ	Exam	4059	6	1	0.00	0.01	1.32
17	LD_CCSAQ	Gasoline	32	2	1	0.00	0.00	0.82
18	LD_CCSAQ	gb12	512	8	20	0.00	3.52	17.48
19	LD_CCSAQ	gb12	512	8	8	103.18	0.02	0.56
20	LD_CCSAQ	HR	120	7	3	0.00	0.01	1.22
21	LD_CCSAQ	Hsb82	7185	5	1	192.73	0.01	0.49
22	LD_CCSAQ	IncBlk	24	8	1	0.56	0.00	0.66
23	LD_CCSAQ	kb07	1790	8	72	8.21	17.47	4.12
24	LD_CCSAQ	Mississippi	37	3	1	0.93	0.00	0.67
25	LD_CCSAQ	mm0	69588	4	6	0.00	4.83	4.40
26	LD_CCSAQ	Oxboys	234	2	3	136.79	0.02	0.71
27	LD_CCSAQ	PBIB	60	15	1	0.00	0.00	1.00
28	LD_CCSAQ	Penicillin	144	1	2	0.00	0.01	4.94
29	LD_CCSAQ	Semiconductor	48	16	1	0.00	0.00	1.05
30	LD_CCSAQ	SIMS	3691	2	3	3.61	0.13	0.99
31	LD_CCSAQ	sleepstudy	180	2	3	0.00	0.01	1.75
32	LD_CCSAQ	sleepstudy	180	2	2	0.00	0.00	1.13
33	LD_CCSAQ	TeachingII	96	12	1	0.00	0.00	0.93
34	LD_CCSAQ	Weights	399	6	3	99.13	0.02	0.51
35	LD_CCSAQ	WWheat	60	2	3	18.20	0.01	0.68

	opt	dsname	n	p	np	excess	time	reltime
560	NLOPT_LN_BOBYQA	Alfalfa	72	12	1	0.00	0.04	27.52
561	NLOPT_LN_BOBYQA	Animal	20	1	2	0.00	0.02	13.92
562	NLOPT_LN_BOBYQA	Assay	60	31	2	0.00	0.03	10.80
563	NLOPT_LN_BOBYQA	AvgDailyGain	32	8	1	0.00	0.02	11.70
564	NLOPT_LN_BOBYQA	AvgDailyGain	32	5	1	0.00	0.02	13.70
565	NLOPT_LN_BOBYQA	BIB	24	8	1	0.00	0.02	12.61
566	NLOPT_LN_BOBYQA	Bond	21	3	1	0.00	0.02	23.27
567	NLOPT_LN_BOBYQA	bs10	1104	4	20	0.00	4.66	18.88
568	NLOPT_LN_BOBYQA	bs10	1104	4	8	0.00	1.06	15.65
569	NLOPT_LN_BOBYQA	cake	270	18	1	0.00	0.05	22.08
570	NLOPT_LN_BOBYQA	Chem97	31022	1	2	0.00	0.63	3.94
571	NLOPT_LN_BOBYQA	Chem97	31022	2	2	0.00	0.56	3.60
572	NLOPT_LN_BOBYQA	Cultivation	24	6	1	0.00	0.02	23.10
573	NLOPT_LN_BOBYQA	d3	130418	2	9	0.00	231.30	2.16
574	NLOPT_LN_BOBYQA	Demand	77	5	2	0.00	0.03	3.81
575	NLOPT_LN_BOBYQA	dialectNL	225866	4	6	0.00	16.88	9.64
576	NLOPT_LN_BOBYQA	Dyestuff2	30	1	1	0.00	0.05	62.58
577	NLOPT_LN_BOBYQA	Dyestuff	30	1	1	0.00	0.02	24.87
578	NLOPT_LN_BOBYQA	egsingle	7230	5	2	0.00	0.17	2.39
579	NLOPT_LN_BOBYQA	ergoStool	36	4	1	0.00	0.02	17.25
580	NLOPT_LN_BOBYQA	Exam	4059	5	1	0.00	0.05	5.40
581	NLOPT_LN_BOBYQA	Exam	4059	6	1	0.00	0.05	6.33
582	NLOPT_LN_BOBYQA	Gasoline	32	2	1	0.00	0.02	14.30
583	NLOPT_LN_BOBYQA	gb12	512	8	20	0.00	1.87	9.28
584	NLOPT_LN_BOBYQA	gb12	512	8	8	0.00	0.42	10.77
585	NLOPT_LN_BOBYQA	Genetics	60	5	2	0.00	0.03	9.60
586	NLOPT_LN_BOBYQA	HR	120	7	3	0.00	0.02	3.29
587	NLOPT_LN_BOBYQA	Hsb82	7185	5	1	0.00	0.07	3.52
588	NLOPT_LN_BOBYQA	IncBlk	24	8	1	0.00	0.02	12.89
589	NLOPT_LN_BOBYQA	InstEval	73421	28	2	0.00	10.06	4.28
590	NLOPT_LN_BOBYQA	InstEval	73421	2	3	0.00	15.82	3.63
591	NLOPT_LN_BOBYQA	kb07	1790	8	72	0.01	311.03	73.43
592	NLOPT_LN_BOBYQA	kb07	1790	8	16	0.00	18.50	26.31
593	NLOPT_LN_BOBYQA	Mississippi	37	3	1	0.00	0.02	21.53
594	NLOPT_LN_BOBYQA	mm0	69588	4	6	0.00	26.20	23.88
595	NLOPT_LN_BOBYQA	Oxboys	234	2	3	0.00	0.03	1.35
596	NLOPT_LN_BOBYQA	Pastes	60	1	2	0.00	0.02	9.51
597	NLOPT_LN_BOBYQA	PBIB	60	15	1	0.00	0.02	13.14
598	NLOPT_LN_BOBYQA	Penicillin	144	1	2	0.00	0.02	8.65
599	NLOPT_LN_BOBYQA	Poems	275996	3	3	0.00	21.31	3.74
600	NLOPT_LN_BOBYQA	ScotsSec	3435	4	2	0.00	0.08	5.04
601	NLOPT_LN_BOBYQA	Semi2	72	2	3	0.00	0.03	9.27
602	NLOPT_LN_BOBYQA	Semiconductor	48	16	1	0.00	0.02	15.96
603	NLOPT_LN_BOBYQA	SIMS	3691	2	3	0.00	0.15	1.10
604	NLOPT_LN_BOBYQA	sleepstudy	180	2	3	0.00	0.04	5.30
605	NLOPT_LN_BOBYQA	sleepstudy	180	2	2	0.00	0.02	8.62
606	NLOPT_LN_BOBYQA	TeachingII	96	12	1	0.00	0.02	15.38
607	NLOPT_LN_BOBYQA	Weights	399	6	3	0.00	0.04	1.13
608	NLOPT_LN_BOBYQA	WWheat	60	2	3	0.00	0.03	2.32

3.1. Proportion Converged

The most important question regarding the optimizers is whether or not they have converged to the global optimum. We cannot test this directly. Instead we use a "crowd-sourced" criterion based on the minimum objective achieved by any of the algorithms. The difference between the objective achieved by a particular algorithm and this minimum is called the excess. In the summaries `excess` is rounded to 5 digits after the decimal so the minimum non-zero `excess` is 10^{-5}.

	opt	dsname	excess
347	LN_BOBYQA	Alfalfa	0.00
348	LN_BOBYQA	Animal	0.00
349	LN_BOBYQA	Assay	0.00
350	LN_BOBYQA	AvgDailyGain	0.00
351	LN_BOBYQA	AvgDailyGain	0.00
352	LN_BOBYQA	BIB	0.00
353	LN_BOBYQA	Bond	0.00
354	LN_BOBYQA	bs10	0.00
355	LN_BOBYQA	bs10	0.00
356	LN_BOBYQA	cake	0.00
357	LN_BOBYQA	Chem97	0.00
358	LN_BOBYQA	Chem97	0.00
359	LN_BOBYQA	Cultivation	0.00
360	LN_BOBYQA	d3	0.00
361	LN_BOBYQA	Demand	0.00
362	LN_BOBYQA	dialectNL	0.00
363	LN_BOBYQA	Dyestuff2	0.00
364	LN_BOBYQA	Dyestuff	0.00
365	LN_BOBYQA	egsingle	0.00
366	LN_BOBYQA	ergoStool	0.00
367	LN_BOBYQA	Exam	0.00
368	LN_BOBYQA	Exam	0.00
369	LN_BOBYQA	Gasoline	0.00
370	LN_BOBYQA	gb12	0.00
371	LN_BOBYQA	gb12	0.00
372	LN_BOBYQA	Genetics	0.00
373	LN_BOBYQA	HR	0.00
374	LN_BOBYQA	Hsb82	0.00
375	LN_BOBYQA	IncBlk	0.00
376	LN_BOBYQA	InstEval	0.00
377	LN_BOBYQA	InstEval	0.00
378	LN_BOBYQA	kb07	0.02
379	LN_BOBYQA	kb07	0.00
380	LN_BOBYQA	Mississippi	0.00
381	LN_BOBYQA	mm0	0.00
382	LN_BOBYQA	Oxboys	0.00
383	LN_BOBYQA	Pastes	0.00
384	LN_BOBYQA	PBIB	0.00
385	LN_BOBYQA	Penicillin	0.00
386	LN_BOBYQA	Poems	0.00
387	LN_BOBYQA	ScotsSec	0.00
388	LN_BOBYQA	Semi2	0.00
389	LN_BOBYQA	Semiconductor	0.00
390	LN_BOBYQA	SIMS	0.00
391	LN_BOBYQA	sleepstudy	0.00
392	LN_BOBYQA	sleepstudy	0.00
393	LN_BOBYQA	TeachingII	0.00
394	LN_BOBYQA	Weights	0.00
395	LN_BOBYQA	WWheat	0.00

If we wish to declare "converged" or "not converged" according to the excess objective value we must establish a threshold. An absolute threshold seems reasonable because the objective, negative twice the log-likelihood, is on a scale where differences in this objective are compared to a χ^2 random variable. Thus an excess of 10^{-9} or even 10^{-5} is negligible.

For each optimizer we can examine which of the data set/model combinations resulted in an excess greater than a threshold.

At this threshold the most reliable algorithm in Julia is `LN_BOBYQA`. In `R` the most reliable algorithms are `NLOPT_LN_BOBYQA`, `optimx:L-BFGS-B` and `optimx:nlminb`. It is interesting that nlminb is reliable as I felt that it wasn't converging well when it was the default optimizer in **lmer**.

Interestingly, the derviative-based algorithms in `NLopt` were not as reliable as the derivative-free algorithms. The most likely explanation is that I don't have the gradient coded properly.

The Nelder-Mead simplex algorithm did not perform well, failing on 8 out of 48 cases. For many of these the value at which convergence was declared was far from the optimum.

```
> print(xtable(subset(res, opt=="Nelder_Mead" & excess > 0.005)[c(1,2,3,5,6,7,8)]),floatin
```

	opt	dsname	n	np	excess	time	reltime
777	Nelder_Mead	bs10	1104	20	71.39	145.37	588.68
783	Nelder_Mead	d3	130418	9	317.59	454.52	4.25
785	Nelder_Mead	dialectNL	225866	6	181.63	54.54	31.16
793	Nelder_Mead	gb12	512	20	78.71	38.21	189.60
801	Nelder_Mead	kb07	1790	72	398.73	2825.46	667.02
802	Nelder_Mead	kb07	1790	16	403.48	269.44	383.09
803	Nelder_Mead	Mississippi	37	1	0.04	0.02	20.40
804	Nelder_Mead	mm0	69588	6	181.63	76.87	70.07

```
> print(xtable(subset(res, opt=="NLOPT_LN_NELDERMEAD" & excess > 0.005)[c(1,2,3,5,6,7,8)])
```

	opt	dsname	n	np	excess	time	reltime
659	NLOPT_LN_NELDERMEAD	Assay	60	2	0.06	0.04	14.18
664	NLOPT_LN_NELDERMEAD	bs10	1104	20	0.97	88.29	357.52
670	NLOPT_LN_NELDERMEAD	d3	130418	9	100.19	627.93	5.87
680	NLOPT_LN_NELDERMEAD	gb12	512	20	0.84	52.41	260.10
688	NLOPT_LN_NELDERMEAD	kb07	1790	72	88.77	2839.07	670.23
689	NLOPT_LN_NELDERMEAD	kb07	1790	16	3.50	198.84	282.72

The `Nelder_Mead` algorithm, either in the native form in **lmer** or in the `NLopt` implementation performed poorly on those cases with many parameters to optimize. It was both unreliable and slow, taking over 45 minutes to reach a spurious optimum on the "maximal" model (in the sense of Barr et al., 2012) for the `kb07` data from Kronmueller and Barr (2007). This is not terribly surprising given that the model is horribly overparameterized, but still it shows that this algorithm is not a good choice in these cases.

We note in passing that all the models involving fitting 20 or more parameters are "maximal" models in the sense of Barr et al., 2012. Such models can present difficult optimization problems because they are severely overparameterized and inevitably converge on the boundary

of the allowable parameter space. Whether or not it is sensible to compare results on such extreme cases is not clear.

The `SBPLX` (subplex) algorithm, which is an enhancement of `Nelder_Mead`, does better in these cases but is still rather slow.

```
> print(xtable(subset(res, opt=="NLOPT_LN_SBPLX" & excess > 0.005)[c(1,2,3,5,6,7,8)]),floa
```

	opt	dsname	n	np	excess	time	reltime
745	NLOPT_LN_SBPLX	gb12	512	20	0.82	3.81	18.92
753	NLOPT_LN_SBPLX	kb07	1790	72	4.97	564.69	133.31

By comparison, the `LN_BOBYQA` algorithm converges quite rapidly on the `kb07` models.

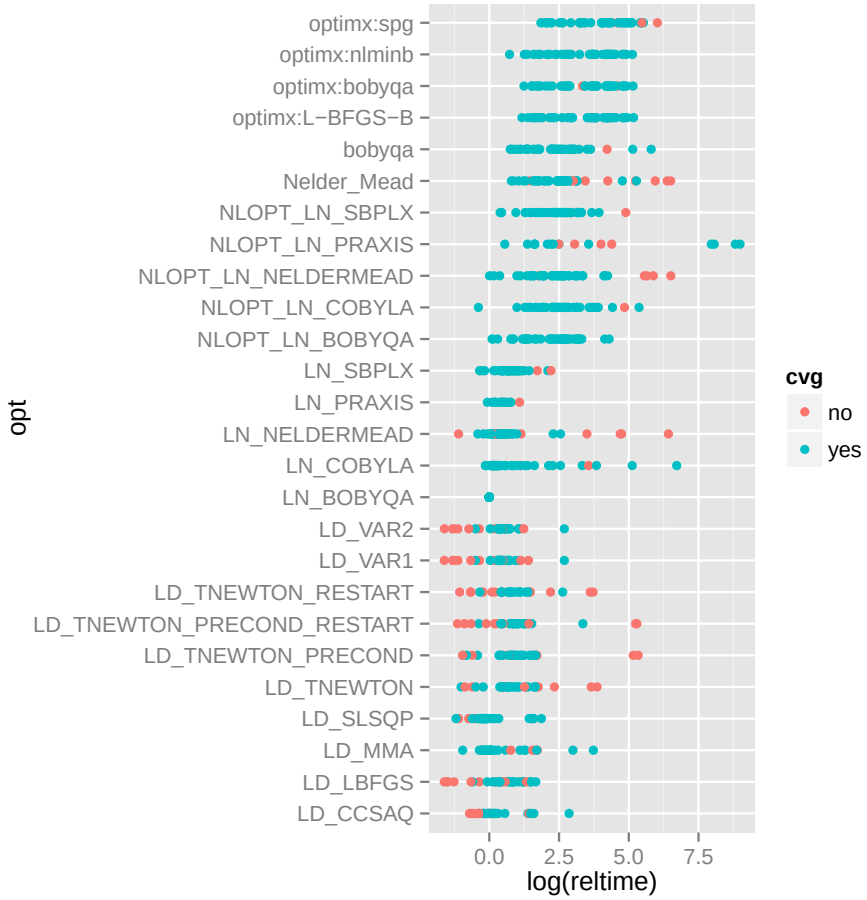
```
> print(xtable(subset(res, opt=="LN_BOBYQA" & dsname == "kb07")[c(1,2,5,6,7,9)]),floating=
```

	opt	dsname	np	excess	time	objective
378	LN_BOBYQA	kb07	72	0.02	4.24	28586.33
379	LN_BOBYQA	kb07	16	0.00	0.70	28670.91

3.2. Relative Speed

We plot the time to convergence, relative to $\mathrm{LN}_BOBYQAandonalogarithmicscale, foreachalgorithm.$

```
> res$cvg<-rep("yes",nrow(res))
> res$cvg[which(res$excess>.02)] <- "no"
> res$cvg<-as.factor(res$cvg)
> k<-ggplot(res, aes(x=log(reltime), y=opt))
> k + geom_point(aes(color=cvg))
```



Many of the cases where LN_BOBYQA is slower than other algorithms are simple problems that converge in less t
We will declare a data set to be non-simple if at least one of the models fit to the data took more than 0.2 seconds to convergence with LN_BOBYQA.

```
> print(xtable(subset(res, opt=="LN_BOBYQA" & time >= 0.2)[c("dsname","time","n","np","mod
```

	dsname	time	n	np	models
354	bs10	0.25	1104	20	Y ~ 1 + U + V + W + ((1 + U + V + W) | G) + ((1 + U + V
360	d3	106.94	130418	9	Y ~ 1 + U + ((1 + U) | G) + ((1 + U) | H) + ((1 + U) | I)
362	dialectNL	1.75	225866	6	Y ~ 1 + A + U + V + W + X + Z + T + (1 | G) + ((0 + V +
370	gb12	0.20	512	20	Y ~ 1 + S + T + U + V + W + X + Z + ((1 + S + U + W) |
376	InstEval	2.35	73421	2	Y ~ 1 + I * A + (1 | G) + (1 | H)
377	InstEval	4.36	73421	3	Y ~ 1 + A + (1 | G) + (1 | H) + (1 | I)
378	kb07	4.24	1790	72	Y ~ 1 + S + T + U + V + W + X + Z + ((1 + S + T + U + V
379	kb07	0.70	1790	16	Y ~ 1 + S + T + U + V + W + X + Z + (1 | G) + ((0 + S) | G
381	mm0	1.10	69588	6	Y ~ 1 + A * U + ((1 + U) | G) + ((1 + U) | H)
386	Poems	5.69	275996	3	Y ~ 1 + U + V + (1 | G) + (1 | H) + (1 | I)

3.3. Reliability

Sed iaculis sodales elit quis vehicula. In et tristique neque, sodales aliquet metus. In posuere

dictum nisl, quis laoreet augue congue a. Aenean in commodo neque, sit amet hendrerit ex. Aliquam id faucibus ante. Vivamus in fermentum nunc. Nam condimentum eros id orci pretium, quis aliquam magna eleifend.

4. Conclusions

5. References

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  author = {Douglas Bates and Martin Maechler and Ben Bolker and Steven Walker},
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Journal of Statistical Software http://www.jstatsoft.org/
published by the American Statistical Association http://www.amstat.org/
Volume VV, Issue II *Submitted:* yyyy-mm-dd
MMMMMM YYYY *Accepted:* yyyy-mm-dd