Bayesian Restricted Likelihood Methods: Conditioning on Insufficient Statistics in Bayesian Regression

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Abstract

Bayesian methods have proven themselves to be successful across a wide range of scientific problems and have many well-documented advantages over competing methods. However, these methods run into difficulties for two major and prevalent classes of problems: handling data sets with outliers and dealing with model misspecification. We outline the drawbacks of previous solutions to both of these problems (e.g., use of heavy-tailed likelihoods) and propose a new method as an alternative. When working with the new method, we summarize the data through a set of insufficient statistics, targeting inferential quantities of interest, and update the prior distribution with the summary statistics rather than the complete data. By careful choice of conditioning statistics, we retain the main benefits of Bayesian methods while reducing the sensitivity of the

*This research has been supported by Nationwide Insurance Company and by the NSF under grant numbers DMS-1007682 and DMS-1209194. The views in this paper are not necessarily those of Nationwide Insurance or the NSF.

analysis to features of the data not captured by the conditioning statistics. For reducing sensitivity to outliers, classical robust estimators (e.g., M-estimators) are natural choices for conditioning statistics. With these choicees, the method can be thought of as a blend of classical robust estimation and Bayesian methods.

A major contribution of this work is the development of a data augmented Markov chain Monte Carlo (MCMC) algorithm for the linear model and a wide range of choices for summary statistics. We demonstrate the method on an insurance agency data set containing many outliers and subject to model misspecification. Success is manifested in better predictive performance for data points of interest as compared to competing methods.
KEYWORDS: Approximate Bayesian computation, Markov chain Monte Carlo, M-estimation, Robust regression.

1 Introduction

Bayesian methods have provided successful solutions to a wide range of scientific problems, with their value having been demonstrated both empirically and theoretically. In simple settings, the success of the methods is often attributed to formal optimality properties, sometimes derived through the laws of subjective probability and sometimes through admissibility and the complete class theorems of decision theory. In complex settings, the hierarchical model allows one to create and fit sophisticated models that may, for example, pool information across similar problems.

The development of Bayesian inference relies on a complete Bayesian model consisting of three elements: the prior distribution, the loss function, and the likelihood or sampling density. While formal optimality of Bayesian methods is unquestioned if one accepts the validity of all three of these elements, a healthy skepticism encourages

us to question each of them. Concern about the prior distribution has been addressed through the development of techniques for subjective elicitation (Garthwaite et al., 2005; O'Hagan et al., 2006) (added the O'Hagan text here) and the rise of objective Bayesian methods (Berger, 2006). Concern about the loss function is reflected in, for example, the extensive literature on Bayesian hypothesis tests (Kass and Raftery, 1995). The sampling density has been given less attention from a specifically Bayesian view, although the work on predictive diagnostics (Box, 1980) departs from classical traditions.

The focus of this work is the development of techniques to handle imperfections in the sampling density. These imperfections often show themselves through the presence of outliers–cases not reflecting the phenomenon under study. There are three main solutions to Bayesian outlier-handling. The first is to replace the basic sampling density with a mixture model which includes one component for the "good" data and a second component for the "bad" data. With this approach, the prior distribution is updated with the likelihood from the mixture model to obtain the complete-data posterior distribution. The good component of the sampling density is used for prediction of future good data. The second approach replaces the basic sampling density with a thick-tailed density in an attempt to discount outliers, yielding techniques that often provide solid estimates of the center of the distribution but do not easily translate to predictive densities for further good data. The third approach fits a flexible (typically nonparametric) model to the data, producing a Bayesian version of a density estimate for both good and bad data. In recent development, inference is made through the use of robust inference functions (Lee and MacEachern, 2014, in press).

The traditional strategies for handling outliers all have their drawbacks. While we view the sampling density for the good data as stable, the outlier-generating

processes may be transitory in nature, constantly shifting as the source of bad data changes. This prevents us from appealing to large-sample arguments to claim that, with enough data, we can nail down a model for both good and bad data combined. Instead of attempting to model both good and bad data, we propose a novel strategy for handling outliers. In a nutshell, we begin with a complete model as if all of the data are good. But rather than driving the move from prior distribution to posterior distribution by the entire likelihood, we use only the likelihood driven by a few summary statistics which typically target inferential quantities of interest. We call this reduced likelihood a restricted likelihood. The update is a formal update from prior distribution to posterior distribution, based on the sampling density of the summary statistics. The novelty of the work is twofold. We make use of classical robust estimators as summary statistics in a formal Bayesian framework, using the sampling density of the estimators as a replacement for the sampling density of the data. Second, we advance the argument that conditioning on an insufficient summary of the data is sound practice, rather than merely being done for computational and modelling convenience.

The sampling density can err due to other forms of model misspecification. The traditional view is that, if the model is inadequate, one should build a better model. In our empirical work, as data sets have become larger and more complex, we have bumped into settings where we cannot realistically build the perfect model. We ask the question "by attempting to improve our model through elaboration, will the overall performance of the model suffer?" If yes, we avoid the elaboration, retaining a model with some level of misspecification. Acknowledging that the model is misspecified implies acknowledging that the sampling density is incorrect, as we do when outliers are present. Thus, outliers are but one form of misspecified model. We recommend a common solution for dealing with outliers and more general forms of model

misspecification.

The remainder of the paper develops Bayesian restricted likelihood (Section 2), shows how it can be applied to a Bayesian linear model (Section 3), illustrates its use on an insurance agencies data set with a novel twist on model evaluation (Section 5), and wraps up with a discussion (Section 6). A major contribution of this work is the computational strategy whose legitimacy is established in Section 3. The technical proofs are in the appendix.

2 Restricted Likelihood

2.1 Examples

To describe the use of the restricted likelihood in a Bayesian framework, we begin with a pair of simple examples for the one-sample problem. Several more examples are detailed in Lewis (2014). For those discussed here, the model takes the data $\boldsymbol{y} = (y_1, \ldots, y_n)$ to be a random sample of size n from a continuous distribution indexed by a parameter vector $\boldsymbol{\theta}$, with pdf $f(y|\boldsymbol{\theta})$. The standard, or full-data, likelihood would be $L(\boldsymbol{\theta}|\boldsymbol{y}) = \prod_{i=1}^{n} f(y_i|\boldsymbol{\theta})$.

As a first example, we consider the case where a subset of the data are known to be bad in the sense of not informing us about $\boldsymbol{\theta}$–and where the subset is known. This case mimics the setting where outliers in a data set are identified and discarded before a formal analysis is done. Without loss of generality, we label the good cases 1 through $n-k$ and the bad cases $n-k+1$ through n. The relevant likelihood to be used to move from prior distribution to posterior distribution is clearly $L(\boldsymbol{\theta}|y_1, \ldots, y_{n-k}) = \prod_{i=1}^{n-k} f(y_i|\boldsymbol{\theta})$. For an equivalent analysis, we rewrite the full likelihood as the product

of two pieces,

$$L(\boldsymbol{\theta}|\boldsymbol{y}) = \left(\prod_{i=1}^{n-k} f(y_i|\boldsymbol{\theta})\right)\left(\prod_{i=n-k+1}^{n} f(y_i|\boldsymbol{\theta})\right). \tag{1}$$

We wish to keep the first piece and drop the second for better inference on $\boldsymbol{\theta}$.

A second example involves deliberate censoring of small and large observations. This is sometimes done as a precursor to the analysis of reaction time experiments (e.g., Ratcliff, 1993) where very small reaction times are physiologically too quick to be true reaction times are usually explained as anticipation, and where implausibly long reaction times are believed due to inattention. With lower and upper censoring times at t_1 and t_2, the post-censoring sampling distribution is of mixed form, with masses $F(t_1|\boldsymbol{\theta})$ at t_1 and $1 - F(t_2|\boldsymbol{\theta})$ at t_2, and density $f(y|\boldsymbol{\theta})$ for $y \in (t_1, t_2)$. We adjust the original data y_i, producing $c(y_i)$ by defining $c(y_i) = t_1$ if $y_i \leq t_1$, $c(y_i) = t_2$ if $y_i \geq t_2$, and $c(y_i) = y_i$ otherwise. The adjusted update is performed with $L(\boldsymbol{\theta}|c(\boldsymbol{y}))$. With slightly non-standard notation, we let $g(t_1|\boldsymbol{\theta}) = F(t_1|\boldsymbol{\theta})$, $g(t_2|\boldsymbol{\theta}) = 1 - F(t_2|\boldsymbol{\theta})$, and $g(y|\boldsymbol{\theta}) = f(y|\boldsymbol{\theta})$ for $y \in (t_1, t_2)$. Hence, we may rewrite the full likelihood as the product of two pieces,

$$L(\boldsymbol{\theta}|\boldsymbol{y}) = \left(\prod_{i=1}^{n} g(c(y_i)|\boldsymbol{\theta})\right)\left(\prod_{i=1}^{n} f(y_i|\boldsymbol{\theta}, c(y_i))\right), \tag{2}$$

and retain only the first for the formal update.

2.2 Generalization

To generalize the approach in (1) and (2), we write the full likelihood in two pieces with a conditioning statistic $T(\boldsymbol{y})$, as indicated below:

$$L(\boldsymbol{\theta}|\boldsymbol{y}) \;\; = \;\; f(T(\boldsymbol{y})|\boldsymbol{\theta}) \; f(\boldsymbol{y}|\boldsymbol{\theta}, T(\boldsymbol{y})). \tag{3}$$

Here, $f(T(\boldsymbol{y})|\boldsymbol{\theta})$ is the conditional pdf of $T(\boldsymbol{y})$ given $\boldsymbol{\theta}$ and $f(\boldsymbol{y}|\boldsymbol{\theta}, T(\boldsymbol{y}))$ is the conditional pdf of $\boldsymbol{y}$ given $\boldsymbol{\theta}$ and $T(\boldsymbol{y})$. In the dropped case example, the conditioning statistic is $T(\boldsymbol{y}) = (y_1, \ldots, y_{n-k})$. In the censoring example, the conditioning statistic is $T(\boldsymbol{y}) = (c(y_1), \ldots, c(y_n))$. We refer to $f(T(\boldsymbol{y})|\boldsymbol{\theta})$ as the restricted likelihood and $L(\boldsymbol{\theta}|\boldsymbol{y}) = f(\boldsymbol{y}|\boldsymbol{\theta})$ as the full likelihood.

Bayesian methods can make use of a restricted likelihood since $T(\boldsymbol{y})$ is a well-defined random variable with a probability distribution indexed by $\boldsymbol{\theta}$. The update from prior distribution to posterior distribution can be made on the basis of $f(T(\boldsymbol{y})|\boldsymbol{\theta})$ rather than $f(\boldsymbol{y}|\boldsymbol{\theta})$. This leads to the restricted likelihood posterior

$$\pi(\boldsymbol{\theta}|T(\boldsymbol{y})) \;\; = \;\; \frac{\pi(\boldsymbol{\theta}) f(T(\boldsymbol{y})|\boldsymbol{\theta})}{m(T(\boldsymbol{y}))}, \tag{4}$$

where $m(T(\boldsymbol{y}))$ is the marginal distribution of $T(\boldsymbol{y})$ under the prior distribution. Predictive statements for further (good) data rely on the model. For another observation, say y_{n+1}, we would have the predictive density

$$f(y_{n+1}|T(\boldsymbol{y})) = \int f(y_{n+1}|\boldsymbol{\theta}) \pi(\boldsymbol{\theta}|T(\boldsymbol{y})) \; d\boldsymbol{\theta}. \tag{5}$$

2.3 Literature review

Direct use of restricted likelihood appears in many areas of the literature. The motivation is often similar to ours: concern about outliers or, more generally, model misspecification. For example, the use of rank likelihoods is discussed by Savage (1969), Pettitt (1983, 1982), and more recently by Hoff et al. (2013). Lewis et al. (2012 xxxx) make use of robust regression estimators for $T(\boldsymbol{y})$. Asymptotic properties of restricted posteriors are studied by Doksum and Lo (1990), Clarke and Ghosh (1995), Yuan and Clarke (2004), and Hwang et al. (2005). The tenor of these asymptotic results is that, for a variety of conditioning statistics with non-trivial regularity conditions on prior, model, and likelihood, the posterior distribution resembles the asymptotic sampling distribution of the conditioning statistic.

Restricted likelihoods have also been used as practical approximations to a full likelihood. For example, Pratt (1965) appeals to heuristic arguments regarding approximate sufficiency to justify the use of the restricted likelihood of the sample mean and standard deviation. Approximate sufficiency is also appealed to in the use of Approximate Bayesian Computation (ABC), which is related to our method. ABC is a collection of posterior approximation methods which has recently experienced success in applications to epidemiology, genetics, and quality control (see, for example, Tavaré et al., 1997; Pritchard et al., 1999; Marjoram et al., 2003; Fearnhead and Prangle, 2012). Interest typically lies in the full data posterior and ABC is used for computational convenience as an approximation. Consequently, effort is made to choose an approximately sufficient $T(\boldsymbol{y})$ and update to the ABC posterior by using the likelihood $L(\boldsymbol{\theta}|\mathcal{B}(\boldsymbol{y}))$, where $\mathcal{B}(\boldsymbol{y}) = \{\boldsymbol{y}^*|\rho(T(\boldsymbol{y}), T(\boldsymbol{y}^*)) < \epsilon\}$, ρ is a metric, and ϵ is a tolerance level. This is the likelihood "conditioned" on the collection of data sets which result in a $T(\cdot)$ within ϵ of the observed $T(\boldsymbol{y})$. By choosing an approximately sufficient $T(\cdot)$ and a small enough ϵ the claim is made that $L(\boldsymbol{\theta}|\mathcal{B}(\boldsymbol{y})) \approx L(\boldsymbol{\theta}|T(\boldsymbol{y})) \approx L(\boldsymbol{\theta}|\boldsymbol{y})$.

Consequently, the ABC posterior approximates the full data posterior. We note that efforts have been made to formalize what is meant by approximate sufficiency (e.g., Joyce and Marjoram, 2008).

ABC is related to our method in that the "conditioning" is on something other than the data $\boldsymbol{y}$. However, the conditioning in ABC is heuristic. For technical reasons, the calculation proceeding from $\pi(\boldsymbol{\theta})$ to $\pi(\boldsymbol{\theta})L(\boldsymbol{\theta}|\mathcal{B}(\boldsymbol{y}))/\int \pi(\boldsymbol{\theta})L(\boldsymbol{\theta}|\mathcal{B}(\boldsymbol{y}))d\boldsymbol{\theta}$ is not a formal conditional update. Simply put, if an external observer told $\mathcal{B}(\boldsymbol{y})$ can supply $T(\boldsymbol{y})$ and vice-versa, the information contained in $\mathcal{B}(\boldsymbol{y})$ is exactly that contained in $T(\boldsymbol{y})$ and proper conditioning will lead to identical posterior distributions. This is not the case with a typical implementation of ABC.

This work extends the development of Bayesian restricted likelihood by arguing that deliberate choice of $T(\boldsymbol{y})$ is sound practice and also by expanding the class of conditioning statistics in which exact conditioning can be achieved. Our methods do not rely on asymptotic properties, nor do they rely on approximate conditioning, nor do they need to correspond to artificial censoring to create incomplete or missing data (e.g., Albert, 1988; Hoff and Wakefield, 2013). Note - fix references here hoffwakefield for asymptotic; albert for ? .

The key to productive use of the restricted likelihood is the choice of $T(\boldsymbol{y})$ and the development of computational strategies that allow us to truly condition on the observed $T(\boldsymbol{y})$ and fit the model in formal Bayesian fashion. In this work, we focus on robustness, and natural choices of $T(\boldsymbol{y})$ for the one-sample problem include a set of middling order statistics, a trimmed mean, or a classical robust estimator of location and/or scale. We have previously implemented several of these methods and have found them to perform well (Lewis et al., 2012). Versions most extensible to the linear model include the M-estimators in the tradition of Huber (1964), least median squares (LMS), and least trimmed squares (LTS). For these choices the restricted

likelihood is not available in closed form, making computation of the restricted posterior a challenge. For low-dimensional statistics $T(\boldsymbol{y})$ and parameters $\boldsymbol{\theta}$, the direct computational strategies described in Lewis (2014) can be used to estimate the incomplete posterior conditioned on essentially any statistic. These strategies rely on generation of complete data sets from different values of $\boldsymbol{\theta}$. Each complete data set leads to a statistic $T(\boldsymbol{y})$ under $\boldsymbol{\theta}$, and these generated statistics are used to estimate the density at $T(\boldsymbol{y}_{obs})$, where $\boldsymbol{y}_{obs}$ is the observed complete data. This estimate is fed into Bayes' theorem for the update from prior distribution to posterior distribution.

These direct sampling techniques rely on density estimation and numerical integration. Density estimation becomes difficult for high dimensional $T(\boldsymbol{y})$ and numerical integration breaks down for high dimensional $\boldsymbol{\theta}$. For these settings, an MCMC algorithm is developed in Section 3.2. Software is available from the authors for use with simultaneous M-estimators of location and scale. At the present time, further software development is required to extend beyond simultaneous M-estimators.

2.4 A first data analysis example

Before discussing computational details of finding restricted posteriors, we begin by analyzing a simple example involving outliers. The data consists of well known measurements of the passage time of light taken by Simon Newcomb in the late nineteenth century and contain two clear outliers on the low end. Details and data are available in the R package `MASS` and previous analyses appear in Stigler (1977), Chan and Rhodin (1980), and Gelman et al. (2004). Letting y_i denote the i^{th} coded measurement of the passage time of light, we assume $y_i \overset{iid}{\sim} N(\beta, \sigma^2)$ for $i = 1, 2, \ldots, n = 66$. The parameter β can be interpreted as the passage time of light with σ^2 representing measurement error. The outliers are a clear indication that this normal model is misspecified. Also, the measurements are coarse, taking on only integer values. For a Bayesian analy-

sis, we must specify prior distributions on the parameters $\boldsymbol{\theta} = (\beta, \sigma)$. For this we assume an independent normal – inverse gamma model. That is, $\beta \sim N(\eta, \tau^2)$ and $\sigma^2 \sim IG(a, b)$. The hyperparameters are fixed for simplicity and taken to be $\eta = 23.6$, $\tau = 2.04$, $a = 5$, and $b = 10$. We note that our computational strategy described in Section 3.2 makes it feasible to fit more complex model structures. The Bayesian model presented here is a special case of the linear model in (7) presented below.

As summary statistics for the restricted likelihood methods, we consider robust simultaneous M-estimators of location and scale as well as LMS (least median squares) and LTS (least trimmed squares) estimators. The simultaneous M-estimators $b(\boldsymbol{y})$ and $s(\boldsymbol{y})$ of β and σ, respectively, are the solutions to the equations

$$\begin{aligned} \sum_{i=1}^{n} \psi\left(\frac{y_i - b(\boldsymbol{y})}{s(\boldsymbol{y})}\right) &= 0 \\ \sum_{i=1}^{n} \chi\left(\frac{y_i - b(\boldsymbol{y})}{s(\boldsymbol{y})}\right) &= 0. \end{aligned} \tag{6}$$

For the first equation we consider two ψ functions: Huber's and Tukey's. These are both coupled with Huber's 'proposal 2' for the χ function in the second equation (for details see Huber and Ronchetti, 2009). Tuning parameters for these functions are set to achieve 95% efficiency under normally distributed data.

LMS minimizes the median squared residual and LTS minimizes the sum of the k smallest squared residuals where k is chosen by the user. These estimators are considered because, unlike the M-estimators above, they can achieve high breakdown. It is well known that LMS has highest possible breakdown but is inefficient. LTS is more efficient and its breakdown properties are determined by k, with highest possible breakdown occurring for $\left\lfloor \frac{n+1}{2} \right\rfloor \leq k \leq \left\lfloor \frac{n+2}{2} \right\rfloor$. For the current analysis we do not choose k to achieve highest possible breakdown. Instead, with $n = 66$ and we choose $k = 62$ (roughly 95% of n) to be more comparable to the tuning parameters

chosen for the M-estimators. The LMS and LTS estimators are also coupled with an estimator of scale for the conditioning. We set the scale estimator to the minimum of the corresponding objective function, appropriately scaled for consistency.

For comparison to a traditional Bayesian outlier approach we also fit a heavy-tailed model by changing the data distribution from a normal to a Student's t with $\nu = 5$ degrees of freedom. We note that the variance of the data under this model is $\frac{\nu}{\nu-2}\sigma^2$. For comparability, it is this quantity that has the prior distribution $IG(a, b)$ given above.

The marginal posteriors for β and σ^2 as well as the predictive distribution (5) under each model are displayed in Figures 1a-1c. Both of the two small outliers and the normal prior on β centered at 23.6 are influential in the results. The normal theory model is most drastically affected with the posterior of β being pulled towards the prior and outliers. Inference on σ^2 under this model is impacted by the outliers (see Figure 1b) resulting in overestimation of σ^2. The heavy-tailed model as well as the restricted likelihood methods with LTS, Huber's, and Tukey's summary statistics are less influenced by the outliers and priors. The marginal posteriors for β are closer to the center of the non-outlying data. Inference on the variance parameter also more closely reflects the variance information in this part of the data (the mean and variance of the data without the two outliers are 27.8 and 25.8, respectively). The posterior of β under LTS is slightly more dispersed than under the two M-estimator methods. This is also reflected in the variance parameter in that under LTS the posterior distribution concentrates on slightly larger values of σ^2 While LMS has high breakdown, it has been more drastically affected by the normal prior centered at 23.6 than the others. This is because LMS achieves high breakdown by discounting much of the information in the data.

Though inference for the main parameter of interest (β) is similar between the tra-

ditional heavy-tailed approach and the new method with LTS, Huber's, and Tukey's summary statistics, the traditional heavy-tailed method has the disadvantage of less precise predictive capability. This is reflected in the heavier tails of its predictive distribution (5) seen in Figure 1c (plotted are the log predictive densities under each method). The predictive distributions under each of the restricted likelihood methods are comparable. Surprisingly, despite the poor inference on β under LMS, the predictive distribution is concentrated more sharply than under the other restricted likelihood methods. This is related to its posterior of σ^2 seen in Figure 1b which is the tightest distribution and shifted the most to the left.

3 Restricted Likelihood for the Linear Model

3.1 The Bayesian linear model

We focus on the use of restricted likelihood for the Bayesian linear model with a standard formulation:

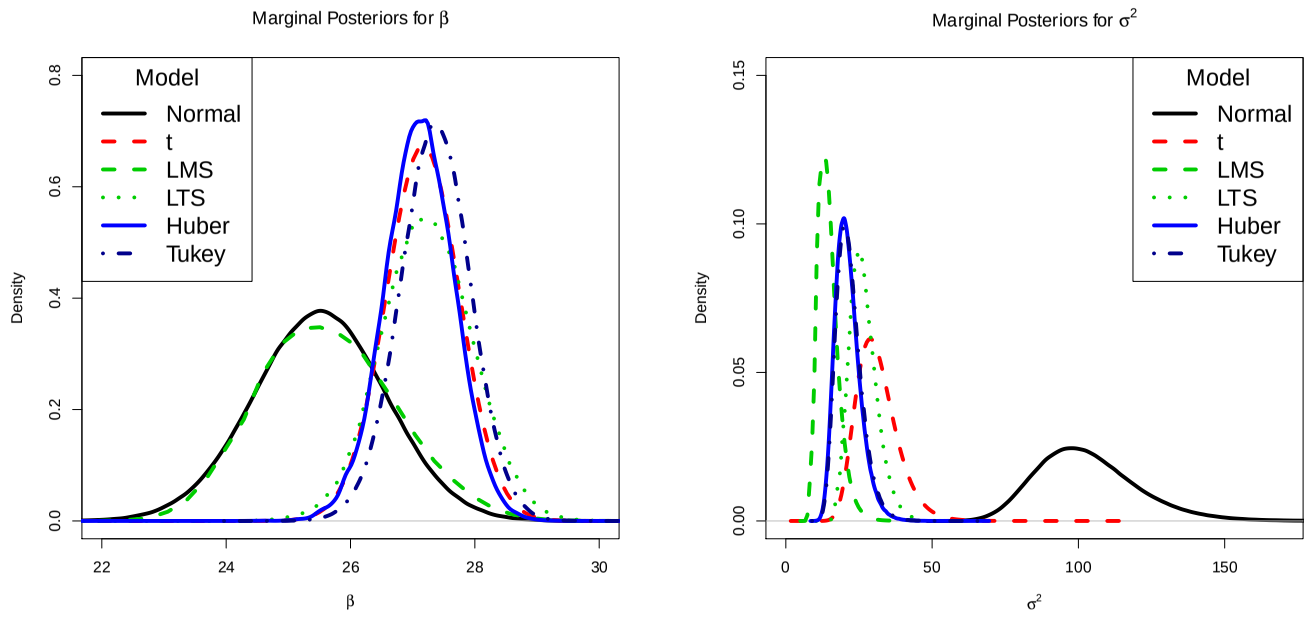
$$\begin{aligned} \boldsymbol{\theta} &= (\boldsymbol{\beta}, \sigma^2) \sim \pi(\boldsymbol{\theta}) \\ y_i &= x_i^\top \boldsymbol{\beta} + \epsilon_i, \text{ for } i = 1, \ldots, n \end{aligned} \tag{7}$$

where x_i and $\boldsymbol{\beta} \in \mathbb{R}^p$, $\sigma^2 \in \mathbb{R}^+$, and the ϵ_i are independent draws from a distribution with center 0 and scale σ. Two conditions are imposed on the model:

C1. The $n \times p$ design matrix, X, whose i^{th} row is $x_i^\top$, is of full column rank.

C2. The ϵ_i are a random sample from some distribution which has a density with respect to Lebesgue measure on the real line and for which the support is the real line.

(a) (b)



(c)

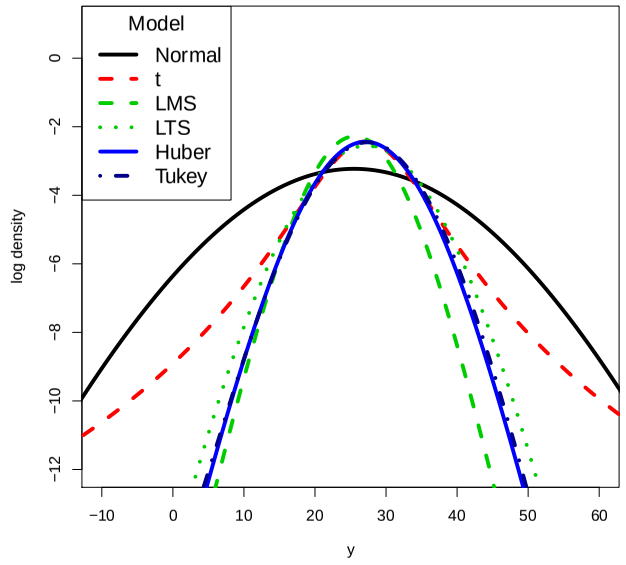


Figure 1: Clockwise from top left: (a) marginal posteriors of β (b) marginal posteriors for σ^2 (c) log predictive distributions.

As summary statistics for the data, we concentrate on robust estimators for the regression coefficients in the linear model and an associated estimator of the scale. In particular, we demonstrate the method using simultaneous M-estimators defined by (6) for the one-sample setting and easily extended to the linear model in (7). The estimator of the regression coefficients is denoted by $\boldsymbol{b}(X, \boldsymbol{y}) \in \mathbb{R}^p$ and that of the scale by ~~$s(X, \boldsymbol{y}) \in \mathbb{R}$~~ $s(X, \boldsymbol{y}) \in \{0\} \cup \mathbb{R}^+$. Thus, $T(\boldsymbol{y}) = (\boldsymbol{b}(X, \boldsymbol{y}), s(X, \boldsymbol{y}))$. The observed complete data is denoted by $\boldsymbol{y}_{obs}$ with observed statistic denoted by $T(\boldsymbol{y}_{obs}) = (\boldsymbol{b}(X, \boldsymbol{y}_{obs}), s(X, \boldsymbol{y}_{obs}))$.

3.2 Computational strategy

As mentioned above, direct computational strategies designed to approximate the restricted posterior break down for high-dimensional statistics $T(\boldsymbol{y})$ or high-dimensional parameters $\boldsymbol{\theta}$. However, Markov chain Monte Carlo (MCMC) methods were developed for exactly these situations. We turn to MCMC to fit the model in these circumstances.

The general style of algorithm that we present is a data augmented MCMC algorithm targeting $f(\boldsymbol{\theta}, \boldsymbol{y}|T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs}))$, the joint distribution of $\boldsymbol{\theta}$ and the full data given the summary statistic $T(\boldsymbol{y}_{obs})$. The Gibbs sampler (Gelfand and Smith, 1990) iteratively samples from the full conditionals $\pi(\boldsymbol{\theta}|\boldsymbol{y}, T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs}))$ and $f(\boldsymbol{y}|\boldsymbol{\theta}, T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs}))$. Alternative algorithms substitute other generations for the full conditionals, such as the Metropolis-Hastings propose and accept/reject framework. Our algorithms are based on the decomposition of the MCMC algorithm into conventional full data sampling steps where $\boldsymbol{\theta}$ is generated given $\boldsymbol{y}$, and steps that allow us to complete the data set where $\boldsymbol{y}$ is generated given $\boldsymbol{\theta}$ and $T(\boldsymbol{y})$. The latter generation relies on the conditioning set $\mathcal{A} = \{\boldsymbol{y} \in \mathbb{R}^n | T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})\}$. The set $\mathcal{A}$ may contain more than one element (i.e., it is not degenerate) when $T(\boldsymbol{y}) : \boldsymbol{y} \to T(\boldsymbol{y})$

is not a $1-1$ function.

When $\boldsymbol{y}$ has the summary statistic ~~$T(\boldsymbol{y})$ matching $T(\boldsymbol{y}_{obs})$~~, $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$, the first full conditional, $\pi(\boldsymbol{\theta}|\boldsymbol{y}, T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs}))$, is the same as the full data posterior $\pi(\boldsymbol{\theta}|\boldsymbol{y})$. In this case, the condition $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$ is redundant. This allows us to make use of conventional MCMC steps for this generation. For ~~In the case of~~ typical regression models, algorithms abound. Details of the recommended algorithms depend on details of the prior distribution and sampling density. As examples, a normal prior distribution and normal likelihood in the regression setting allow one to alternate conditional generations of σ^2 and $\boldsymbol{\beta}$, and blocking the generation of $\boldsymbol{\beta}$ generally leads to quicker convergence and mixing (Liu, 1994); a thick-tailed scale mixture of normal distributions in the style of the hyper-g/n prior (Liang et al., 2008) necessitates an additional stage for the sampler where the scale g/n is generated; a thick-tailed sampling density such as a t distribution can be handled with the addition of a scale parameter for each case and an extra stage where these scale parameters are generated.

For a typical model and conditioning statistic, the second full conditional $f(\boldsymbol{y}|\boldsymbol{\theta}, T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs}))= f(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{y} \in \mathcal{A})$ is not available in closed form. As a consequence, we turn to Metropolis-Hastings (Hastings, 1970), using the strategy of proposing full data $\boldsymbol{y}$ ~~in the sample space of the distribution~~ for which $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$ and either accepting or rejecting the proposal. Let $\boldsymbol{y}_p$ and $\boldsymbol{y}_c$ represent the proposed and current full data, respectively. In subsequent algorithms, we propose only from the set $\mathcal{A}$. Denote the proposal distribution for $\boldsymbol{y}_p$ by $p(\boldsymbol{y}_p|\boldsymbol{\theta}, T(\boldsymbol{y}_p) = T(\boldsymbol{y}_{obs}))= p(\boldsymbol{y}_p|\boldsymbol{\theta}, \boldsymbol{y}_p \in \mathcal{A}) = p(\boldsymbol{y}_p|\boldsymbol{\theta})$. The last equality follows from the fact that our $p(\cdot|\boldsymbol{\theta})$ assigns probability one to the event $\{\boldsymbol{y}_p \in \mathcal{A}\}$. These equalities still hold if the dummy argument $\boldsymbol{y}_p$ is replaced

with $\boldsymbol{y}_c$. The conditional density is

$$\begin{aligned} f(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{y} \in \mathcal{A}) &= \frac{f(\boldsymbol{y}|\boldsymbol{\theta}) I(\boldsymbol{y} \in \mathcal{A}|\boldsymbol{y}, \boldsymbol{\theta})}{\int_{\mathcal{A}} f(\boldsymbol{y}|\boldsymbol{\theta}) d\boldsymbol{y}} \\ &= \frac{f(\boldsymbol{y}|\boldsymbol{\theta})}{\int_{\mathcal{A}} f(\boldsymbol{y}|\boldsymbol{\theta}) d\boldsymbol{y}} \end{aligned}$$

for $\boldsymbol{y} \in \mathcal{A}$. This includes both $\boldsymbol{y}_p$ and $\boldsymbol{y}_c$.

The Metropolis-Hastings acceptance probability is the minimum of 1 and R where,

$$R = \frac{f(\boldsymbol{y}_p|\boldsymbol{\theta}, \boldsymbol{y}_p \in \mathcal{A})}{f(\boldsymbol{y}_c|\boldsymbol{\theta}, \boldsymbol{y}_c \in \mathcal{A})} \frac{p(\boldsymbol{y}_c|\boldsymbol{\theta}, \boldsymbol{y}_c \in \mathcal{A})}{p(\boldsymbol{y}_p|\boldsymbol{\theta}, \boldsymbol{y}_p \in \mathcal{A})} \tag{8}$$

$$= \frac{f(\boldsymbol{y}_p|\boldsymbol{\theta})}{\int_{\mathcal{A}} f(\boldsymbol{y}|\boldsymbol{\theta}) d\boldsymbol{y}} \frac{\int_{\mathcal{A}} f(\boldsymbol{y}|\boldsymbol{\theta}) d\boldsymbol{y}}{f(\boldsymbol{y}_c|\boldsymbol{\theta})} \frac{p(\boldsymbol{y}_c|\boldsymbol{\theta})}{p(\boldsymbol{y}_p|\boldsymbol{\theta})} \tag{9}$$

$$= \frac{f(\boldsymbol{y}_p|\boldsymbol{\theta})}{f(\boldsymbol{y}_c|\boldsymbol{\theta})} \frac{p(\boldsymbol{y}_c|\boldsymbol{\theta})}{p(\boldsymbol{y}_p|\boldsymbol{\theta})}. \tag{10}$$

Note: Above expression changed. Check argument again.

For the models we consider, evaluation of $f(\boldsymbol{y}|\boldsymbol{\theta})$ is straightforward. Therefore, the difficulty in implementing this Metropolis-Hastings step manifests itself in the ability to simulate proposals that guarantee $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$ and on the evaluation of the proposal density derived from the method used to simulate $\boldsymbol{y}$. We now discuss such an implementation method for the linear model in (7).

3.2.1 Construction of the proposal

Our computational strategy is easiest to envision in a location-scale setting where the design matrix in model (7) consists of a single column of ones. Robust estimation techniques along with model (7) suggest a conditioning statistic $T(\boldsymbol{y})$ which consists of estimates of the scalars β and σ, say $T(\boldsymbol{y}) = (b(X, \boldsymbol{y}), s(X, \boldsymbol{y}))$. It is not a simple matter to directly sample the required proposal $\boldsymbol{y}$ satisfying $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$. How-

ever, with equivariance/invariance properties of $T(\boldsymbol{y})$, we will see in Theorem 3.1 below that it is possible to scale and shift any ~~$\boldsymbol{z}^* \in \mathbb{R}^n$~~ $\boldsymbol{z}^*$ which generates a positive scale estimate to such a $\boldsymbol{y}$. Hence, to obtain $\boldsymbol{y}$ from $\mathcal{A}$, we proceed in two steps. First, a vector $\boldsymbol{z}^*$ is sampled from a known distribution (examples of which are described later). This vector has summary statistic $T(\boldsymbol{z}^*) = (b(X, \boldsymbol{z}^*), s(X, \boldsymbol{z}^*))$ which may not match the observed summary $T(\boldsymbol{y}_{obs})$. Second, $\boldsymbol{z}^*$ is mapped into $\boldsymbol{y} = h(\boldsymbol{z}^*)$ using Theorem 3.1 so that $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$. To evaluate the proposal density $p(\boldsymbol{y}|\boldsymbol{\theta})$, we need to adjust the known density of $\boldsymbol{z}^*$, $p(\boldsymbol{z}^*)$, with the Jacobian of the transformation $h(\cdot)$ to $\boldsymbol{y}$. We choose the distribution of the ~~intermediate~~ data vector $\boldsymbol{z}^*$ to have support on a subset of $\mathbb{R}^n$ so that the transformation to $\boldsymbol{y}$ is one-to-one and the Jacobian, $\left|\dfrac{\partial h^{-1}(\boldsymbol{y})}{\partial \boldsymbol{y}}\right|$, can be computed from first principles. It is the calculation of this Jacobian which is described in the section. We will repeatedly return to an artificial low-dimensional example in the location-scale setting to help visualize this calculation.

The strategy described in the previous paragraph extends to full-blown regression models. Robust regression methods lead naturally to a conditioning statistic in the form of a classical M-estimator for $\boldsymbol{\beta}$ and a companion estimator for σ. We denote the resulting estimator which involves the covariates through the design matrix and the response as $T(\boldsymbol{y}) = (\boldsymbol{b}(X, \boldsymbol{y}), s(X, \boldsymbol{y}))$, with $\boldsymbol{b}(X, \boldsymbol{y}) = (b_1(X, \boldsymbol{y}), \cdots, b_p(X, \boldsymbol{y}))^\top$. Simultaneous M-estimators have a number of standard properties C3-C8 which prove useful in the sequel (Huber and Ronchetti, 2009; Maronna et al., 2006).

C3. $\boldsymbol{b}(X, \boldsymbol{y})$ is almost surely continuous and differentiable with respect to $\boldsymbol{y}$.

C4. $s(X, \boldsymbol{y})$ is almost surely positive, continuous, and differentiable with respect to $\boldsymbol{y}$.

C5. $\boldsymbol{b}(X, \boldsymbol{y} + X\boldsymbol{v}) = \boldsymbol{b}(X, \boldsymbol{y}) + \boldsymbol{v}$ for all $\boldsymbol{v} \in \mathbb{R}^p$.

C6. $\boldsymbol{b}(X, a\boldsymbol{y}) = a\boldsymbol{b}(X, \boldsymbol{y})$ for all constants a.

C7. $s(X, \boldsymbol{y} + X\boldsymbol{v}) = s(X, \boldsymbol{y})$ for all $\boldsymbol{v} \in \mathbb{R}^p$.

C8. $s(X, a\boldsymbol{y}) = |a|s(X, \boldsymbol{y})$ for all constants a.

Properties C5 and C6 of $\boldsymbol{b}$ are called *regression* and *scale equivariance*, respectively. Properties C7 and C8 of s are called *regression invariance* and *scale equivariance*. Many other estimators satisfy these properties, and our subsequent results apply equally well to them. With more cumbersome statements, the upcoming results can be adjusted to handle a relaxation of C4 that $s(X, \boldsymbol{y}_{obs}) > 0$ and $P(s(X, \boldsymbol{y}) > 0) > 0$.

We have stated that any vector $\boldsymbol{z}^* \in \mathbb{R}^n$ can be transformed to a proposal $\boldsymbol{y}$ satisfying $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$. The properties above ensure that this can be done through the mechanism presented in the following theorem. The proof of this and other results appear in the appendix.

Theorem 3.1. *Assume that conditions C4-C8 hold. Then, any vector $\boldsymbol{z}^* \in \mathbb{R}^n$ with conditioning statistic $T(\boldsymbol{z}^*)$ for which $s(X, \boldsymbol{z}^*) > 0$ can be transformed into $\boldsymbol{y}$ with conditioning statistic $T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})$ through the transformation*

$$\boldsymbol{y} = \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^* + X\left(\boldsymbol{b}(X, \boldsymbol{y}_{obs}) - \boldsymbol{b}(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^*)\right).$$

The mapping described in the theorem is many-to-one in general. Its range is the collection of data sets which match the observed summary statistic:

$$\mathcal{A} = \{\boldsymbol{y} \in \mathbb{R}^n | T(\boldsymbol{y}) = T(\boldsymbol{y}_{obs})\}. \tag{11}$$

To see this, note that the theorem shows that any $\boldsymbol{y}$ expressed as in the theorem is an element of $\mathcal{A}$. Further, any $\boldsymbol{y} \in \mathcal{A}$ can be expressed as in the theorem by simply

replacing $\boldsymbol{z}^*$ with $\boldsymbol{y}$. That is, any vector already in $\mathcal{A}$ requires no shifting or scaling. The set $\mathcal{A}$ is an $n-p-1$ dimensional space: there are p constraints imposed by the regression coefficients and one further constraint imposed by the scale. The form of the set is determined by the statistic $T(\cdot)$. Figure 2 provides an artificial low-dimensional visualization of such a set $\mathcal{A}$ with a location-scale model. In the figure, $n = 3$, and the conditioning statistic is $T(\boldsymbol{y}) = (\min(\boldsymbol{y}), \sum(y_i - \min(\boldsymbol{y}))^2)$. The set $\mathcal{A}$ is depicted for $T(\boldsymbol{y}_{obs}) = (0, 1)$ and is a "warped triangle" in light blue, with each side corresponding to a particular coordinate of $\boldsymbol{y}$ being the minimum value of zero. The other two coordinates are restricted by the scale statistic to lie on the quarter circle of radius one in the positive orthant. In general, this set may be compact and given by a closed curve, as in the figure, or it may be unbounded, depending on the choice of $T(\boldsymbol{y})$. The other sets labeled in the figure will be described shortly.

The set $\mathcal{A}$ typically does not lie in a linear space of dimension $n-p-1$, and so we must account for both the many-to-one nature of the mapping and a Jacobian when deriving the proposal density. We handle the first point by sampling the initial $\boldsymbol{z}^*$ from a reduced $n-p-1$ dimensional space which, through the scaling and shifting of the above theorem, maps uniquely to a point in $\mathcal{A}$. This reduced space is chosen so that the range of the map is the entirety of $\mathcal{A}$. The Jacobian does not cancel in (8), since the scaling depends on the initial proposal.

The reduced space from which the initial sample is taken is simply the unit sphere ~~restricted to~~ in the orthogonal complement of the column space of the design matrix (i.e., the least squares residual space). To help understand the density of the proposal derived from the transformation of this initial sample we introduce the following notation. Denote the column space of the design matrix X by $\mathcal{C}(X)$ and its orthogonal complement by $\mathcal{C}^{\perp}(X)$. ~~This~~ The latter is the least squares residual space which we will often refer to as the 'deviation space'. The projection of the set $\mathcal{A}$ onto the

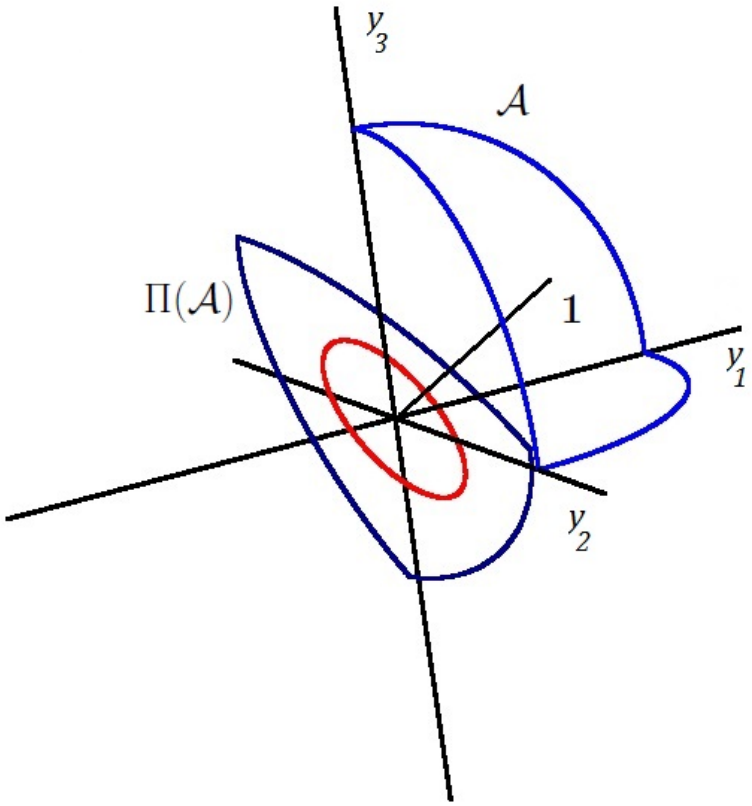


Figure 2: A depiction of $\mathcal{A}$, $\Pi(\mathcal{A})$, and the unit circle for the illustrative example where $b_1(\mathbf{1}, \boldsymbol{y}) = \min(\boldsymbol{y}) = 0$ and $s(\mathbf{1}, \boldsymbol{y}) = \sum(y_i - b_1(\mathbf{1}, \boldsymbol{y}))^2 = 1$. $\mathcal{A}$ is the combination of three quarter circles, one on each plane defined by $y_i = 0$. The projection of this manifold onto the deviation space is depicted by the bowed triangular shape in the plane defined by $\sum y_i = 0$. The circle in this plane represents the sample space for the intermediate sample $\boldsymbol{z}^*$. Also depicted is the vector $\mathbf{1}$, the design matrix for the location and scale setting.

deviation space is

$$\Pi(\mathcal{A}) = \{\boldsymbol{z} \in \mathbb{R}^n | \ \exists \ \boldsymbol{y} \in \mathcal{A} \ s.t. \ \boldsymbol{z} = Q\boldsymbol{y}\} \tag{12}$$

where Q is the projection matrix onto $\mathcal{C}^{\perp}(X)$. Explicitly, $Q = I - H$ with $H = XX^{\top}$ where we assume, without loss of generality following condition C1, that the columns of X form an orthonormal basis for $\mathcal{C}(X)$ (i.e., $X^{\top}X = I$). It will also be helpful at times to write $Q = WW^{\top}$ where the columns of W form an orthonormal basis for $\mathcal{C}^{\perp}(X)$. This set has been introduced because we will first transform the initial

distribution on the sphere to the distribution on this set. Then we will transform to the ~~sample space~~ set $\mathcal{A}$.

Returning to the artificial example, Figure 2 depicts $\Pi(\mathcal{A})$ as well as the sphere from which we obtain the initial sample. The column vector $X = \mathbf{1}$ spans $\mathcal{C}(X)$ and is shown as a reference. The triangle with bowed sides in dark blue is $\Pi(\mathcal{A})$, the projection of $\mathcal{A}$ onto the plane orthogonal to $\mathbf{1}$ (i.e., $\mathcal{C}^{\perp}(X)$). The unit sphere from which the initial sample is taken is depicted as the red circle in this plane. In general, this is the unit sphere in the $n - p$ dimensional space $\mathcal{C}^{\perp}(X)$.

For the transformation of the initial proposal $\boldsymbol{z}^*$ on the surface of the sphere to $\boldsymbol{y} \in \mathcal{A}$, we first move to a point on $\Pi(\mathcal{A})$ through a simple scaling of $\boldsymbol{z}^*$. This is followed by undoing the projection with a move from $\Pi(\mathcal{A})$ to its (unique) preimage on $\mathcal{A}$. Together, these two steps correspond to the transformation in Theorem 3.1. The introduction of the sphere in $\mathcal{C}^{\perp}(X)$ as the initial proposal surface along with properties C5-C8 ensure that the mapping is 1-1. In particular, property C8 ensures the scaling to be unique and C7 implies that the scale statistic is unchanged when undoing the projection. Property C5 ensures the uniqueness of undoing the projection. The general proposal strategy is summarized as follows:

1. Sample $\boldsymbol{z}^*$ from a distribution with known density on the unit sphere in $\mathcal{C}^{\perp}(X)$.

2. Calculate the Jacobian of the transformation in Theorem 3.1 in two steps.

   (a) Scale from unit sphere to $\Pi(\mathcal{A})$: $\boldsymbol{z} = \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)} \boldsymbol{z}^*$

   (b) Shift from $\Pi(\mathcal{A})$ to $\mathcal{A}$: $\boldsymbol{y} = \boldsymbol{z} + X\left(\boldsymbol{b}(X, \boldsymbol{y}_{obs}) - \boldsymbol{b}(X, \boldsymbol{z})\right)$

3.2.2 Evaluation of the proposal density

Calculation of the appropriate Jacobian of the transformation is absolutely vital and also non-trivial. Writing the transformation from the unit sphere in deviation space

to $\mathcal{A}$ in two steps facilitates calculation of the Jacobian in two steps as written above. We now explain each step, keeping in mind that the Jacobian of a transformation is simply the ratio of infinitesimal volumes along the tangents of the domain and range of the transformation.

Scale from unit sphere to $\Pi(\mathcal{A})$

The first step is constrained to $\mathcal{C}^{\perp}(X)$ where the unit sphere is transformed to $\Pi(\mathcal{A})$. We further break this ~~piece~~ step into ~~in two steps~~ into two substeps: first, the distribution on the unit sphere is transformed to that along a sphere of radius $r = \|\boldsymbol{z}\| = s(X, \boldsymbol{y}_{obs})/s(X, \boldsymbol{z}^*)$. This contributes a factor of $r^{-(n-p-1)}$ to the Jacobian. Second, the new sphere is then deformed to $\Pi(\mathcal{A})$. This deformation contributes an attenuation to the Jacobian equal to the ratio of infinitesimal volumes in the tangent spaces of the sphere and $\Pi(\mathcal{A})$ at $\boldsymbol{z}$. Restricting ourselves to the $n-p$ dimensional space $\mathcal{C}^{\perp}(X)$, this ratio is the cosine of the angle between the normal vectors of the two sets at $\boldsymbol{z}$. The normal to the sphere is its radius vector $\boldsymbol{z}$. The normal to $\Pi(\mathcal{A})$ is given in the following lemma.

Lemma 3.2. *Assume that conditions C1-C2, C4, and C7 hold. Let $\boldsymbol{y} \in \mathcal{A}$. Let $\nabla s(X, \boldsymbol{y})$ denote the gradient of the scale statistic with respect to the data vector evaluated at $\boldsymbol{y}$. Then $\nabla s(X, \boldsymbol{y}) \in \mathcal{C}^{\perp}(X)$ and is normal to $\Pi(\mathcal{A})$ at $\boldsymbol{z} = Q\boldsymbol{y}$ in $\mathcal{C}^{\perp}(X)$.*

As a result of the lemma, the contribution to the Jacobian of this attenuation is

$$\cos(\gamma) = \frac{\nabla s(X, \boldsymbol{y})^{\top} \boldsymbol{z}}{\|\nabla s(X, \boldsymbol{y})\| \|\boldsymbol{z}\|}, \tag{13}$$

where γ is the angle between the two normal vectors. This step is illustrated in Figure 3 for the toy location-scale example. The figure ~~only~~ pictures only the deviation space which in this case is a plane. The original unit sphere (here, the solid circle) is

first stretched to the dashed sphere contributing $r^{-(n-p-1)}$ to the Jacobian as seen in panel (a). In panel (b), the dashed circle is transformed onto $\Pi(\mathcal{A})$ contributing $\cos(\gamma)$ to the Jacobian. The normal vectors in panel (b) are orthogonal to the tangent vectors of $\Pi(\mathcal{A})$ and the circle. As stated above, the Jacobian is the ratio of infinitesimal lengths along these tangent vectors. This is the same as the ratio of the infinitesimal lengths of the normal vectors (i.e., $\cos(\gamma)$). This generalization extends to higher dimensions where the 'lengths' along the tangent vectors become volumes along the tangent spaces.

Shift from $\Pi(\mathcal{A})$ to $\mathcal{A}$

The final piece of the Jacobian comes from the transformation from $\Pi(\mathcal{A})$ to $\mathcal{A}$. This step involves a shift of $\boldsymbol{z}$ to $\boldsymbol{y}$ along the column space of X. Since the shift depends on $\boldsymbol{z}$, the density on the set $\Pi(\mathcal{A})$ is deformed by the shift. The contribution of this deformation to the Jacobian is, again, the ratio of the infinitesimal volume along $\Pi(\mathcal{A})$ at $\boldsymbol{z}$ to the corresponding volume along $\mathcal{A}$ at $\boldsymbol{y}$. The ratio is calculated by considering the volume of the projection of a unit hypercube in the tangent space of $\mathcal{A}$ at $\boldsymbol{y}$ onto $\mathcal{C}^{\perp}(X)$. Computational details are given in the following lemmas and subsequent theorem. Throughout, let $\mathcal{T}_y(\mathcal{A})$ and $\mathcal{T}_y^{\perp}(\mathcal{A})$ denote the tangent space to $\mathcal{A}$ at $\boldsymbol{y}$ and its orthogonal complement respectively.

Lemma 3.3. *Assume that conditions C1-C5 and C7-C8 hold. Then the $p+1$ gradient vectors $\nabla s(X, \boldsymbol{y}), \nabla b_1(X, \boldsymbol{y}), \ldots, \nabla b_p(X, \boldsymbol{y})$ form a basis for $\mathcal{T}_y^{\perp}(\mathcal{A})$ with probability one.*

The lemma describes construction of a basis for $\mathcal{T}_y^{\perp}(\mathcal{A})$. This leads to a basis for $\mathcal{T}_y(\mathcal{A})$. Both of these bases can be orthonormalized. Let $A = [a_1, \ldots, a_{n-p-1}]$ and $B = [b_1, \ldots, b_{p+1}]$ denote the matrices whose columns contain the orthonormal bases for $\mathcal{T}_y(\mathcal{A})$ and $\mathcal{T}_y^{\perp}(\mathcal{A})$, respectively. The columns in A define a unit hypercube in

$\mathcal{T}_y(\mathcal{A})$ and their projections onto $\mathcal{C}^{\perp}(X)$ define a parallelepiped. We defer construction of A until later.

Lemma 3.4. *Assume that conditions C1-C5 and C7-C8 hold. Then the* $n \times (n-p-1)$ *dimensional matrix* $P = QA$ *is of full column rank.*

As a consequence of this lemma, the parallelepiped spanned by the columns of P is not degenerate (it is $n-p-1$ dimensional), and its volume is given by

$$\text{Vol}(P) := \sqrt{\det(P^{\top}P)} = \prod_{i=1}^{r} \sigma_i \tag{14}$$

where $r = \text{rank}(P) = n-p-1$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_r > 0$ are the singular values of P (e.g., Miao and Ben-Israel (1992)). Combining Lemmas 3.3 and 3.4 above leaves us with the following result concerning the calculation of the desired Jacobian.

Theorem 3.5. *Assume that conditions C1-C5 and C7-C8 hold. Then the Jacobian of the transformation from the distribution along* $\Pi(\mathcal{A})$ *to that along* $\mathcal{A}$ *is equal to the volume given in* (14).

The proposal density

Putting all the pieces of the Jacobian together we have the following result. Any dependence on other variables, including current states in the Markov chain, is made implicit.

Theorem 3.6. *Assume that conditions C1-C8 hold. Let* $\boldsymbol{z}^*$ *be sampled on the unit sphere in* $\mathcal{C}^{\perp}(X)$ *with density* $p(\boldsymbol{z}^*)$. *Using the transformation of* $\boldsymbol{z}^*$ *to* $\boldsymbol{y} \in \mathcal{A}$ *described in Theorem 3.1, the density of* $\boldsymbol{y}$ *is*

$$p(\boldsymbol{y}) = p(\boldsymbol{z}^*) r^{-(n-p-1)} \cos(\gamma)\, Vol(P) \tag{15}$$

where $r = s(X, \boldsymbol{y}_{obs})/s(X, \boldsymbol{z}^*)$*, and* $\cos(\gamma)$ *and Vol*(P) *are as in equations* (13) *and* (14)*, respectively.*

In practice, computing A directly to find P and $\text{Vol}(P)$ is computationally intensive as it involves orthogonalization of n vectors in n-dimensional space. To find a matrix A, supplement B with a set of n linearly independent columns on the right, and apply Gram-Schmidt orthonormalization to the matrix. This algorithm is infeasibly slow when n is large because it is $\mathcal{O}(n^3)$ and must be repeated at each iterate of the MCMC when a complete data set is drawn. Fortunately, we can make use of results related to *principal angles* found in Miao and Ben-Israel (1992) to compute the volume in (14) using B and an orthonormal basis for $\mathcal{C}(X)$ (The definition of principal angles can be found in the cited text). Recall, B is constructed by orthogonalization of a basis for $\mathcal{T}_y^{\perp}(\mathcal{A})$. Since this space is of dimension $p+1$, applying Gram-Schmidt to find the orthonormal basis is much faster, the algorithm is $\mathcal{O}(np^2)$, and there is a considerable reduction in computational burden when $n \gg p$. Further, the singular values of $P = QA$ are also the singular values of $W^\top A$ (recall, $Q = WW^\top$), which can be easily obtained through B. The following corollary formally states how computation of A can be circumvented.

Corollary 3.7. *Let* U *be a matrix whose columns form an orthonormal basis for* $\mathcal{C}(X)$*. Then the non-unit singular values of* $U^\top B$ *are the same as the non-unit singular values of* $W^\top A$*.*

Thus, we can compute $\text{Vol}(P)$ by finding the singular values of $U^\top B$, reducing the computational burden substantially.

4 Simulations

4.1 Simulation 1

4.2 Simulation 2

Data generating model:

$$\begin{aligned} \theta_i \sim & N(\mu, \tau^2),\ i = 1, 2, \ldots, 90 \\ y_{ij} \sim & (1 - p_i)N(\theta_i, \sigma^2) + p_i N(\theta_i, m_i\sigma^2), j = 1, 2, ..., n_i \end{aligned} \tag{16}$$

with $\mu = 0, \tau^2 = 1, \sigma^2 = 4$. The values of p_i, m_i, and n_i depend on the group and are formed using 5 replicates of the full factorial design over factors p_i, m_i, n_i with levels $p_i = .1, .2, .3$, $m_i = 9, 25$, and $n_i = 25, 50, 100$. The full model for fitting is a corresponding normal model without contamination:

$$\begin{aligned} \mu \propto 1,\ \tau^2 \propto \tau^{-2}, \\ \theta_i \sim N(\mu, \tau^2),\ \sigma_i^2 \sim IG(a_s, b_s),\ i = 1, 2, \ldots, 90, \\ y_{ij} \sim N(\theta_i, \sigma_i^2),\ j = 1, 2, \ldots, n_i \end{aligned} \tag{17}$$

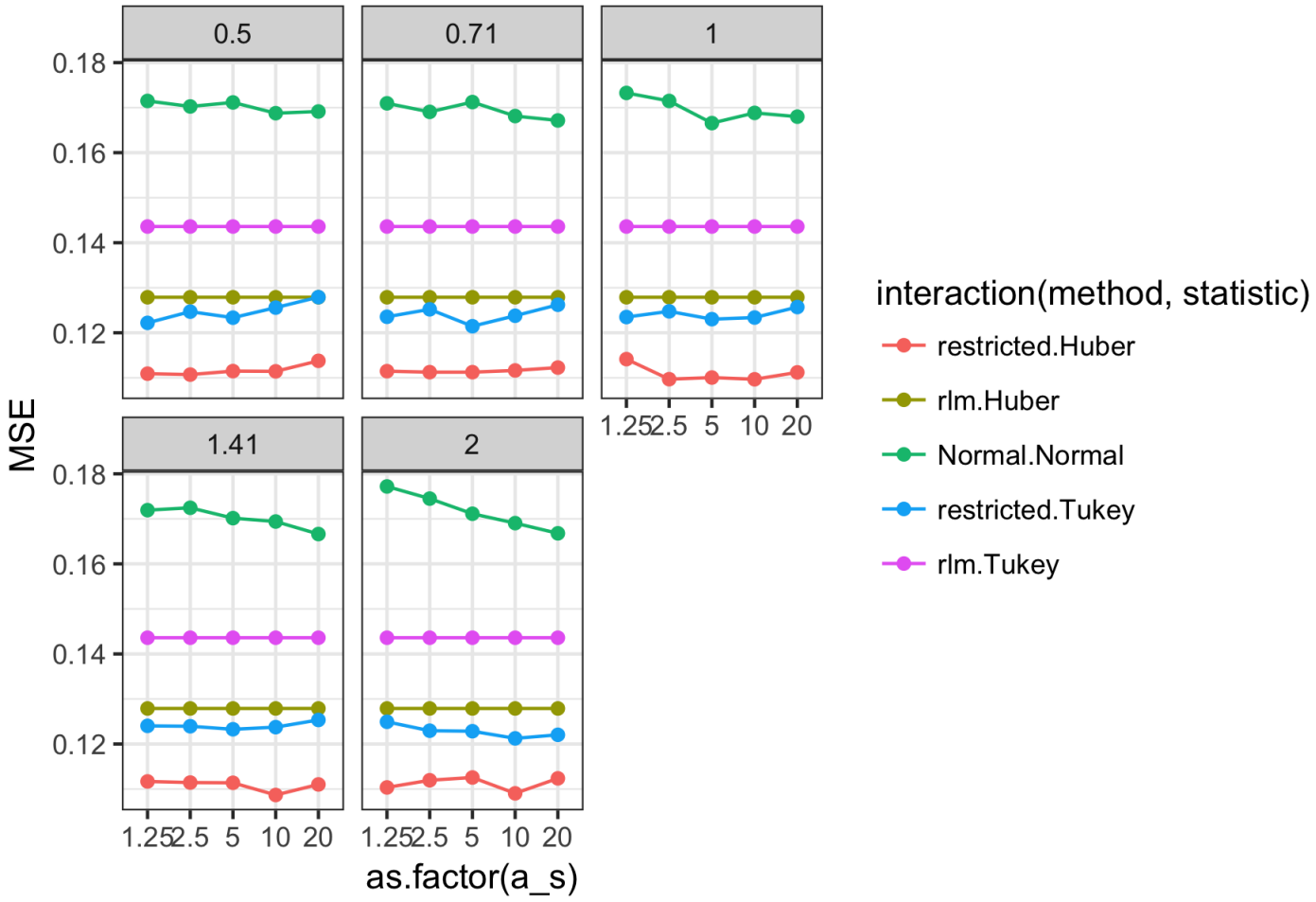
For the restricted likelihood versions we condition on robust M-estimators of location and scale in each group: $T_i(\boldsymbol{y}_i) = (\hat{\theta}_i, \hat{\sigma}_i^2), i = 1, 2, ..., 90$. The two versions used are Huber's and Tukey's location estimator both coupled with Huber's scale estimator. The estimates from the Bayesian models are compared to these estimates. To complete the specification of model (17) we must specify a_s and b_s. For this we use a variety of values representing different levels of prior knowledge. For each we set $b_s = 4a_s c_s$ resulting in a prior mean for each σ_i^2 of $\frac{4c_s a_s}{a_s - 1},\ a_s > 1$. The larger a_s, the more informative the prior. With $c_s = 1$ the shrinkage (for large a_s) is to the true

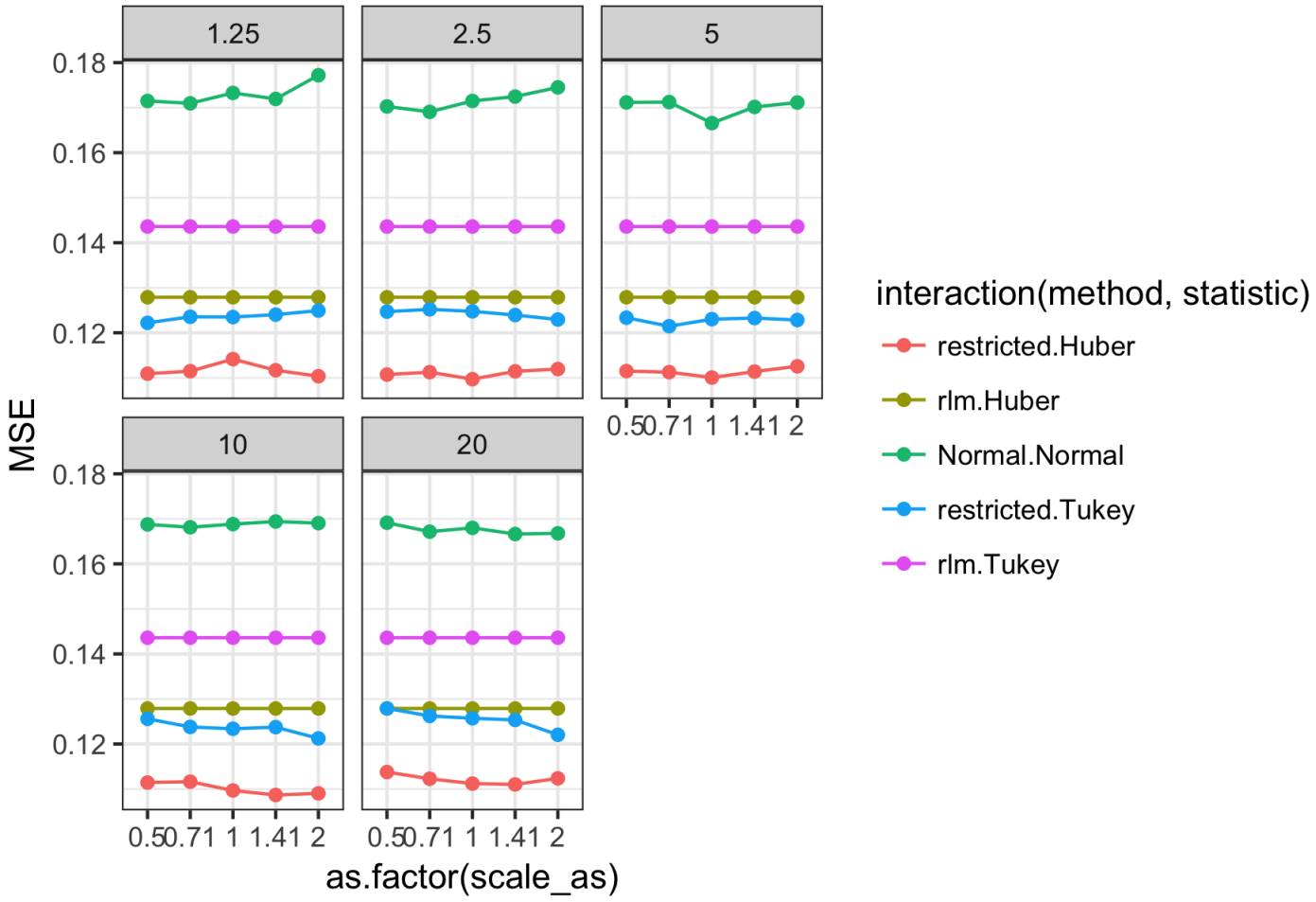
value of $\sigma^2 = 4$ of the variance of the good component of data in the data generating model. We consider $a_s = 1.25, 2.5, 5, 10, 20$ and $c_s = 1/2, 1/\sqrt{2}, 1, \sqrt{2}, 2$. Values of $c_s \neq 1$ will result in shrinkage towards the wrong value of σ^2 with strength growing with a_s.

A single (maybe need to do more...each run through takes about 3 hours on my laptop and current code, maybe 10 different sets would suffice) set of data is generated from (16). The models compared are: the full model (17), the two restricted likelihood versions of this full model, classical robust linear models fit individually to each group.

We compare fits of each model using $MSE = \frac{1}{90}\sum_{i=1}^{90}(\hat{\theta}_i - \theta_i)^2$ with $\hat{\theta}_i$ the estimate of θ_i from the corresponding model.

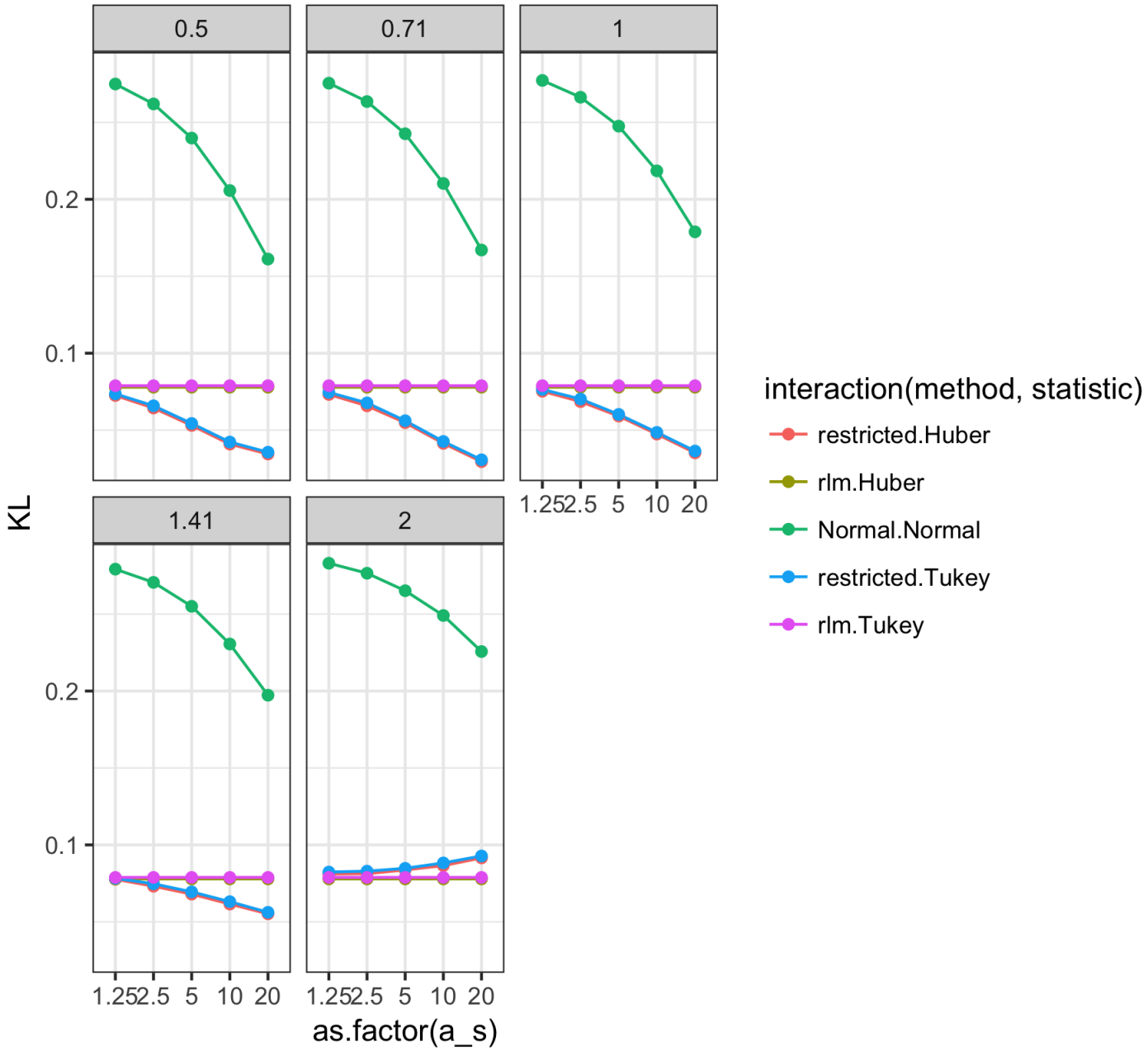
Results for MSE

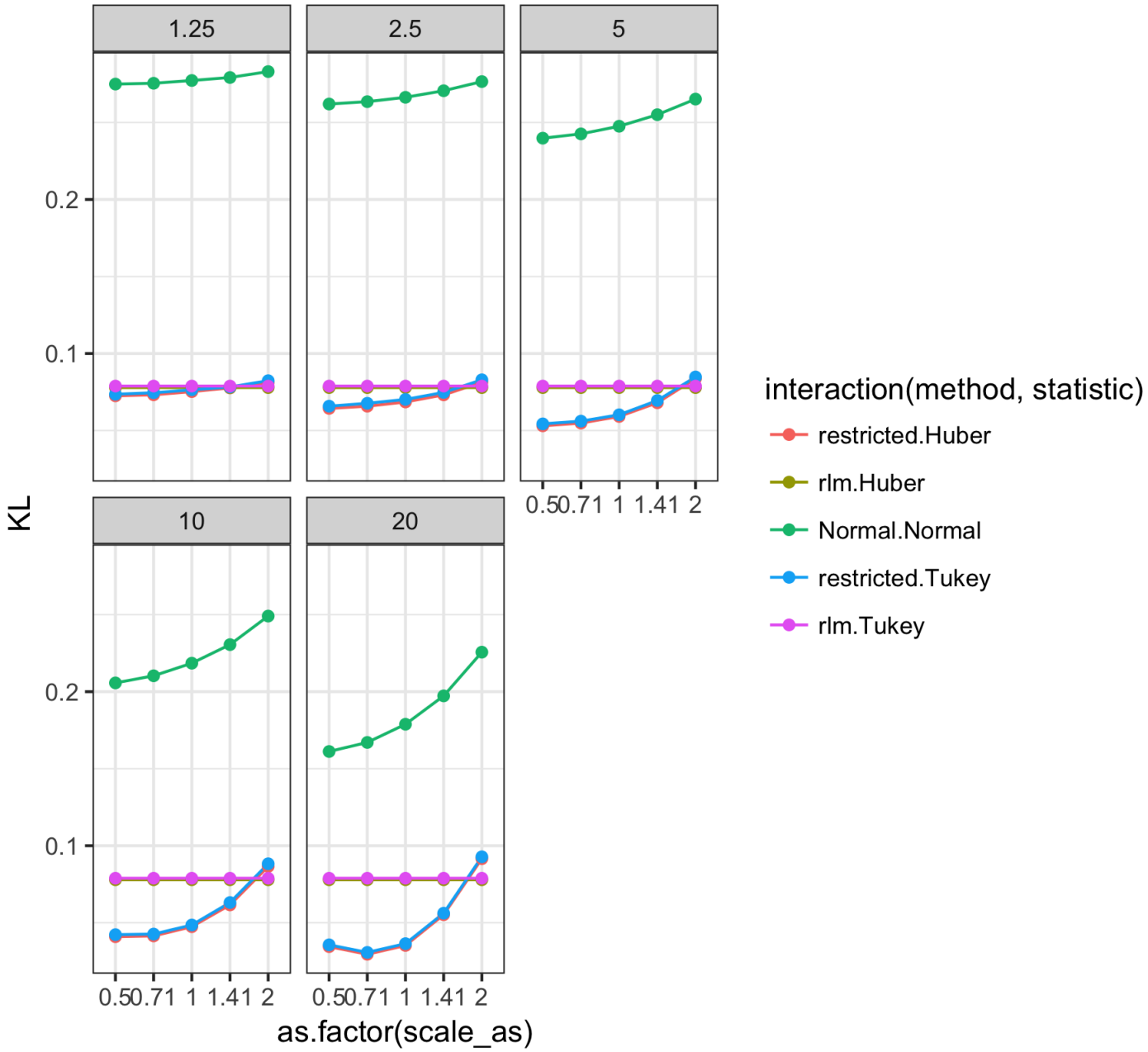

0.5
0.71
1
1.41
2
MSE
0.18
0.16
0.14
0.12
1.25
2.5
5
10
20
as.factor(a_s)
interaction(method, statistic)
restricted.Huber
rlm.Huber
Normal.Normal
restricted.Tukey
rlm.Tukey



Big picture - restricted methods beating corresponding robust regressions (labeled rlm). MSE robustness to prior on σ_i^2

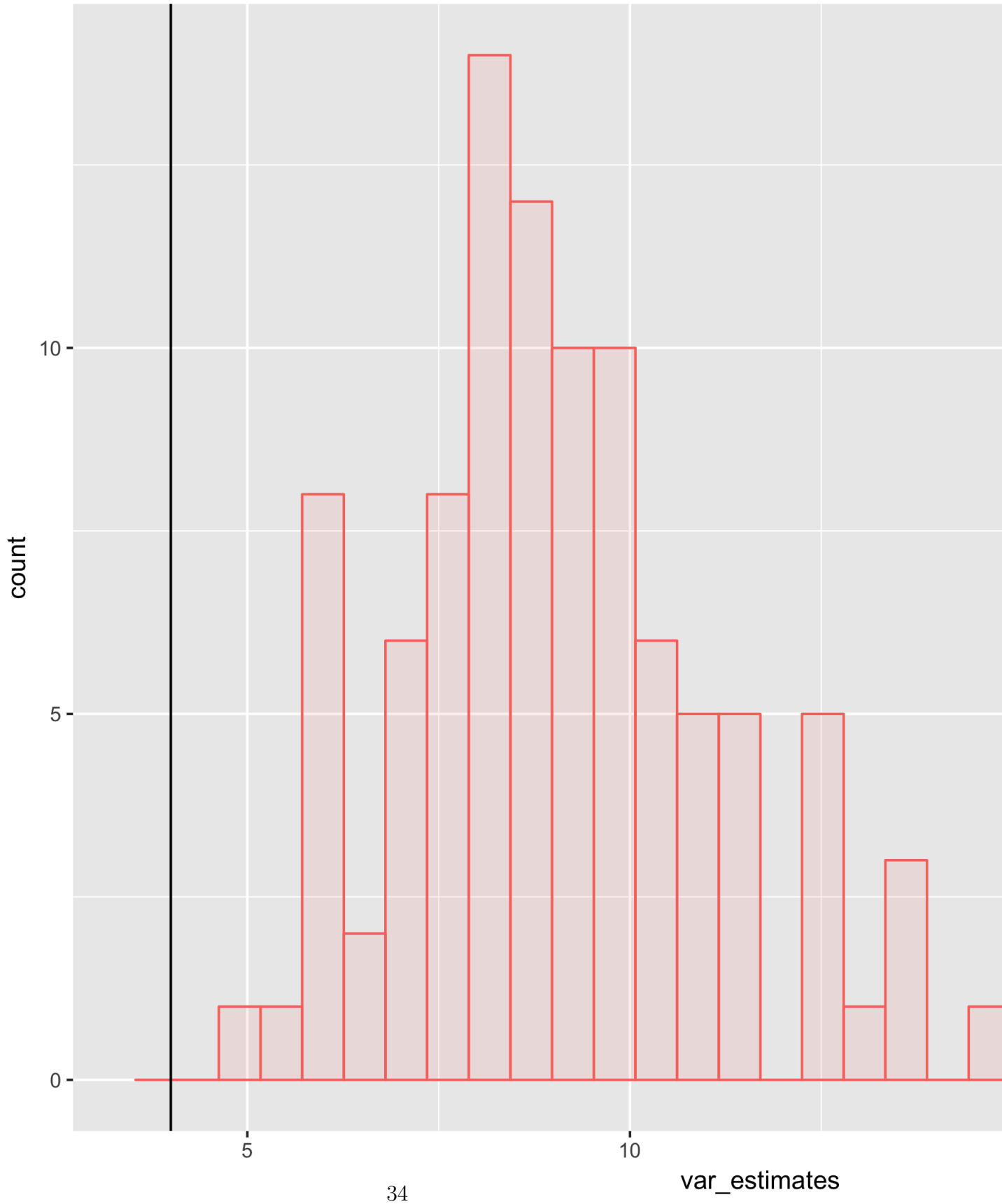
Results for KL (plots are average of the KLs computed for each group):


0.5
0.71
1
1.41
2
0.2
0.1
KL
1.25
2.5
5
10
20
as.factor(a_s)
interaction(method, statistic)
restricted.Huber
rlm.Huber
Normal.Normal
restricted.Tukey
rlm.Tukey



One explaination for the idea that 'shrinking towards smaller values' may do slightly better than shrinking toward the true value is the fact that we used default tuning parameters to define M-Estimators. For the amount of contaimination in each group, the expected value of the variance estimate (Huber's proposal 2) is larger that $\sigma^2 = 4$. The histogram below demonstrates a sample of variaince estimates for data

generated from one of the contamination groups....the estimates are consitently above 4. Thus it appears the prior mean must be smaller than the true value to get the 'correct' amount of shrinkage. There is a suggestion that if the prior is too strong (large a_s), at some point, shrinking to too small a value degrades performance....which would be expected.


count
10
5
0
5
10
var_estimates

5 Applications

We illustrate the methods developed in Sections 2 and 3 with a pair of regression models for data from Nationwide Insurance Company, which concern prediction of the performance of insurance agencies. The data contain outliers and are subject to model misspecification. In particular, a group of the data do not follow the same generative process as the data of interest. It would be extremely challenging to model some features of the data. In our analysis, we follow the standard practice when demonstrating the benefits of robust methods. We work with a naive model for the data which ignores certain features of the problem. We do this both to create a situation where all can agree that the model for the full data $\boldsymbol{y}$ is imperfect and to preserve the confidentiality of selected aspects of modelling done by Nationwide. We wish to provide inference for the 'good' portion of the data. The two models we fit either treat the analysis as a single regression or as a collection of related regressions. Details of the models, prior distributions, and conditioning statistics are given in the next two subsections.

5.1 Nationwide Data

The Nationwide Insurance Company sells many of its insurance policies through agencies which provide direct service to policy holders. The contractual agreements between Nationwide and these agencies vary. Of major interest to Nationwide is the prediction of future performance of agencies where, for our purposes, performance is measured by the total number of households an agency services ('household count'). A serviced household is one in which at least one person living at that residence has at least one policy written through the agency. We used data from previous years to build a model to forecast future household count. In particular, we use agency char-

acteristics, as measured during a single month in 2010, to predict household counts in the corresponding month in 2012. The characteristics used are household count and two measurements of agency size/experience. The two measurements of agency size/experience are, roughly, the number of employed persons at the agency and the length of time the agency has been affiliated with Nationwide. The household counts (response and predictor) have been square rooted to stabilize variance. The data are proprietary, and to mask them all variables have been individually centered and scaled and identifiers (agency/agent names and state labels) have been removed. All subsequent analysis is done on this scale. As an exploratory view, a plot of the square root of count in 2012, against that in 2010 is shown in Figure 4. The different colors represent the varying contractual agreements as they stood in 2010. 'Type 1' agencies are of special interest. Among the open agencies, a strong linear correlation exists. The specific linear relationship depends on agency type. The data are characterized by a large number of agencies which were open in 2010 but closed sometime before 2012, as represented by the horizontal band at 0. We use these data as a test bed for our techniques, fitting models that do not account for agency closures or contract type. Our expectation is that ~~the incomplete~~ restricting the likelihood will facilitate prediction for the good part of the data.

5.2 Regression model

The first analysis that we consider is based on a single regression. We use the following standard normal theory regression model

$$\boldsymbol{\beta} \sim N_p(\boldsymbol{\mu}_0, \Sigma_0); \;\; \sigma^2 \sim IG(a_0, b_0); \;\; y_i = \boldsymbol{x}_i^\top \boldsymbol{\beta} + \epsilon_i, \;\; \epsilon_i \overset{iid}{\sim} N(0, \sigma^2), \; i = 1, \ldots, n, \quad (18)$$

where $\boldsymbol{\beta}$ is a four dimensional vector ($p = 4$) of regression coefficients for the intercept, square root of count in 2010, and the two size/experience measures, and y_i is the square rooted household count in 2012 for the i^{th} agency with covariate vector $\boldsymbol{x}_i$. Although the mean of covariates and response have been removed, we include the intercept as fitting is done on a holdout set to evaluate predictive performance. The hyper-parameters $a_0, b_0, \boldsymbol{\mu}_0$ and Σ_0 are all fixed and set from a robust regression fit to the data from the time period two years before. Letting $\hat{\boldsymbol{\beta}}$ represent the estimate of the coefficients from this fit we set $\boldsymbol{\mu}_0 = \hat{\boldsymbol{\beta}}$ and $\Sigma_0 = n \cdot \text{var}(\hat{\boldsymbol{\beta}})$ where here n is the sample size of the prior data set. The hyperparameters for σ^2 are set so that the prior mean is s^2, the estimated variance from the robust regression, and the spread of the prior covers the range of plausible values with high probability. All values are then transformed appropriately to match the current scale of the data. In the end we take $\boldsymbol{\mu}_0 = (0.18, 0.81, 0.01, -0.02)^\top$ and set the mean of σ^2 to 0.014 and standard deviation to 0.033.

We compare four Bayesian models: the standard Bayesian normal theory model, two restricted likelihood models, both with simultaneous M-estimators, and a heavy-tailed model. For the restricted likelihood methods we use the same simultaneous M-estimators as in Section 2.4 adapted to linear regression. The heavy-tailed model replaces the normal sampling density in (18) with a t-distribution with $\nu = 3$ degrees of freedom. We also fit the corresponding classical robust regressions and a least squares regression.

5.2.1 Method of model comparison

We wish to examine the performance of the models in a fashion that preserves the essential features of the problem. Since we are concerned with outliers and model misspecification, we understand that our models are imperfect and so prefer to use

an out-of-sample measure of fit. This leads us to cross-validation. We repeatedly split the data into training and validation sets. We fit the model to the training data and assess its performance on the validation data.

The presence of numerous outliers in the data implies that both training and validation data will contain outliers. For this reason, the evaluation must be robust to a certain fraction of bad data. The two main strategies are to robustify the evaluation function (e.g., Ronchetti et al., 1997) or to retain the desired evaluation function and trim cases (Jung et al., 2014). Here, we pursue the trimming approach with log predictive density for the Bayesian models and log plug-in maximum likelihood for the classical fits used as the evaluation function.

The trimmed evaluation proceeds as follows in our context. The evaluation function for case i in the hold-out data is the log predictive density, say $\log(f(y_i))$, with the conditioning on the summary statistic suppressed. The trimming fraction is set at $0 \leq \alpha < 1$. To score a method, we first identify a base method. Denote the predictive density under this method by $f_b(y)$. Under the base method, $\log(f_b(y_i))$ is computed for each case in the validation sample, say $i = 1, \ldots, M$. Order the validation sample according to the ordering of $\log(f_b(y_i))$ and denote this ordering by $y^b_{(1)}, y^b_{(2)}, \ldots, y^b_{(M)}$. That is, for $i < j$ $\log(f_b(y^b_{(i)})) < \log(f_b(y^b_{(j)}))$. All of the methods are then scored on the validation sample with the mean trimmed log marginal pseudo likelihood,

$$TLM_b(A) = (M - [\alpha M])^{-1} \sum_{i=[\alpha M]+1}^{M} \log(f_A(y^b_{(i)})),$$

where f_A corresponds to the predictive distribution under the method "A" being scored. In other words, the $[\alpha M]$ observations with the smallest values of $\log(f_b(y))$ are removed from the validation sample and all of the methods are scored using only the remaining $M - [\alpha M]$ observations. This process is advantageous to the base

method. A method that performs poorly when it is the base method is discredited. For a complete evaluation, we allow each method to appear as the base method. For brevity, we present only a selection of results in our subsequent analyses.

5.2.2 Comparison of predictive performance

Model performance is assessed using the mean and standard deviation of the TLM across 100 different splits into training and validation samples. First, we include all observations in each validation sample to calculate TLM for each split. We then repeat the evaluation using only certain subsets of the validation sample that are of special interest. Subsets include open agencies, open 'Type 1' agencies, and 'Type 1' agencies. For brevity, we include results for the 'Type 1' agencies only. As noted, assessing model predictions on this set of agencies is of special interest to the company. A range of training sample sizes was used and we include results from $n = 25, 100, 1000,$ and 2000 out of a total of 3180 agencies. The trimming fraction, α, ranges from 0 to 0.3. A classical robust regression to the prior data assigns zero weight to around 16% of observations; in essence removing these from the analysis. This informed the range of trimming fractions chosen. In practice, we would set α slightly larger than 0.16.

Model evaluation for 'Type 1' agencies is shown in Figure 5 for training sample sizes $n = 25, 100,$ and 1000. The t-model is used as the base method to compute TLM. The models pictured are: classical robust regression with Tukey's ψ function (rlm-T), restricted likelihood with Tukey ψ (restr.-T), classical robust regression with Huber's ψ function (rlm-H), restricted likelihood with Huber's ψ (restr.-H), and the thick tailed t-model (t). The normal theory models perform poorly due to the numerous outliers and are left out of the figures. Appearing in the figures are the mean TLM across validations set for each model and each trimming fraction, α (along the x-axis).

The error bars depicted are one standard deviation of the TLM above and below the mean. The range of the vertical axis is chosen to enhance important features and as a result, some evaluation measures extend below this range. In particular, the restricted likelihood methods perform poorly if no trimming is done; reflecting that these methods are not intended to fit well to outliers. Recall that we expect about 15-16% outliers in the validation sets, thus trimming fractions slightly larger than this amount are needed in order to assess fits to the 'good' data. For $n = 25$, the thick tailed model prevails across trimming fractions, although less so for $\alpha \geq 0.15$. For sample sizes as low as $n = 100$, the restricted likelihood methods outperform the heavy-tailed model with the Tukey version performing the best. The stronger performance of restricted likelihood based on Tukey's method and the t model is to be expected, as many of the residuals are so extreme that trimming is better than winsorizing (as Huber's method effectively does). As expected, with enough data, the Bayesian methods and their classical counterparts perform similarly, although there is a persistent slight edge in favor of the Bayesian restricted likelihood methods. We attribute this advantage to the weakly informative prior distribution which pulls the estimates slightly toward better values. The similarity occurs as early as $n = 100$.

5.3 Hierarchical regression model

Nationwide agencies span many states and insurance regulations and the competitive environment varies between states. A natural extension to the previous analysis is a hierarchical regression model, grouping agencies within each state to reflect similar business environments. Using the same study design with the same training and validation splits, we re-analyze the data using the following hierarchical regression

model:

$$\begin{aligned} &\boldsymbol{\beta} \sim N_p(\boldsymbol{\mu}_0, a\Sigma_0); \quad \boldsymbol{\beta}_j \overset{iid}{\sim} N_p(\boldsymbol{\beta}, b\Sigma_0); \quad \sigma_j^2 \sim IG(a_0, b_0); \\ &\boldsymbol{y}_{ij} = \boldsymbol{x}_{ij}^\top \boldsymbol{\beta}_j + \epsilon_{ij}, \quad \epsilon_{ij} \overset{iid}{\sim} N(0, \sigma_j^2), \ i = 1, \ldots, n_j, \ j = 1, \ldots, J \end{aligned} \tag{19}$$

where y_{ij} represents the i^{th} observation in the j^{th} state, n_j is the total number of agencies in each state, and J is the number of states. $\boldsymbol{x}_{ij}$ is a four dimensional vector comprised of the same covariates as above. $\boldsymbol{\beta}_j$ represents the individual regression coefficient vector for state j. We match this model to the non-hierarchical model in several ways. First, $\boldsymbol{\mu}_0$, Σ_0, a_0, and b_0 are fixed as before. We constrain $a+b = 1$ in an attempt to partition the total variance between the individual $\boldsymbol{\beta}_j$'s and the overall $\boldsymbol{\beta}$. We take $b \sim \text{beta}(v_1, v_2)$. Using the previous data set, we assess the variation between individual estimates of the β_j to set v_1 and v_2 to allow for a reasonable amount of shrinkage. To allow for dependence across the σ_j^2 we first take $(z_1, \ldots, z_J) \sim N_J(\mathbf{0}, \Sigma_\rho)$ with $\Sigma_\rho = (1-\rho)I + \rho\mathbf{1}\mathbf{1}^\top$. Then we set $\sigma_j^2 = H^{-1}(\Phi(z_j))$ where H is the cdf of an $IG(a_0, b_0)$ and Φ is the cdf of a standard normal. This results in the specified marginal distribution, while introducing correlation via ρ. We assume $\rho \sim \text{beta}(a_\rho, b_\rho)$ with mean $\mu_\rho = a_\rho/(a_\rho + b_\rho)$ and precision $\psi_\rho = a_\rho + b_\rho$. The parameters μ_ρ and ψ_ρ are given beta and gamma distributions, respectively. We fix the parameters of these distributions by again considering fits to individual states from the previous data set. More precise details on setting v_1, v_2 and the the priors on μ_ρ and ψ_ρ are given in the appendix. We note that we tried a range of other fixed hyper-parameters resulting in negligible differences in the results.

Using the same techniques as in the previous section, we fit the normal theory hierarchical model above, a thick tailed t version with $\nu = 3$ d.f., and two restricted likelihood versions (Huber's and Tukey's) of the model. For the incomplete restricted

methods, we condition on robust regression estimates fit separately within each state. We also fit classical robust regression counterparts and a least squares regression separately within each state.

We digress briefly to note that for the restricted likelihood methods no additional computational strategies outside of those discussed in Section 3.2 are needed to fit the hierarchical models described here. Since we condition on statistics which are computed within each state, the model's conditional independence between the states allows the data augmentation described earlier to be performed independently within each state. Updates of hyperparameters follow conventional MCMC procedures. We note that different types of statistics could be chosen for each state, if desired, allowing for a large amount of flexibility.

Selected results for the hierarchical fits appear in Figure 6. Hierarchical models naturally require more data and so we consider only training sizes of $n = 1000$ and 2000. Again, the t-model is used as the base method for computing TLM. Trimming fractions between 0.15 and 0.3 are displayed, as patterns for smaller trimming fractions are similar to those from the non-hierarchical fits. That is, without sufficient trimming, the Bayesian restricted likelihood fits' evaluation measure is poor. Again, the normal theory fits, both Bayesian and classical, perform poorly and are left out of the figures. We see that the restricted likelihood with Tukey's estimator performs best in each case (assuming sufficient trimming). Huber's version also tops the thick tailed model for $n = 2000$. The Bayesian restricted likelihood fits considerably outperform their respective individual classical robust fits for training size of $n = 1000$. This observation remains, though marginally so, for $n = 2000$. The advantage of the hierarchical models seen here is due to the pooling of information across states, resulting in better predictive performance as compared to both the thick tailed competitor as well the respective classical fits.

5.4 Comparison of hierarchical and non-hierarchical fits

The performance of the methods for the hierarchical and non-hierarchical models can be contrasted through our cross validations studies. We focus on Tukey's and Huber's conditioning statistic and concentrate our evaluation on the 'Type 1' agencies. Table 1 displays the mean TLM for each model and range of trimming fractions. Our summary below focuses exclusively on realistic trimming fractions, $\alpha \geq 0.15$, and Tukey's conditioning statistic.

We first note that for the non-hierarchical model, there is little difference between mean TLM for $n = 1000$ and $n = 2000$, with the numbers differing only in the third decimal place (see rows 1 and 3 of the table). This is due to the posterior predictive distributions having stabilized. The mean TLMs for the hierarchical model show a greater change with increases of about 0.05 to 0.08 as the training sample size changes from 1000 to 2000 (see rows 2 and 4 of the table). For calibration, the mean TLM for a normal with mean 0.5 and variance 1 is approximately this size when trimming is done under a standard normal base model. Thus, the increase in mean TLM is substantial. We attribute the change for the hierarchical model to the improvement in fits, particularly for states with fewer agencies.

Direct comparison of the hierarchical and non-hierarchical models shows that, for $n = 1000$, the non-hierarchical model has uniformly (for α of interest) better mean TLM (rows 1 and 2). The differences are substantial, and the summaries primarily reflect greater stability of fits on a state-by-state basis under the non-hierarchical model. To a lesser extent, they reflect variation in the evaluation criterion which stems from modest validation sample size, particularly with larger trimming fractions. The trimmed cases are not proportionally distributed across states. The pattern changes for $n = 2000$ (rows 3 and 4), with the hierarchical model showing larger mean TLMs for trimming fractions 0.15 and 0.20. The improvement reflects the

	Trimming fraction (α)			
	0.15	0.2	0.25	0.3
Tukey ($n = 1000$)				
Non-Hier.	1.072 (0.014)	1.179 (0.022)	1.226 (0.029)	1.255 (0.033)
Hier.	1.021 (0.063)	1.110 (0.070)	1.157 (0.067)	1.187 (0.065)
Tukey ($n = 2000$)				
Non-Hier.	1.068 (0.029)	1.178 (0.007)	1.225 (0.011)	1.254 (0.014)
Hier.	1.094 (0.041)	1.189 (0.036)	1.221 (0.033)	1.242 (0.028)
Huber ($n = 1000$)				
Non-Hier.	1.020 (0.020)	1.114 (0.035)	1.157 (0.041)	1.184 (0.045)
Hier.	0.861 (0.073)	0.937 (0.079)	1.001 (0.074)	1.063 (0.064)
Huber ($n = 2000$)				
Non-Hier.	1.015 (0.021)	1.112 (0.014)	1.154 (0.019)	1.181 (0.023)
Hier.	0.930 (0.041)	1.014 (0.043)	1.080 (0.035)	1.148 (0.027)

Table 1: Mean (standard deviation) of TLM for 'Type 1' agencies for the Bayesian restricted likelihood non-hierarchical and hierarchical models for $n = 1000$ and 2000.

ability of the hierarchical model to capture differences in regressions across the states which is realized when the training sample size is large enough. We attribute the better performance of the non-hierarchical model for the largest trimming fractions to variation in the evaluation.

6 Discussion

Many routine choices in an analysis react to the gap between reality and the statistical model, where a bit of set-up work improves inferential performance. Often, these choices can be recast in the framework of restricted likelihood presented here, lending them more formality and facilitating development of theoretical results. But a much greater benefit of our framework is that it leads us to blend classical estimation with Bayesian methods. Here, we use the likelihood from robust regression estimators to move from prior distribution to posterior distribution. Conditioning on the estimator, the update follows Bayes' Theorem exactly. Computation is driven by MCMC meth-

ods, requiring only a modest supplement to existing algorithms. In another context, we might condition on the results of a set of estimating equations, designed to enforce lexical preferences for those features of the analysis considered most important, yet still producing inferences for secondary aspects of the problem. For example, the computational strategies we devised here allow us to apply the method to inference on quantiles of a regression model. In other settings, we envision conditioning on a mix of estimators and some of the observed data.

The framework we propose allows us to retain many benefits of Bayesian methods: it requires a full and complete model for the data; it lets us combine various sources of information both through the use of a prior distribution and through creation of a hierarchical model; it guarantees admissibility of our decision rules among the class based on the summary statistic $T(\boldsymbol{y})$; and it naturally leads us to focus on predictive inference.

This same framework retains many of the benefits of classical estimation. Great ingenuity has been used to create a wide variety of estimators in this tradition, many of which are designed to handle specific flaws in the model. The estimators are typically accompanied by asymptotic results on consistency and distribution. Many of these results carry over to our blend of classical and Bayesian methods, although regularity conditions differ. We expect our procedures to have strong large sample performance, especially in settings where pooling of information is of value.

This framework opens a number of questions, including a need to revisit such issues as model selection, model averaging for predictive performance, and the role of diagnostics. Perhaps the biggest question is which summary statistic to choose. For this, we recommend a choice based on the analyst's understanding of the problem, model, reality, deficiencies in the model, inferences to be made, and the relative importance of various inferences. In our words, to provide desireable inference, we recommend

use of robust and relevant summary statistics in conjunction with Bayesian models.

7 Appendix

7.1 Proofs

Proof of Theorem 3.1.

Proof.

$$
\begin{aligned}
s(X, \boldsymbol{y}) &= s\left(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^* + X\left(\boldsymbol{b}(X, \boldsymbol{y}_{obs}) - \boldsymbol{b}(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^*)\right)\right) && (20)\\
&= \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)} s(X, \boldsymbol{z}^*) = s(X, \boldsymbol{y}_{obs}), \qquad \text{and} && (21)\\
\boldsymbol{b}(X, \boldsymbol{y}) &= \boldsymbol{b}\left(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^* + X\left(\boldsymbol{b}(X, \boldsymbol{y}_{obs}) - \boldsymbol{b}(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^*)\right)\right) && (22)\\
&= \boldsymbol{b}(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^*) + \boldsymbol{b}(X, \boldsymbol{y}_{obs}) - \boldsymbol{b}(X, \frac{s(X, \boldsymbol{y}_{obs})}{s(X, \boldsymbol{z}^*)}\boldsymbol{z}^*) && (23)\\
&= \boldsymbol{b}(X, \boldsymbol{y}_{obs}) && (24)
\end{aligned}
$$

□

Proof of Lemma 3.2.

Proof. We first show that $\nabla s(X, \boldsymbol{y}) \in \mathcal{C}^{\perp}(X)$. Recall that $H = I - Q$. By the regression invariance property C7 of s, we have

$$
s(X, \boldsymbol{y}) = s(X, Q\boldsymbol{y} + H\boldsymbol{y}) = s(X, Q\boldsymbol{y}). \tag{25}
$$

Thus, by the chain rule $\nabla s(X, \boldsymbol{y}) = Q\nabla s(X, Q\boldsymbol{y}) = Q\nabla s(X, \boldsymbol{z})$. Hence $X^{\top}\nabla s(X, \boldsymbol{y}) = 0$ as desired. From equation (25), all vectors $\boldsymbol{z}' \in \Pi(\mathcal{A})$ satisfy $s(X, \boldsymbol{z}') = s(X, \boldsymbol{y}) = s(X, \boldsymbol{y}_{obs})$, and so all directional derivatives of s along each tangent $\boldsymbol{v}$ to $\Pi(\mathcal{A})$ in

$\mathcal{C}^{\perp}(X)$ at $\boldsymbol{z}$ are equal to 0 (i.e., $\nabla s(X, \boldsymbol{z}) \cdot \boldsymbol{v} = 0$). Thus $\nabla s(X, \boldsymbol{z})$ is orthogonal to $\Pi(\mathcal{A})$ at $\boldsymbol{z}$. Since $\Pi(\mathcal{A})$ has dimension $n - p - 1$, $\nabla s(X, \boldsymbol{z})$ gives the unique (up to scaling and reversing direction) normal in the $n - p$ dimensional $\mathcal{C}^{\perp}(X)$. □

Proof of Lemma 3.3

Proof. Without loss of generality, assume the columns of X form an orthonormal basis for $\mathcal{C}(X)$ and likewise the columns of W form and orthonormal basis for $\mathcal{C}^{\perp}(X)$. With earlier notation, $H = XX^{\top}$ and $Q = WW^{\top}$. The set $\mathcal{A}$ is defined by the $p + 1$ equations $s(X, \boldsymbol{y}) = s(X, \boldsymbol{y}_{obs})$, $b_1(X, \boldsymbol{y}) = b_1(X, \boldsymbol{y}_{obs}), \ldots, b_p(X, \boldsymbol{y}) = b_p(X, \boldsymbol{y}_{obs})$. Consequently, the gradients are orthogonal to $\mathcal{A}$. Let $\nabla \boldsymbol{b}(X, \boldsymbol{y})$ denote the $n \times p$ matrix with columns $\nabla b_1(X, \boldsymbol{y}), \ldots, \nabla b_p(X, \boldsymbol{y})$. We seek to show the $n \times (p + 1)$ matrix $[\nabla \boldsymbol{b}(X, \boldsymbol{y}), \nabla s(X, \boldsymbol{y})]$ has rank $p + 1$. Using property C5, we have that

$$\boldsymbol{b}(X, \boldsymbol{y}) = \boldsymbol{b}(X, Q\boldsymbol{y} + H\boldsymbol{y}) = \boldsymbol{b}(X, Q\boldsymbol{y}) + X^{\top}\boldsymbol{y}$$

Then $\nabla \boldsymbol{b}(X, \boldsymbol{y}) = Q \nabla \boldsymbol{b}(X, Q\boldsymbol{y}) + X$ and

$$[XX^{\top}, WW^{\top}]^{\top}[\nabla \boldsymbol{b}(X, \boldsymbol{y}), \nabla s(X, \boldsymbol{y})] = \begin{pmatrix} X & \mathbf{0} \\ WW^{\top}\nabla b(X, \boldsymbol{y}) & \nabla s(X, \boldsymbol{y}) \end{pmatrix} \tag{26}$$

The last column comes from Lemma 3.2. The matrix $[XX^{\top}, WW^{\top}]^{\top}$ is of full column rank (rank n), and so the rank of $[\nabla \boldsymbol{b}(X, \boldsymbol{y}), \nabla s(X, \boldsymbol{y})]$ is the same as the rank of the matrix on the right hand side of (26). This last matrix has rank $p + 1$ since $\nabla s(X, \boldsymbol{y}) \neq \mathbf{0}$ by C8, and so does $[\nabla b(X, \boldsymbol{y}), \nabla s(X, \boldsymbol{y})]$. □

Proof of Lemma 3.4

Proof. P is the projection of the columns of A onto $\mathcal{C}^{\perp}(X)$. For this to result in a loss of rank, a subspace of $\mathcal{T}_y(\mathcal{A})$ must belong to $\mathcal{C}(X)$. Following property C5, for

an arbitrary vector $X\boldsymbol{v} \in \mathcal{C}(X)$, $\boldsymbol{b}(X, \boldsymbol{y} + X\boldsymbol{v}) = \boldsymbol{b}(X, \boldsymbol{y}) + \boldsymbol{v}$. From the property, we can show that the directional derivative of $\boldsymbol{b}$ along $X\boldsymbol{v}$ with $\boldsymbol{v} \neq \mathbf{0}$ is $\boldsymbol{v}$, which is a nonzero vector. Hence $X\boldsymbol{v} \notin \mathcal{T}_y(\mathcal{A})$. □

Proof of Corollary 3.7

Proof. The corollary relies on a lemma and theorem from Miao and Ben-Israel (1992) which we restate slightly for brevity of presentation. The principal angles between subspaces pluck off a set of angles between subspaces, from smallest to largest. The number of such angles is the minimum of the dimensions of the two subspaces. Miao and Ben-Israel's first result (their Lemma 1) connects these principal angles to a set of singular values, and hence to volumes.

Lemma 7.1. *(Miao, Ben-Israel) Let the columns of $Q_L \in \mathbb{R}^{n\times l}$ and $Q_M \in \mathbb{R}^{n\times m}$ form orthonormal bases for linear subspaces L and M respectively, with $l \leq m$. Let $\sigma_1 \geq \cdots \geq \sigma_l \geq 0$ be the singular values of $Q_M^\top Q_L$. Then $\cos\theta_i = \sigma_i, i = 1, \ldots, l$ where $0 \leq \theta_1 \leq \theta_2 \leq \cdots \leq \theta_l \leq \frac{\pi}{2}$ are the principal angles between L and M.*

Miao and Ben-Israel's second result (their Theorem 3) makes a match between the principal angles between a pair of subspaces and the principal angles between their orthogonal complements.

Theorem 7.2. *(Miao, Ben-Israel) The nonzero principal angles between subspace L and M are equal to the nonzero principal angles between $L^\perp$ and $M^\perp$.*

To establish the corollary, we appeal to Lemma 7.1 and Theorem 7.2. Translating Miao and Ben Israel's notation, we have $M = \mathcal{C}^\perp(X)$, $Q_M = W$, $L = \mathcal{T}_{\boldsymbol{y}}(\mathcal{A})$, and $Q_L = A$. By Theorem 7.2, the nonzero principal angles between $\mathcal{T}_{\boldsymbol{y}}(\mathcal{A})$ and $\mathcal{C}^\perp(X)$ are the same as the nonzero principal angles between $\mathcal{T}_{\boldsymbol{y}}^\perp(\mathcal{A})$ and $\mathcal{C}(X)$. By 7.1,

the non-unit singular values of $W^\top A$ are the same as the non-unit singular values of $U^\top B$. □

7.2 Setting the hierarchical prior values

In setting the priors we use the same previous data set used to set the priors for the non-hierarchical model (Section 5.2) and several heuristic arguments. While the analyses in Section 5.3 set the hyper-parameters using what is described here, the results were not sensitive to these choices. This section describes the heuristics used in setting these prior parameters and is given for completeness. Using the previous data set we fit separate (robust) regressions to each state and a regression to the ~~entire~~ entirety of the data at once. Let the estimates for the fits to each state be $\hat{\beta}_1, \ldots, \hat{\beta}_J, \hat{\sigma}_1, \ldots, \hat{\sigma}_J$ and the estimates from the single regression be $\hat{\beta}$ and $\hat{\sigma}$. These are classical robust estimates using Tukey's regression and Huber's scale. Let n_j denote the number of observations in the j^{th} state and set $n = \sum n_j$.

First, consider v_1 and v_2 in the prior $b \sim \text{beta}(v_1, v_2)$. In the hierarchical model (19), $b = 0$ implies all the $\boldsymbol{\beta}_j's$ are equal (no variation between states) and $b = 1$ implies the $\boldsymbol{\beta}_j's$ vary about μ_0 according to $\Sigma_0 = n \cdot \text{var}(\hat{\beta})$ (see Section 5.2). We seek a prior measure for what we think b should be. In other words, how much prior uncertainty should we allow in $\boldsymbol{\beta}$ as opposed to the uncertainty amongst the $\boldsymbol{\beta}_j's$? Using the prior fit, a measure for uncertainty for $\boldsymbol{\beta}$ is $\Sigma_{\hat{\beta}} = \text{var}(\hat{\beta})$, the estimate of the covariance from the single regression. For the $\boldsymbol{\beta}_j's$, take $\delta_j = \hat{\beta}_j - \hat{\beta}$ and set the prior uncertainty to $\Sigma_\delta = n^{-1} \sum n_j \delta_j \delta_j^\top$. Consider the value $g = \left(|\Sigma_\delta| / |\Sigma_{\hat{\beta}}| \right)^{1/p}$. Heuristically, g is measure of the amount of uncertainty between the $\boldsymbol{\beta}_j's$ to the amount of uncertainty in $\boldsymbol{\beta}$. Now in the prior, we heuristically set the uncertainty in the $\boldsymbol{\beta}_j's$ ($b\Sigma_0$) to be approximately equal to $g \cdot \text{var}(\hat{\beta})$. That is, $b\Sigma_0 \approx g \cdot \text{var}(\hat{\beta}) = \frac{g}{n}\Sigma_0$, suggesting $b \approx \frac{g}{n}$. Hence we set $E[b] = \frac{g}{n}$. The precision, $v_1 + v_2$, is set to be relatively high at 20,

completing the specification for the prior on b.

In setting the parameters for the beta prior on μ_ρ and gamma prior on ψ_ρ we first take $\hat{z}_j = \Phi^{-1}(H(\hat{\sigma}_j^2))$. As in the prior we assume $(\hat{z}_1, \ldots, \hat{z}_J) \sim N_J(\mathbf{0}, \Sigma_\rho)$ with $\Sigma_\rho = (1-\rho)I + \rho\mathbf{1}\mathbf{1}^\top$ and find the MLE, $\hat{\rho}_{mle}$, and observed inverse Fisher information, $I^{-1}(\rho_{mle})$. The mean of the beta prior on μ_ρ is set to $\hat{\rho}_{mle}$. Its variance is inflated somewhat and set to $2I^{-1}(\hat{\rho}_{mle})$. Since $\text{var}(\rho|\mu_\rho, \psi_\rho) = \mu_\rho(1-\mu_p)/(\psi_\rho+1)$ we replace μ_ρ with $\hat{\rho}_{mle}$, $\text{var}(\rho|\mu_\rho, \psi_\rho)$ with $2I^{-1}(\hat{\rho}_{mle})$, and set the mean of the gamma prior on ψ_ρ equal to $\hat{\rho}_{mle}(1-\hat{\rho}_{mle})/(2I^{-1}(\hat{\rho}_{mle})) - 1$. Finally, we arbitrarily set the variance of the gamma prior to be approximately the same as the mean.

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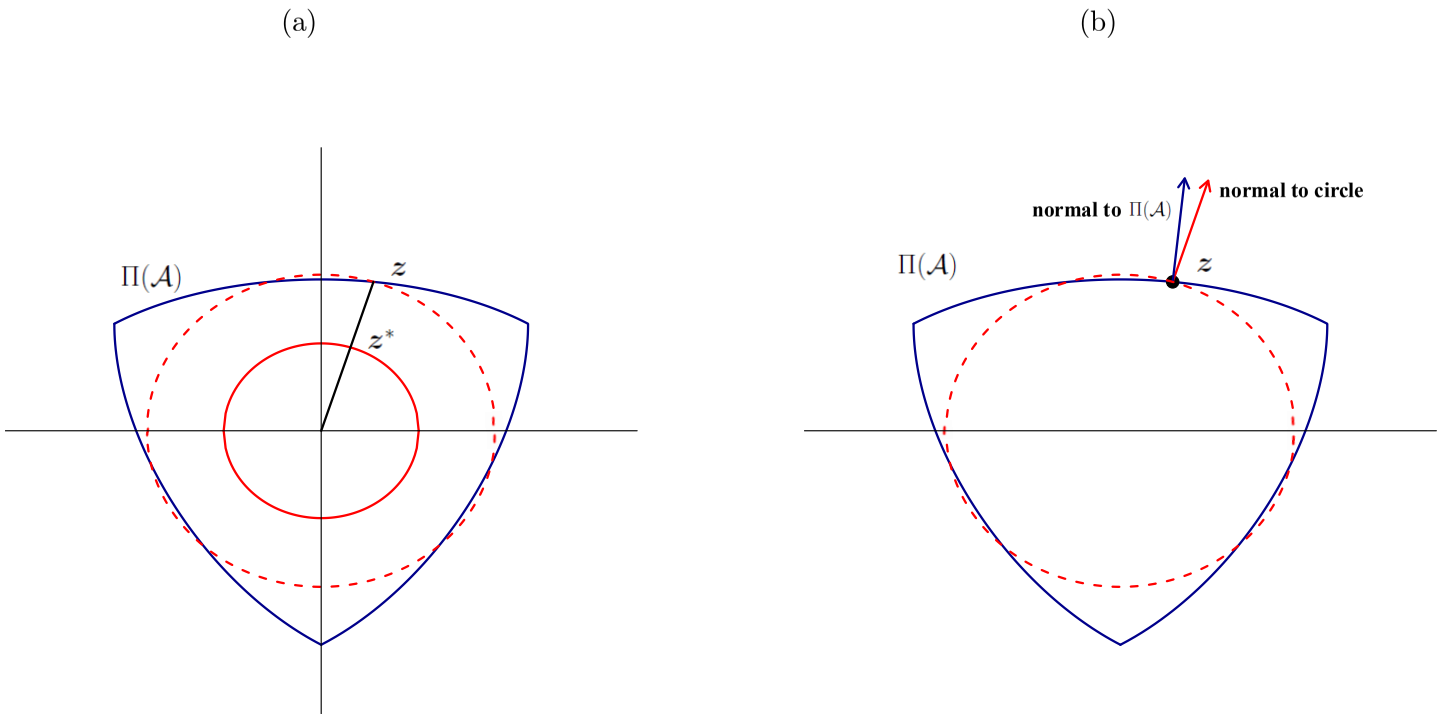


Figure 3: Panel (a) contains a depiction of the stretch from $\boldsymbol{z}^*$ to $\boldsymbol{z}$. The adjustment for the stretch transforms the density along the unit circle to the density along the circle of radius $\|\boldsymbol{z}\|$ (dashed circle). Panel (b) contains a depiction of the deformation from the distribution along the circle to the distribution along $\Pi(\mathcal{A})$. The adjustment can be seen to be the cosine of the angle between the normals to each manifold.

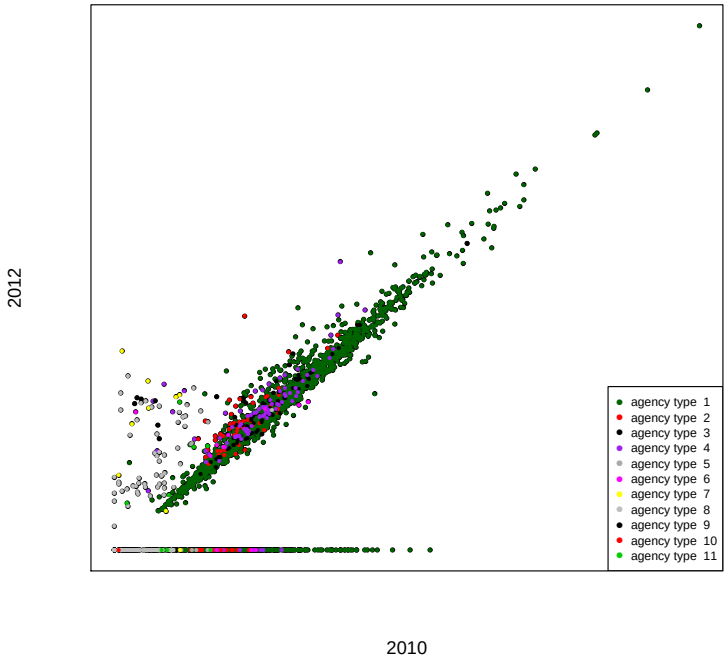
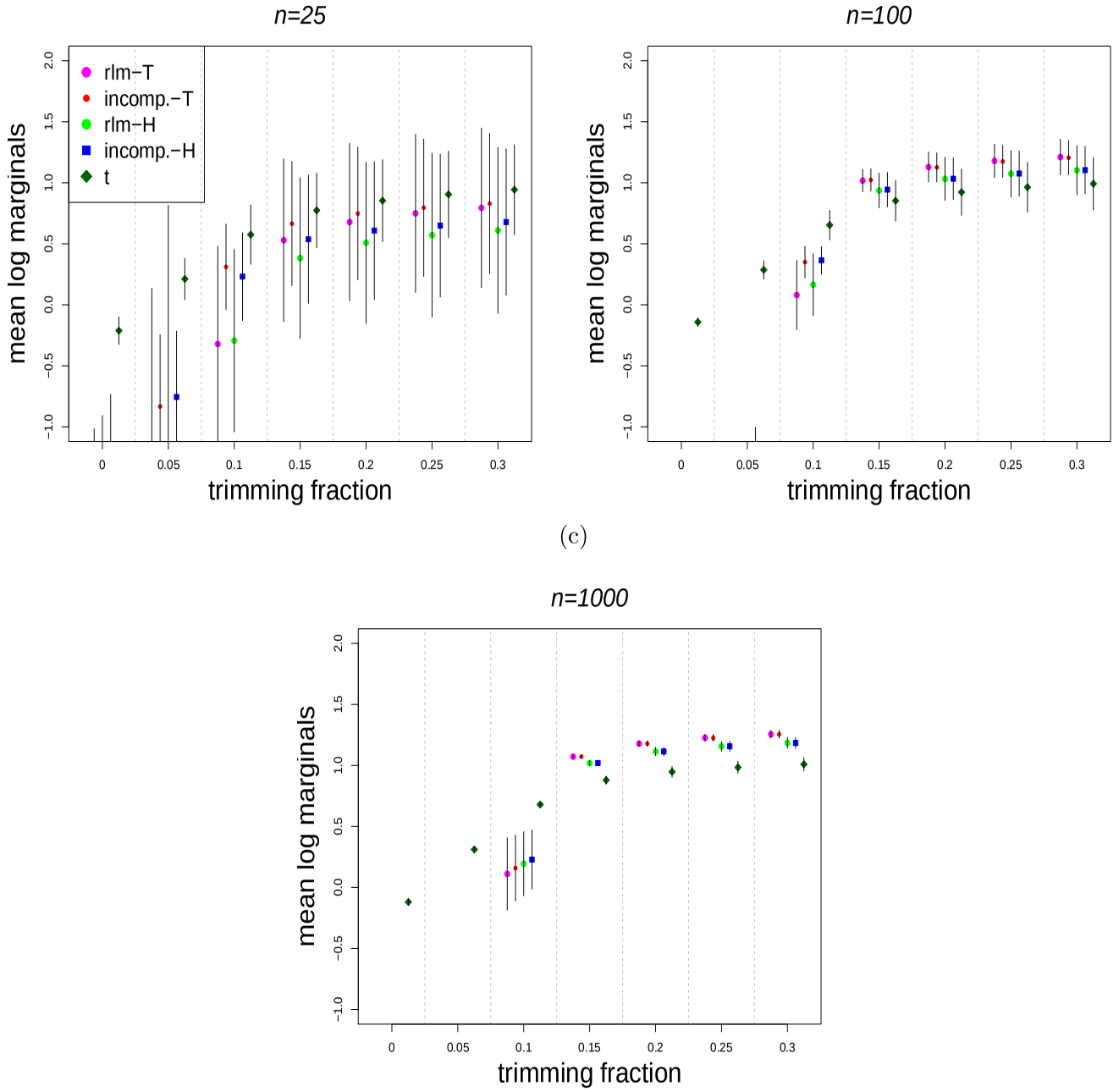


Figure 4: The square root of count in 2012 versus that in 2010 (after centering and scaling). The colors represent the varying contractual agreements as they stood in 2010. Agencies that closed during the 2010-2012 period are represented by the zero counts for 2012. Scalings on the axes are purposely left off for proprietary reasons.



(c)

Figure 5: Model evaluation for 'Type 1' agencies for training sample sizes of $n = 25, 100$, and 1000. The t-model is used as the base method to compute TLM. Plotted are the mean TLM for each model against the trimming fraction across the 100 cross-validation samples. Error bars correspond to one standard deviation of TLM above and below the mean. Models are labeled with the following abbreviations: 'rlm' corresponds to a classical robust fit, 'restr.' corresponds to our restricted likelihood method, and 't' corresponds to the heavy-tailed t-distribution model. The letters 'T' and 'H' appearing after 'rlm' and 'restr.' correspond to the use of Tukey's and Huber's ψ respectively.

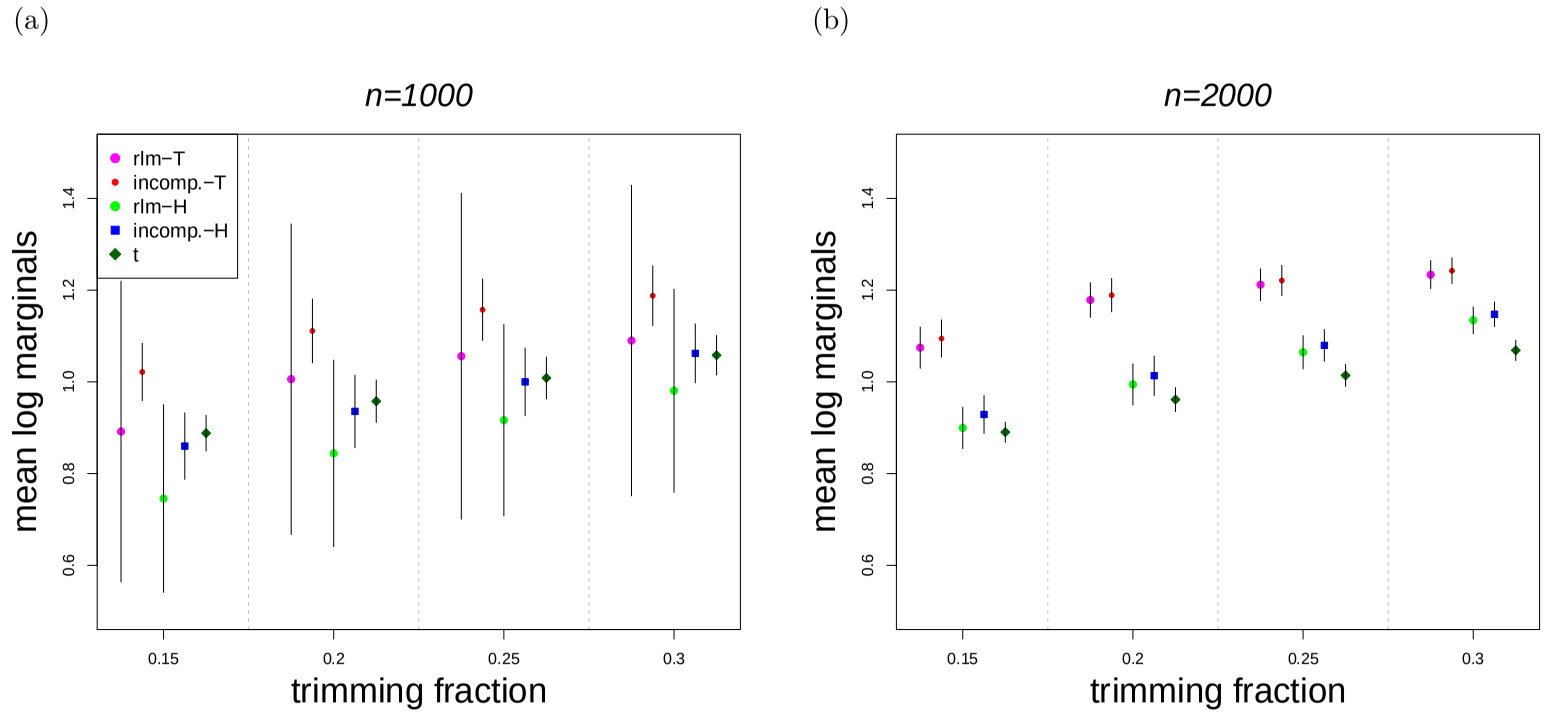


Figure 6: Model evaluation for 'Type 1' agencies under the hierarchical model for $n = 1000$ and 2000. The t-model is used as the base method to compute TLM. Plotted are the mean TLM for each model against the trimming fraction across the 100 cross-validation samples. Error bars correspond to one standard deviation of TLM above and below the mean. Models are labeled using the same notation as the previous figure. Only the relevant trimming fractions ($\alpha \geq .15$) are pictured.