

# 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 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 choices, 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.

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\*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.

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**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](#)) and 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 focus of this work is the development of techniques to handle imperfections in the likelihood. 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 mixture model likelihood to obtain the complete-data posterior distribution and 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](#)).

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. Rather than driving the move from prior to posterior by the full likelihood, we use only the likelihood driven by a few summary statistics which typically target inferential quantities of interest. We call this likelihood a restricted because conditioning is done on a restricted set of data; the set which satisfies the observed summary statistics. This is a formal update of the prior 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 remainder of the paper develops....

## 2 Restricted Likelihood

### 2.1 Examples

To describe the use of the restricted likelihood, we begin with a pair of simple examples for the one-sample problem. For both, the model takes the data  $\mathbf{y} = (y_1, \dots, y_n)$  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, likelihood is  $L(\boldsymbol{\theta}|\mathbf{y}) = \prod_{i=1}^n f(y_i|\boldsymbol{\theta})$ .

The first example considers the case where a known subset of the data are known to be bad in the sense of not informing us about  $\boldsymbol{\theta}$ . This case mimics the setting where outliers are identified and discarded before doing a formal analysis. 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  $L(\boldsymbol{\theta}|y_1, \dots, y_{n-k}) = \prod_{i=1}^{n-k} f(y_i|\boldsymbol{\theta})$ . For an equivalent analysis, we rewrite the full likelihood as the product of two pieces:

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

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

The 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 and large reaction times are physiologically implausible; explained by either anticipation or lack of attention of the subject. 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  $L(\boldsymbol{\theta}|c(\mathbf{y}))$ . Letting  $g(t_1|\boldsymbol{\theta}) = F(t_1|\boldsymbol{\theta})$ ,  $g(t_2|\boldsymbol{\theta}) = 1 - F(t_2|\boldsymbol{\theta})$ , and  $g(y|\boldsymbol{\theta}) = f(y|\boldsymbol{\theta})$  for  $y \in (t_1, t_2)$ , we may rewrite the full likelihood as the product of two pieces

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

Only the first part is retained the analysis. Several more examples are detailed in [Lewis \(2014\)](#).

## 2.2 Generalization

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

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

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

Bayesian methods can make use of a restricted likelihood since  $T(\mathbf{y})$  is a well-defined random variable with a probability distribution indexed by  $\boldsymbol{\theta}$ . This leads to the restricted likelihood posterior

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

where  $m(T(\mathbf{y}))$  is the marginal distribution of  $T(\mathbf{y})$  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

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

## 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. \(2012\)](#) make use order statistics and robust estimators for  $T(\mathbf{y})$  in the location-scale setting. 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  $T(\mathbf{y})$  and update to the ABC posterior by using the likelihood  $L(\boldsymbol{\theta}|\mathcal{B}(\mathbf{y}))$ , where  $\mathcal{B}(\mathbf{y}) = \{\mathbf{y}^* | \rho(T(\mathbf{y}), T(\mathbf{y}^*)) < \epsilon\}$ ,  $\rho$  is a metric, and  $\epsilon$  is a tolerance level. This is the likelihood “conditioned” on the collection of data sets which result in a  $T(\cdot)$  within  $\epsilon$  of the observed  $T(\mathbf{y})$ . With an approximately sufficient  $T(\cdot)$  and a small enough  $\epsilon$ , heuristically  $L(\boldsymbol{\theta}|\mathcal{B}(\mathbf{y})) \approx L(\boldsymbol{\theta}|T(\mathbf{y})) \approx L(\boldsymbol{\theta}|\mathbf{y})$ . Consequently, the ABC posterior approximates the full data posterior and 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  $\mathbf{y}$ . However, we specifically seek to condition on an insufficient statistic to guard against misspecification in parts of the likelihood. Additionally, we develop methods where the conditioning is exact (i.e.  $\epsilon = 0$ ).

This work extends the development of Bayesian restricted likelihood by arguing that deliberate choice of  $T(\mathbf{y})$  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.

### 3 Illustrative Examples

Before discussing computational details, the method is applied to two simple examples on well known data sets to demonstrate its effectiveness in situations where outliers are a major concern. The full model in each case fits into the Bayesian linear regression framework discussed in [Section 4](#).

The first example is an analysis of Simon Necomb’s 66 measurements of the speed of light; two of which are significant outliers in the lower tail. The full model is a standard location-scale Bayesian model:

$$\beta \sim N(23.6, 2.04^2), \sigma^2 \sim IG(5, 10), y_i \stackrel{iid}{\sim} N(\beta, \sigma^2), i = 1, 2, \dots, n = 66, \quad (6)$$

where  $y_i$  denotes the  $i^{th}$  measurement of the passage time of light.  $\beta$  is interpreted as the passage time of light with  $\sigma^2$  representing measurement error. Four versions of the restricted likelihood are fit with conditioning statistics: 1) Huber's M-estimator for location with Huber's 'proposal 2' for scale 2) Tukey's M-estimator for location with Huber's 'proposal 2' for scale 3) LMS (least median squares) for location with associated estimator of scale and 4) LTS (least trimmed squares) for location with associated estimator of scale. Associated tuning parameters for the M-estimators are chosen to achieve 95% efficiency under normality (Huber and Ronchetti, 2009) and for comparability, roughly 5% of the residuals are trimmed for LTS. Additionally, two other common approaches to outlier handling are fit: 1) replacing the normal distribution with a t-distribution and, 2) replacing the normal distribution with a mixture of two normals. The t-model assumes  $y_i \stackrel{iid}{\sim} t_\nu(\beta, \sigma^2)$  with  $\nu = 5$ . The prior on  $\sigma^2$  is  $IG(5, \frac{\nu-2}{\nu}10)$  so the prior on the variance is the same as the other models. The mixture takes the form:  $y_i \stackrel{iid}{\sim} pN(\beta, \sigma^2) + (1-p)N(\beta, 10\sigma^2)$  assuming the prior  $p \sim \beta(20, 1)$  on the probability of belonging to the 'good' component.

The posteriors of  $\beta$  under each model appear in Figure 1. As expected, the posterior under the normal model is pulled downward by the two outliers while the heavy tailed model provides robustness against them. The restricted likelihood methods using the M-estimators and LTS statistics also achieve robustness against the outliers. Conditioning on LMS however, results in a posterior similar to the one under the normal model. The M-estimators provide the most precise posteriors in this case. This is reflected in more precise predictions than the heavy-tailed and mixture model as illustrated by the predictive distributions displayed in Figure ??.

As a second example, a data set measuring the number of telephone calls in Belgium from 1950-1973 is analyzed. The outliers in this case are due to a change in units on which calls were recorded for part of the dataset. The full model is a standard normal Bayesian linear regression:

$$\beta \sim N_2(\mu_0, \Sigma_0), \sigma^2 \sim IG(a, b), \mathbf{y} \sim N(X\beta, \sigma^2 I), \quad (7)$$

where  $\beta = (\beta_0, \beta_1)^\top$ ,  $\mathbf{y}$  is the vector of the logarithm of the number of calls, and  $X$  is the  $n \times 2$  design matrix. Prior parameters are fixed via a fit to the first 3 data points. In particular,  $\Sigma_0 =$

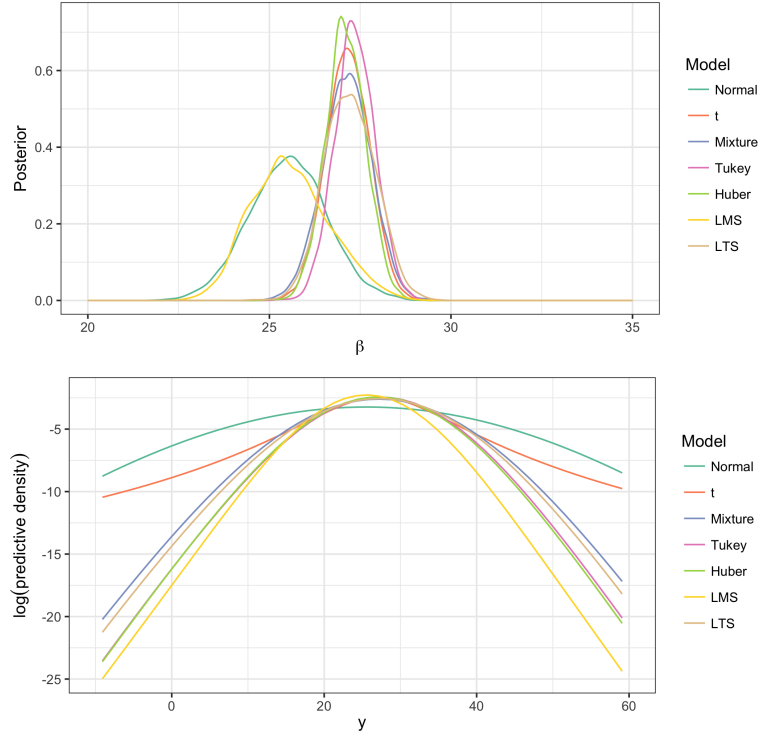


Figure 1: asdfdfa

$g\sigma_0^2(X^\top X)^{-1}$ , with  $\sigma_0 = 0.03$  and  $\mu_0 = (1.87, 0.03)^\top$ ; the MLEs fit to the first three data points. There are  $n = 21$  remaining data points and the parameter  $g$  is set to 21 reflecting a unit information prior (Kass and Wasserman, 1995). Finally  $a = 2$  and  $b = 1$  for the normal theory and restricted likelihood models.

Four models are compared: 1) the normal theory base model 2) A two component normal mixture model, 3) a t-model, and 4) a restricted likelihood model conditioning on Tukey's M-estimator for the slope and intercept with Huber's 'proposal 2' for scale. The mixture model assumes different mean regression functions and variances for each component, but keeps the same, relatively non-informative priors. The probability of belonging to the first component is given a  $\beta(5, 1)$  prior. The heavy-tailed model fixes the degrees of freedom to 5 with the same adjustment to the prior on  $\sigma^2$  as above.



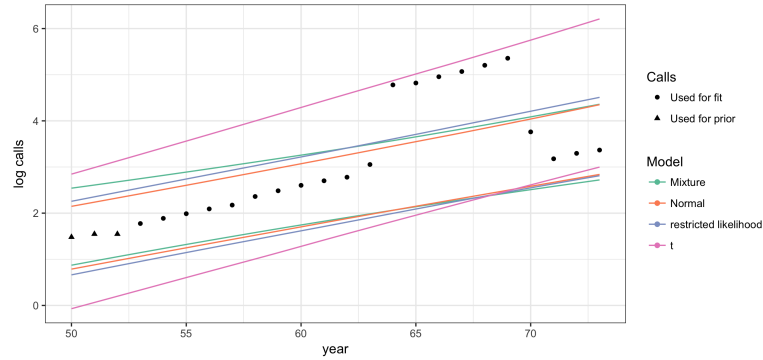


Figure 2: Predictive distribution of  $\log(\text{calls})$  under the Normal theory model fit to the non-outliers, the restricted likelihood model with Tukey’s M-estimator for the slope and intercept with Huber’s ‘proposal 2’ for scale, and a heavy-tailed t-distribution model. The first three data points were used to specify the prior with the remaining points used in the posterior fits. See details in the Appendix.

The data and 95% credible bands of the posterior predictive distribution under each model are displayed in Figure 2. The normal theory model is only fit to the obvious non-outlying points. Since the t-model assumes the data are heavy-tailed, the posterior predictive distribution is much wider. On the other hand, the predictive distribution under the restricted likelihood approach is much more precise and is close to that of the normal theory fit that discards the outliers. It is also close to the two component mixture results where the predictive distribution is formulated using only the good component. The mixture model involves explicitly modeling the outlier generating mechanism. In more more complex situations where the outlier generating mechanism is transient (i.e. ever changing and more complex than just a unit error in the recording), modeling the outliers becomes more difficult. Like classical robust estimation, the restricted likelihood approach avoids explicitly modeling the outliers.

## 4 Restricted Likelihood for the Linear Model

The simple examples in the previous section highlight that productive use of the restricted likelihood relies on a good choice of  $T(\mathbf{y})$ . This work focuses on robustness in linear models where natural choices include many used above: 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  $T(\mathbf{y})$  and parameters  $\boldsymbol{\theta}$ , direct computational strategies described in Lewis (2014) can be used to estimate the restricted posterior conditioned on essentially any statistic. These strategies rely on density estimation  $f(T(\mathbf{y})|\boldsymbol{\theta})$  using samples of  $T(\mathbf{y})$  for many values of  $\boldsymbol{\theta}$ ; a strategy which breaks down in higher dimensions. This section outlines a data-augmented MCMC algorithm that can be applied to the Bayesian linear model when  $T(\mathbf{y})$  consists of estimates of the regression coefficients and scale parameter.

#### 4.1 The Bayesian linear model

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

$$\begin{aligned}\boldsymbol{\theta} &= (\boldsymbol{\beta}, \sigma^2) \sim \pi(\boldsymbol{\theta}) \\ y_i &= \mathbf{x}_i^\top \boldsymbol{\beta} + \epsilon_i, \text{ for } i = 1, \dots, n\end{aligned}\tag{8}$$

where  $x_i$  and  $\boldsymbol{\beta} \in \mathbb{R}^p$ ,  $\sigma^2 \in \mathbb{R}^+$ , and the  $\epsilon_i$  are independent draws from a distribution with center 0 and scale  $\sigma$ .  $X$  denotes the design matrix whose rows are  $x_i^\top$ .

For the restricted likelihood model, conditioning statistics are assumed to be of the form  $T(\mathbf{y}) = (\mathbf{b}(X, \mathbf{y}), s(X, \mathbf{y}))$  where  $\mathbf{b}(X, \mathbf{y}) = (b_1(X, \mathbf{y}), \dots, b_p(X, \mathbf{y}))^\top \in \mathbb{R}^p$  is an estimator for the regression coefficients and  $s(X, \mathbf{y}) \in \{0\} \cup \mathbb{R}^+$  is an estimator of the scale. Throughout, observed data and summary statistic is denoted by  $\mathbf{y}_{obs}$  and  $T(\mathbf{y}_{obs}) = (\mathbf{b}(X, \mathbf{y}_{obs}), s(X, \mathbf{y}_{obs}))$ , respectively. Several conditions are imposed on the model and statistic to ensure validity of the MCMC algorithm:

- C1.** The  $n \times p$  design matrix,  $X$ , whose  $i^{th}$  row is  $x_i^\top$ , is of full column rank.
- C2.** The  $\epsilon_i$  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.
- C3.**  $\mathbf{b}(X, \mathbf{y})$  is almost surely continuous and differentiable with respect to  $\mathbf{y}$ .
- C4.**  $s(X, \mathbf{y})$  is almost surely positive, continuous, and differentiable with respect to  $\mathbf{y}$ .

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

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

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

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

Properties **C5** and **C6** of  $\mathbf{b}$  are called *regression* and *scale equivariance*, respectively. Properties **C7** and **C8** of  $s$  are called *regression invariance* and *scale equivariance*. Many estimators satisfy the above properties, including simultaneous M-estimators (Huber and Ronchetti, 2009; Maronna et al., 2006) for which the R package `brlm` ([github.com/jrlewi/brlm](https://github.com/jrlewi/brlm)) is available to implement the MCMC described here. Further software development is required to extend the MCMC implementation beyond these M-estimators. The package also implements the direct computational methods described in Lewis (2014). These methods are effective in lower dimensional problems and were used in several of the examples in Section 3.

## 4.2 Computational strategy

The general style of algorithm we present is a data augmented MCMC targeting  $f(\boldsymbol{\theta}, \mathbf{y} | T(\mathbf{y}) = T(\mathbf{y}_{obs}))$ , the joint distribution of  $\boldsymbol{\theta}$  and the full data given the summary statistic  $T(\mathbf{y}_{obs})$ . The Gibbs sampler (Gelfand and Smith, 1990) iteratively samples from the full conditionals 1)  $\pi(\boldsymbol{\theta} | \mathbf{y}, T(\mathbf{y}) = T(\mathbf{y}_{obs}))$  and 2)  $f(\mathbf{y} | \boldsymbol{\theta}, T(\mathbf{y}) = T(\mathbf{y}_{obs}))$ . When  $\mathbf{y}$  has the summary statistic  $T(\mathbf{y}) = T(\mathbf{y}_{obs})$ , the first full conditional is the same as the full data posterior  $\pi(\boldsymbol{\theta} | \mathbf{y})$ . In this case, the condition  $T(\mathbf{y}) = T(\mathbf{y}_{obs})$  is redundant. This allows us to make use of conventional MCMC steps for this generation. For typical regression models, algorithms abound. Details of the recommended algorithms depend on details of the prior distribution and sampling density and we assume this can be done (see e.g., Liu, 1994; Liang et al., 2008).

For a typical model and conditioning statistic, the second full conditional  $f(\mathbf{y} | \boldsymbol{\theta}, T(\mathbf{y}) = T(\mathbf{y}_{obs}))$  is not available in closed form. We turn to Metropolis-Hastings (Hastings, 1970), using the strategy

of proposing full data  $\mathbf{y} \in \mathcal{A} := \{\mathbf{y} \in \mathbb{R}^n | T(\mathbf{y}) = T(\mathbf{y}_{obs})\}$  from a well defined distribution with support  $\mathcal{A}$  and either accepting or rejecting the proposal. Let  $\mathbf{y}_p, \mathbf{y}_c \in \mathcal{A}$  represent the proposed and current full data, respectively. Denote the proposal distribution for  $\mathbf{y}_p$  by  $p(\mathbf{y}_p | \boldsymbol{\theta}, T(\mathbf{y}_p) = T(\mathbf{y}_{obs})) = p(\mathbf{y}_p | \boldsymbol{\theta}, \mathbf{y}_p \in \mathcal{A}) = p(\mathbf{y}_p | \boldsymbol{\theta})$ . The last equality follows from the fact that our  $p(\cdot | \boldsymbol{\theta})$  assigns probability one to the event  $\{\mathbf{y}_p \in \mathcal{A}\}$ . These equalities still hold if the dummy argument  $\mathbf{y}_p$  is replaced with  $\mathbf{y}_c$ . The conditional density is

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

for  $\mathbf{y} \in \mathcal{A}$ . This includes both  $\mathbf{y}_p$  and  $\mathbf{y}_c$ . The Metropolis-Hastings acceptance probability is the minimum of 1 and  $R$  where,

$$R = \frac{f(\mathbf{y}_p | \boldsymbol{\theta}, \mathbf{y}_p \in \mathcal{A}) p(\mathbf{y}_c | \boldsymbol{\theta}, \mathbf{y}_c \in \mathcal{A})}{f(\mathbf{y}_c | \boldsymbol{\theta}, \mathbf{y}_c \in \mathcal{A}) p(\mathbf{y}_p | \boldsymbol{\theta}, \mathbf{y}_p \in \mathcal{A})} \quad (9)$$

$$= \frac{f(\mathbf{y}_p | \boldsymbol{\theta})}{\int_{\mathcal{A}} f(\mathbf{y} | \boldsymbol{\theta}) d\mathbf{y}} \frac{\int_{\mathcal{A}} f(\mathbf{y} | \boldsymbol{\theta}) d\mathbf{y}}{f(\mathbf{y}_c | \boldsymbol{\theta})} \frac{p(\mathbf{y}_c | \boldsymbol{\theta})}{p(\mathbf{y}_p | \boldsymbol{\theta})} \quad (10)$$

$$= \frac{f(\mathbf{y}_p | \boldsymbol{\theta}) p(\mathbf{y}_c | \boldsymbol{\theta})}{f(\mathbf{y}_c | \boldsymbol{\theta}) p(\mathbf{y}_p | \boldsymbol{\theta})}. \quad (11)$$

For the models we consider, evaluation of  $f(\mathbf{y} | \boldsymbol{\theta})$  is straightforward. Therefore, the difficulty in implementing this Metropolis-Hastings step manifests itself in the ability to both simulate from and evaluate  $p(\mathbf{y}_p | \boldsymbol{\theta})$ ; the well defined distribution with support  $\mathcal{A}$ . We now discuss such an implementation method for the linear model in (8).

### Construction of the proposal

Our computational strategy relies on proposing  $\mathbf{y}$  such that  $T(\mathbf{y}) = T(\mathbf{y}_{obs})$  where  $T(\cdot) = (\mathbf{b}(X, \cdot), s(X, \cdot))$  satisfies the conditions C3-C8. It is not a simple matter to do this directly, but with the specified conditions, it is possible to scale and shift any  $\mathbf{z}^*$  which generates a positive scale estimate to such a  $\mathbf{y}$  via the following Theorem, whose proof is in the appendix.

**Theorem 4.1.** *Assume that conditions C4-C8 hold. Then, any vector  $\mathbf{z}^* \in \mathbb{R}^n$  with conditioning statistic  $T(\mathbf{z}^*)$  for which  $s(X, \mathbf{z}^*) > 0$  can be transformed into  $\mathbf{y}$  with conditioning statistic  $T(\mathbf{y}) =$*

$T(\mathbf{y}_{obs})$  through the transformation

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

Using the theorem, the general idea is to first start with an initial vector  $\mathbf{z}^*$  drawn from a known distribution, say  $p(\mathbf{z}^*)$ , and transform via  $h(\cdot)$  to  $\mathbf{y} \in \mathcal{A}$ . The proposal density  $p(\mathbf{y}|\boldsymbol{\theta})$  is then a change-of-variables adjustment on  $p(\mathbf{z}^*)$  derived from  $h(\cdot)$ . In general however, the mapping  $h(\cdot)$  is many-to-one: for any  $\mathbf{v} \in \mathbb{R}^n$  and any  $c \in \mathbb{R}^+$ ,  $c\mathbf{z}^* + X\mathbf{v}$  map to the same  $\mathbf{y}$ . This makes the change-of-variables adjustment difficult. We handle this point by first noticing that 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. Hence, we restrict the initial  $\mathbf{z}^*$  to an easily understood  $n - p - 1$  dimensional space. Specifically, this space is the unit sphere in the orthogonal complement of the column space of the design matrix:  $\mathbb{S} := \{\mathbf{z}^* \in \mathcal{C}^\perp(X) \mid \|\mathbf{z}^*\| = 1\}$ , where  $\mathcal{C}(X)$  and  $\mathcal{C}^\perp(X)$  are the column space of  $X$  and its orthogonal complement, respectively. With  $\mathbf{z}^* \in \mathbb{S}$ ,  $c\mathbf{z}^* + X\mathbf{v}$  is not (unless  $c = 1$  and  $\mathbf{v} = \mathbf{0}$ ); the scaling by  $c$  and/or the affine transformation in the direction of  $\mathcal{C}(X)$  takes the point off  $\mathbb{S}$ . The mapping  $h : \mathbb{S} \rightarrow \mathcal{A}$  is one-to-one making the change of variables more feasible.

With the domain of  $h(\cdot)$  restricted to  $\mathbb{S}$ , the range is still the entirety of  $\mathcal{A}$ . This is important so that the support of the proposal distribution (which is the range of  $h(\cdot)$ ) contains the support of the target  $f(\mathbf{y}|\boldsymbol{\theta}, \mathbf{y} \in \mathcal{A})$ ; a necessary condition for convergence of the Metropolis-Hastings algorithm (in this case the supports are both  $\mathcal{A}$ ). To see that the range of  $h(\cdot)$  is  $\mathcal{A}$ , consider any  $\mathbf{y} \in \mathcal{A}$  and its projection onto  $\mathcal{C}^\perp(X)$ :  $Q\mathbf{y}$  where  $Q = I - XX^\top$ .<sup>1</sup> It is easy to show that  $\mathbf{z}^* = Q\mathbf{y}/\|Q\mathbf{y}\| \in \mathbb{S}$  and  $h(\mathbf{z}^*) = \mathbf{y}$ .

Given the one-to-one and onto mapping  $h : \mathbb{S} \rightarrow \mathcal{A}$ , the general proposal strategy is summarized as follows:

1. Sample  $\mathbf{z}^*$  from a distribution with known density on  $\mathbb{S}$ .

---

<sup>1</sup>We have used condition C1 to assume without loss of generality that the columns of  $X$  form an orthonormal basis for  $\mathcal{C}(X)$  (i.e.,  $X^\top X = I$ ).

2. Set  $\mathbf{y} = h(\mathbf{z}^*)$  and calculate the Jacobian of this transformation in two steps.

- (a) Scale from  $\mathbb{S}$  to the set  $\Pi(\mathcal{A}) := \{\mathbf{z} \in \mathbb{R}^n \mid \exists \mathbf{y} \in \mathcal{A} \text{ s.t. } \mathbf{z} = Q\mathbf{y}\}$ .  $\Pi(\mathcal{A})$  is the projection of  $\mathcal{A}$  onto  $\mathcal{C}^\perp(X)$  and, by condition C7, every element of this set has  $s(X, \mathbf{z}) = s(X, \mathbf{y}_{obs})$ . Specifically, set  $\mathbf{z} = \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*$ . There are two pieces of this Jacobian: one for the scaling and one for the mapping of the sphere onto  $\Pi(\mathcal{A})$ . The latter piece is given in equation (12).
- (b) Shift from  $\Pi(\mathcal{A})$  to  $\mathcal{A}$ :  $\mathbf{y} = \mathbf{z} + X(\mathbf{b}(X, \mathbf{y}_{obs}) - \mathbf{b}(X, \mathbf{z}))$ . This shift is along the column space of  $X$  to the unique element in  $\mathcal{A}$ . The Jacobian of this transformation is given by equation (13).

The final proposal distribution including the complete Jacobian is given in equation (14) with details in the next section. Before giving these details we provide a visualization in Figure 3 of each of the sets described above to aid in the understanding of the strategy we are taking. In the figure,  $n = 3$ ,  $p = 1$ , and the conditioning statistic is  $T(\mathbf{y}) = (\min(\mathbf{y}), \sum (y_i - \min(\mathbf{y}))^2)$ . The set  $\mathcal{A}$  is depicted for  $T(\mathbf{y}_{obs}) = (0, 1)$  which we describe as a “warped triangle” in light blue, with each side corresponding to a particular coordinate of  $\mathbf{y}$  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 this example, the column vector  $X = \mathbf{1}$  (shown as a reference) spans  $\mathcal{C}(X)$  and  $\mathbb{S}$  is a unit circle on the orthogonal plane (shown in red).  $\Pi(\mathcal{A})$  is depicted as the bowed triangle in dark blue. We will come back to this artificial example in the next section in an attempt to visualize the Jacobian calculations.

### Evaluation of the proposal density

We now explain each step in computing the Jacobian described above.

#### Scale from $\mathbb{S}$ to $\Pi(\mathcal{A})$

The first step is constrained to  $\mathcal{C}^\perp(X)$  and scales the initial  $\mathbf{z}^*$  to  $\mathbf{z} = \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*$ . For the Jacobian, we consider two substeps: first, the distribution on  $\mathbb{S}$  is transformed to that along a sphere of radius

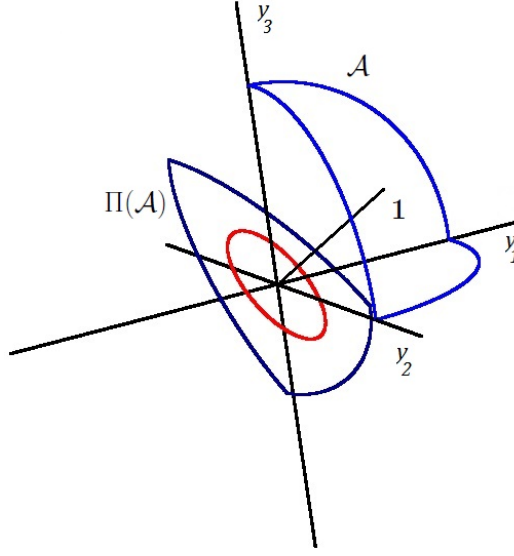


Figure 3: A depiction of  $\mathcal{A}$ ,  $\Pi(\mathcal{A})$ , and the unit circle for the illustrative example where  $b_1(\mathbf{1}, \mathbf{y}) = \min(\mathbf{y}) = 0$  and  $s(\mathbf{1}, \mathbf{y}) = \sum (y_i - b_1(\mathbf{1}, \mathbf{y}))^2 = 1$ .  $\mathcal{A}$  is the combination of three 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  $\mathbf{z}^*$ . Also depicted is the vector  $\mathbf{1}$ , the design matrix for the location and scale setting.

$r = \|\mathbf{z}\| = s(X, \mathbf{y}_{obs})/s(X, \mathbf{z}^*)$ . By comparison of the volumes of these spheres, this transformation contributes a factor of  $r^{-(n-p-1)}$  to the Jacobian. For the second substep, the sphere of radius  $r$  is deformed onto  $\Pi(\mathcal{A})$ . 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  $\mathbf{z}$ . Restricting to  $\mathcal{C}^\perp(X)$ , this ratio is the cosine of the angle between the normal vectors of the two sets at  $\mathbf{z}$ . The normal to the sphere is its radius vector  $\mathbf{z}$ . The normal to  $\Pi(\mathcal{A})$  is given in the following lemma.

**Lemma 4.2.** *Assume that conditions C1-C2, C4, and C7 hold and  $\mathbf{y} \in \mathcal{A}$ . Let  $\nabla s(X, \mathbf{y})$  denote the gradient of the scale statistic with respect to the data vector evaluated at  $\mathbf{y}$ . Then  $\nabla s(X, \mathbf{y}) \in \mathcal{C}^\perp(X)$  and is normal to  $\Pi(\mathcal{A})$  at  $\mathbf{z} = Q\mathbf{y}$  in  $\mathcal{C}^\perp(X)$ .*

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

$$\cos(\gamma) = \frac{\nabla s(X, \mathbf{y})^\top \mathbf{z}}{\|\nabla s(X, \mathbf{y})\| \|\mathbf{z}\|}, \quad (12)$$

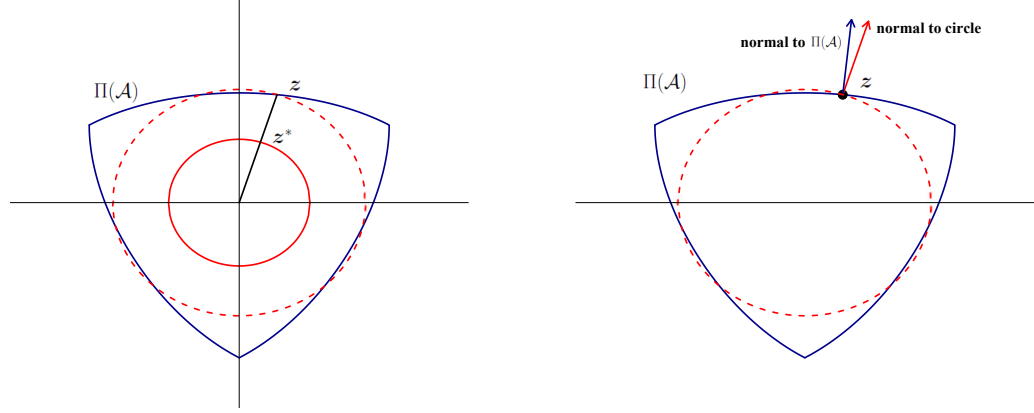


Figure 4: sdsfda

where  $\gamma$  is the angle between the two normal vectors. This step is visualized in Figure 4.2 for the artificial location-scale example. The figure pictures only the  $\mathcal{C}^\perp(X)$ , which in this case is a plane. The unit sphere (here, the solid circle) is 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.

#### 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  $\mathbf{z}$  to  $\mathbf{y}$  along the column space of  $X$ . Since the shift depends on  $\mathbf{z}$ , 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 volumes along  $\Pi(\mathcal{A})$  at  $\mathbf{z}$  to the corresponding volume along  $\mathcal{A}$  at  $\mathbf{y}$ . The ratio is calculated by considering the volume of the projection of a unit hypercube in the tangent space of  $\mathcal{A}$  at  $\mathbf{y}$  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  $\mathbf{y}$  and its orthogonal complement respectively. All gradients denote with  $\nabla$  are with respect to the data vector.



**Lemma 4.3.** *Assume that conditions C1-C5 and C7-C8 hold. Then the  $p + 1$  gradient vectors  $\nabla s(X, \mathbf{y}), \nabla b_1(X, \mathbf{y}), \dots, \nabla b_p(X, \mathbf{y})$  form a basis for  $\mathcal{T}_y^\perp(\mathcal{A})$  with probability one.*

The lemma describes construction of a basis for  $\mathcal{T}_y^\perp(\mathcal{A})$ , leading to a basis for  $\mathcal{T}_y(\mathcal{A})$ . Both of these bases can be orthonormalized. Let  $A = [a_1, \dots, a_{n-p-1}]$  and  $B = [b_1, \dots, b_{p+1}]$  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 4.4.** *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

$$\text{Vol}(P) := \sqrt{\det(P^\top P)} = \prod_{i=1}^r \sigma_i \quad (13)$$

where  $r = \text{rank}(P) = n - p - 1$  and  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$  are the singular values of  $P$  (e.g., Miao and Ben-Israel (1992)). Combining Lemmas 4.3 and 4.4 above leaves us with the following result concerning the calculation of the desired Jacobian.

**Theorem 4.5.** *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 (13).*

### 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 4.6.** *Assume that conditions C1-C8 hold. Let  $\mathbf{z}^*$  be sampled on the unit sphere in  $\mathcal{C}^\perp(X)$  with density  $p(\mathbf{z}^*)$ . Using the transformation of  $\mathbf{z}^*$  to  $\mathbf{y} \in \mathcal{A}$  described in Theorem 4.1, the density of  $\mathbf{y}$  is*

$$p(\mathbf{y}) = p(\mathbf{z}^*) r^{-(n-p-1)} \cos(\gamma) \text{Vol}(P) \quad (14)$$

where  $r = s(X, \mathbf{y}_{\text{obs}})/s(X, \mathbf{z}^*)$ , and  $\cos(\gamma)$  and  $\text{Vol}(P)$  are as in equations (12) and (13), respectively.

A few details for computing the needed quantities are worth further explanation. Computing  $\text{Vol}(P)$  involves finding an orthonormal matrix  $A$  whose columns span  $\mathcal{T}_y(\mathcal{A})$ . This matrix can be found by supplementing  $B$  with a set of  $n$  linearly independent columns on the right, and apply Gram-Schmidt orthonormalization. This is  $\mathcal{O}(n^3)$  and is infeasibly slow when  $n$  is large because it must be repeated at each iterate of the MCMC when a complete data set is drawn. However, using results related to *principal angles* found in [Miao and Ben-Israel \(1992\)](#) the volume (13) can be computed using only  $B$ .  $B$  is constructed by Gram-Schmidt orthogonalization of  $\nabla s(X, \mathbf{y}), \nabla b_1(X, \mathbf{y}), \dots, \nabla b_p(X, \mathbf{y})$ , which is  $\mathcal{O}(np^2)$ ; a considerable reduction in computational burden when  $n \gg p$ . The following corollary formally states how computation of  $A$  can be circumvented.

**Corollary 4.7.** *Let  $U$  be a matrix whose columns form an orthonormal basis for  $\mathcal{C}(X)$  and set  $Q = WW^\top$  where the columns of  $W$  form an orthonormal basis for  $\mathcal{C}^\perp(X)$ . Then the non-unit singular values of  $U^\top B$  are the same as the non-unit singular values of  $W^\top A$ .*

The lemma implies the  $\text{Vol}(P)$  is the product of the singular values of  $U^\top B$ .

Second, the gradients of  $\nabla s(X, \mathbf{y}), \nabla b_1(X, \mathbf{y}), \dots, \nabla b_p(X, \mathbf{y})$  are easily computed. For example, below we consider M-estimators defined by the estimating equations:

$$\begin{aligned} \sum_{i=1}^n \psi \left( \frac{y_i - x_i^\top \mathbf{b}(\mathbf{y}, X)}{s(\mathbf{y}, X)} \right) &= 0 \\ \sum_{i=1}^n \chi \left( \frac{y_i - x_i^\top \mathbf{b}(\mathbf{y}, X)}{s(\mathbf{y}, X)} \right) &= 0, \end{aligned} \tag{15}$$

where  $\psi$  and  $\chi$  are almost surely differentiable. Differentiating this system of equations with respect to each  $y_i$  can be used to find the gradients. In theory, finite differences could also be used.

## 5 Simulated Data

We study the performance of the restricted likelihood in a hierarchical setting contaminated with outliers. Specifically, simulated data come from the following data generating model:

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

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  $n_i = 25, 50, 100$ . This results in 90 groups that have varying levels of outlier contamination and sample size. We wish to build models that offer good prediction for the good portion of data within each group. The full model for fitting is a corresponding normal model without contamination:

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

For the restricted likelihood versions we condition on robust M-estimators of location and scale in each group:  $T_i(y_{i1}, \dots, y_{in_i}) = (\hat{\theta}_i, \hat{\sigma}_i^2), i = 1, 2, \dots, 90$ . These estimators are solutions to equation (15) (where  $x_i \equiv 1$ ) with user specified  $\psi$  and  $\chi$  functions designed to discount outliers. The two versions use Huber's and Tukey's  $\psi$  function, while both versions use Huber's  $\chi$  function. The tuning parameters associate with these functions are chosen so that the estimators are 95% efficient under normally distributed data. Both of these are well known M-estimators used in robust regression settings (Huber and Ronchetti, 2009).

To complete the specification of model (17),  $a_s$  and  $b_s$  are fixed to a variety of values representing different levels of prior knowledge. For each we set  $b_s = 4a_sc$  resulting in a prior mean for each  $\sigma_i^2$  of  $\frac{4ca_s}{a_s-1}$ ,  $a_s > 1$ . The precision is  $\frac{(a_s-1)^2(a_s-2)}{(4ca_s)^2}$ ; meaning the larger  $a_s$ , the more informative the prior. With  $c = 1$  the shrinkage (for large  $a_s$ ) is to the true value of  $\sigma^2 = 4$ . We consider  $a_s = 1.25, 5, 10$  and  $c = 0.5, 1, 2$ .

$K = 30$  data sets are generated from (16). For each data set and each pair  $(a_s, c)$ , the Bayesian models are fit using MCMC. The MCMC for the restricted likelihood version requires no further

computational details other than those described for the traditional Bayesian model in Section 4. This is because there are conditioning statistics for each group and the model's conditional independence between the groups allows the data augmentation described earlier to be performed independently within each group. That is, there is a separate Gibbs step for each group generating group level data matching the statistics for that group.

To assess the predictive capability, the models are compared using Kullback-Leibler (KL) divergence from the distribution of good data to the posterior predictive distribution. Specifically, for the  $i^{th}$  group of the  $k^{th}$  simulated data set  $\mathbf{y}_k$  compute:

$$KL_{ik}^{(M)} = \int \log \frac{f(\tilde{y}|\theta_i, \sigma^2)}{f_i(\tilde{y}|M, \mathbf{y}_k)} f(\tilde{y}|\theta_i, \sigma^2) dy \quad (18)$$

where  $M$  indexes the fitting model,  $f(\tilde{y}|\theta_i, \sigma^2) = N(\tilde{y}|\theta_i, \sigma^2)$ ; the mean  $\theta_i$ , variance  $\sigma^2$  normal pdf evaluated at  $\tilde{y}$ . For the Bayesian models  $f_i(\tilde{y}|M, \mathbf{y}_k) = \int f(\tilde{y}|\theta_i, \sigma_i^2) \pi(\theta_i, \sigma_i^2|M, \mathbf{y}_k) d\theta_i d\sigma_i^2$  where  $\pi(\theta_i, \sigma_i^2|M, \mathbf{y}_k)$  is the posterior for the  $i^{th}$  group model parameters under model  $M$  for the  $k^{th}$  data set.  $M$  denotes either the full normal theory model (17) or one of the two restricted likelihood versions, along with  $a_s$  and  $c$ . For the classical robust fits, we set  $f_i(\tilde{y}|M, \mathbf{y}_k) = N(\tilde{y}|\hat{\theta}_i, \hat{\sigma}_i^2)$  as a groupwise plug-in estimator for the predictive distribution. The classical fits are done separately for each group with no consideration of the hierarchical structure between the groups. The overall mean  $\overline{KL}_{..}^{(M)} = \frac{1}{90K} \sum_{k=1}^K \sum_{i=1}^{90} KL_{ik}^{(M)}$  is used to compare the models where smaller means correspond to better fits. Sampling variation is summarized with the standard error  $SE(\overline{KL}_{..}^{(M)}) = \sqrt{\frac{1}{K(K-1)} \sum_{k=1}^K (\overline{KL}_{.k}^{(M)} - \overline{KL}_{..}^{(M)})^2}$  where  $\overline{KL}_{.k}^{(M)} = \frac{1}{90} \sum_{i=1}^{90} KL_{ik}^{(M)}$ .

Figure 5 displays  $\overline{KL}_{..}^{(M)}$  with error-bars plus/minus one  $SE(\overline{KL}_{.k}^{(M)})$  for each  $a_s = 1.25, 5, 10$  and  $c = 0.5, 1, 2$ . The values of  $a_s$  and  $c$ , do not effect the classical robust linear models. The normal theory model results are left out as they perform significant worse. Overall, the results are strikingly in favor of the restricted likelihood methods for the range of hyper-parameter values studied. Undoubtably, the most precise and accurate prior studied is  $c = 1$  and  $a_s = 10$  and this results in the lowest (and best) average KL for both the Tukey and Huber restricted likelihood versions ((shown in the middle panel).  $c = 0.5$  performs the worst, but still better than the classical fits. There is evidence that performance starts to degrade as  $a_s = 10$  as reflected in a larger average

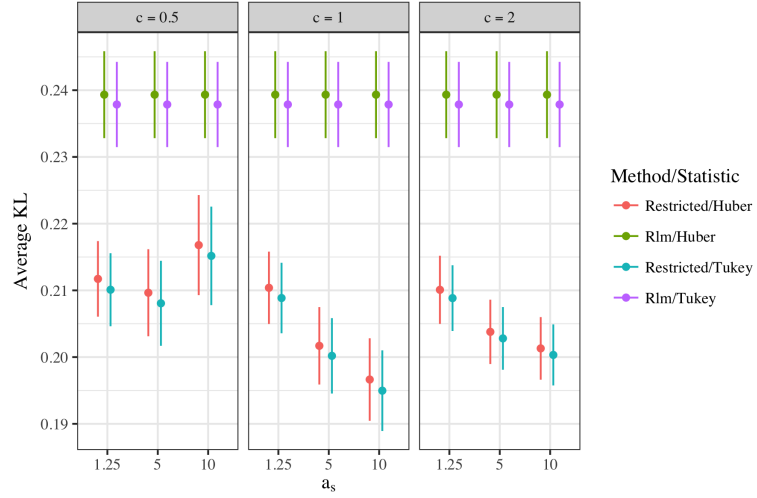


Figure 5: Average KL - divergence plus/minus one standard error for each value of  $a_s$  and  $c$ . The panels correspond to  $c = 0.5$  (left),  $c = 1$  (middle), and  $c = 2$  (right) with the values of  $a_s$  on the horizontal axis.

KL for  $a_s = 10$ . Here, the prior mean and precision are 2.22 and 1.62 and we suspect this is starting to put too much mass on  $\sigma_i^2$  values much smaller than  $\sigma^2 = 4$ . For  $c = 2$ , the performance still improves from  $a_s = 5$  to  $a_s = 10$ . Here the mean is 8.89 and precision is only 0.1; apparently not yet large enough to degrade the performance due to an incorrect mean. Lastly, Tukey's statistic performs marginally better than Huber's. This is likely due to the fact that Tukey's estimator trims extreme outliers completely in the estimation procedure (Huber and Ronchetti, 2009).

It is also interesting to consider the effects of factors  $n_i$ ,  $p_i$ , and  $m_i$ . For a given factor and simulation, the  $KL_{ik}^{(M)}$  are averaged by factor level. For the Bayesian models, the averages are also taken over the different values of  $a_s$  and  $c$ . Figure 6 displays these averages for  $m$ ,  $n$ , and  $p$  with error bars plus/minus one standard error. The restricted likelihood versions consistently perform better than their classical counterparts. Intuitively, as the amount of contamination ( $p$ ) increases performance degrades as it becomes more difficult to identify the good data. Likewise, as  $n$  increases, the performance for the Bayesian methods become closer to that of their classical counterparts reflecting the diminishing effect of the prior. However, the decrease of KL-divergence with  $m$  and increase with  $n$  is somewhat surprising. To investigate, Figure 7 and 8 display boxplots of  $(\theta_i - \hat{\theta}_i)$

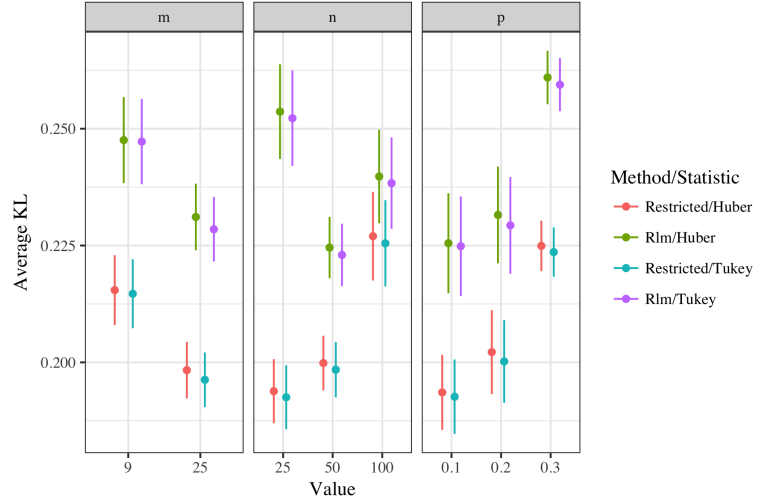


Figure 6: Average KL - divergence plus/minus one standard error grouped by the factors  $m$  (left),  $n$  (middle), and  $p$  (right)

and  $\hat{\sigma}_i$  for each simulated data set. The  $\hat{\theta}_i$ 's have no systematic bias however the  $\hat{\sigma}_i$ 's do; consistently biased upward from the value of  $\sigma = 2$  for the good portion of data. As  $n$  increases, the bias remains the same and the variation in the estimates gets smaller. Thus, the estimates are getting more certain about an incorrect value; explaining the degradation of the KL - divergence. As  $m$  increases, the variance in the estimates gets larger and there is a marginal increase in the bias. Thus, for  $m = 9$  there is more certainty about an incorrect value and the increased uncertainty at  $m = 25$  helps to improve the KL-divergence.

This simulation shows the potential of the restricted likelihood while highlighting some interesting observations. Specifically, the choice of summary statistics, along with corresponding tuning parameters is important. For the tuning parameters, the standard choice of 95% efficiency at the normal was used. Under the data generating model here, this choice results in bias in the scale estimation which affects the performance of the method. These choices must be made in both the classical and Bayesian settings. The Bayesian setting allows for the incorporation of informative prior information which, as shown in this example, can dramatically improve prediction. The results are sensitive to the prior, but here we have observed good relative improvement over the classical

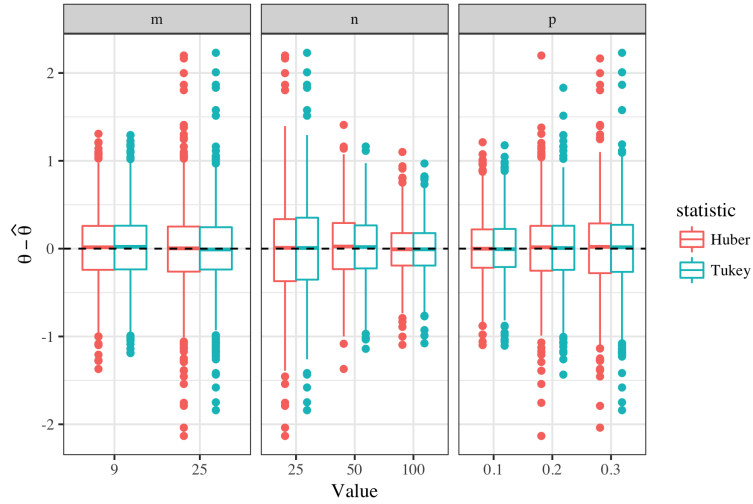


Figure 7: Boxplots  $(\theta_i - \hat{\theta}_i)$  across all simulations separated by the values for  $m$  (left),  $n$  (middle),  $p$  (right) where  $\hat{\theta}_i$  are the classical robust estimators (Huber's and Tukey's).

counterparts for a range of prior choices.

## 6 Real Data

We illustrate our methods with a pair of regression models for data from Nationwide Insurance Company, which concern prediction of the performance of insurance agencies. Nationwide sells many of its insurance policies through agencies which provide direct service to policy holders. The contractual agreements between Nationwide and these agencies vary. Our interest is the prediction of future performance of agencies where performance is measured by the total number of households an agency services ('household count'). The data are grouped by states with a varying number of agencies by state. Identifiers such as agency/agent names are removed. Likewise, state labels and agency types (identifying the varying contractual agreements) have been made generic to protect the proprietary nature of the data. As an exploratory view, a plot of the square root of household count in 2012, against that in 2010 is shown in Figure 9 for four states. The states have varying number of agencies and the different colors represent the varying types of contractual agreements as they stood in 2010

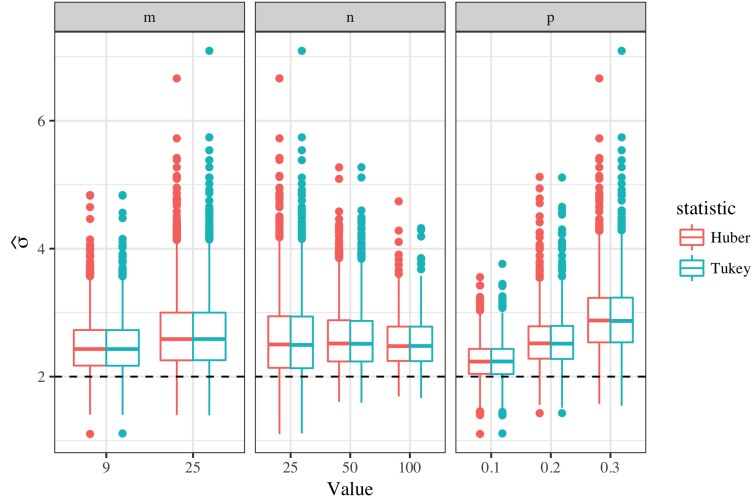


Figure 8: Boxplots of the classical robust estimators (Huber's and Tukey's) for  $\sigma_i$  across all simulations separated by the values for  $m$  (left),  $n$  (middle),  $p$  (right). The horizontal line at  $\sigma = 2$  highlights the true standard deviation of the 'good' data.

('Type'). A significant number of agencies closed sometime before 2012, as represented by the 0 counts for 2012. Among the open agencies, linear correlations exist with strength depending on agency type and state. 'Type 1' agencies open in 2012 are of special interest and one could easily subset the analysis to only these agencies, removing the others. However, we leave them and use the data as a test bed for our techniques by fitting models that do not account for agency closures or contract type. Our expectation is that the restricting likelihood will facilitate prediction for the 'good' part of the data (i.e. open, 'type 1' agencies).

## 6.1 State Level Regression model

The first analysis considered is based on individual regressions fit separately within states. The following normal theory regression model is used as the full model for a single state:

$$\beta \sim N(\mu_0, \sigma_0^2); \quad \sigma^2 \sim IG(a_0, b_0); \quad y_i = \beta x_i + \epsilon_i, \quad \epsilon_i \stackrel{iid}{\sim} N(0, \sigma^2), \quad i = 1, \dots, n, \quad (19)$$



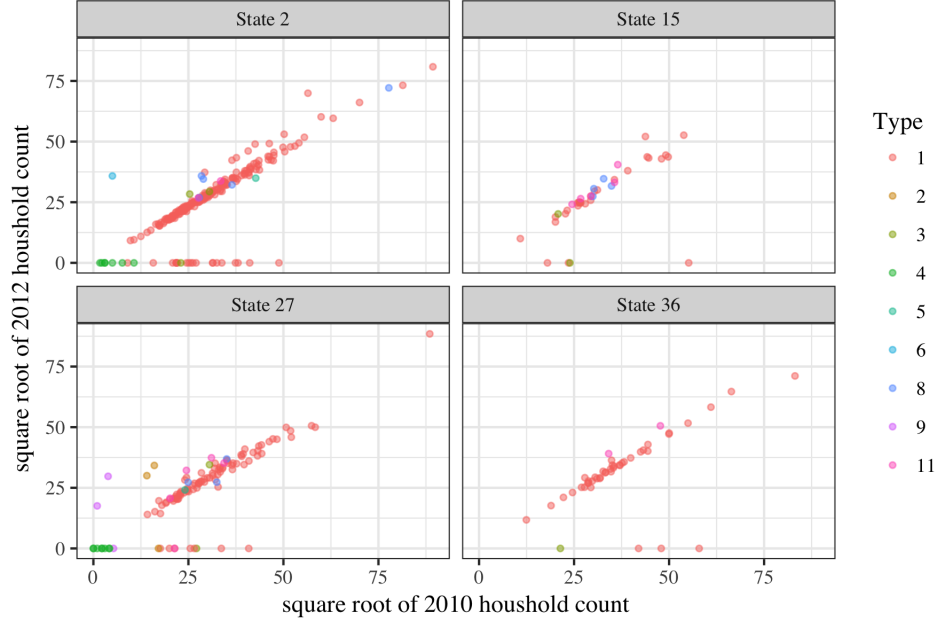


Figure 9: The square root of count in 2012 versus that in 2010 (after centering and scaling). The colors represent the varying contractual agreements as they stood in 2010. Agencies that closed during the 2010-2012 period are represented by the zero counts for 2012. Scalings on the axes are purposely left off for proprietary reasons.

where  $y_i$  and  $x_i$  are the square rooted household count in 2012 and 2010 for the  $i^{th}$  agency, respectively. The hyper-parameters  $a_0, b_0, \mu_0$  and  $\sigma_0^2$  are all fixed and set from a robust regression fit to the corresponding state's data from the time period two years before. Specifically, Let  $\hat{\beta}$  and  $\hat{\sigma}^2$  be estimates from the robust linear regression of 2010 counts on 2008 counts. We fix  $a_0 = 5$  and set  $b_0 = \hat{\sigma}^2(a_0 - 1)$  so the prior mean is  $\hat{\sigma}^2$ . We set  $\mu_0 = \hat{\beta}$  and  $\sigma_0^2 = n_p se(\hat{\beta})^2$  where  $n_p$  is the number of agencies in the prior data set and  $se(\hat{\beta})$  is the standard error of  $\hat{\beta}$  derived from the robust regression. This prior is in the spirit of the Zellner's  $g$ -prior (Zellner, 1986; Liang et al., 2008); in general scaling the prior variance  $se(\hat{\beta})^2$  by a factor  $g$ .  $g = n_p$  is analogous to the unit-information prior (Kass and Wasserman, 1995), with the difference that we are using a prior data set, not the current data set, to set the prior.

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 the simulation of Section 5 adapted to linear regression. The heavy-tailed model replaces the normal sampling density in (19) with a  $t$ -distribution with  $\nu = 5$  degrees of freedom. The Bayesian models are all fit using MCMC, with the restricted versions using the algorithm presented in Section 4.2. We also fit the corresponding classical robust regressions and a least squares regression.

### 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 prefer to use an out-of-sample measure of fit. This leads us to cross-validation. We repeatedly split the data into training and holdout data sets; fitting the model to the training data and assessing performance on the holdout 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 holdout 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 holdout sample, say  $i = 1, \dots, M$ . Order the holdout sample according to the ordering of  $\log(f_b(y_i))$  and denote this ordering by  $y_{(1)}^b, y_{(2)}^b, \dots, y_{(M)}^b$ . That is, for  $i < j$   $\log(f_b(y_{(i)}^b)) < \log(f_b(y_{(j)}^b))$ . All of the methods are then scored on the holdout sample

with the mean trimmed log marginal pseudo likelihood,

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

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 since the smallest scores from this method are guaranteed to be trimmed. A method that performs poorly when it is the base method is discredited.

### Comparison of predictive performance

‘Type 1’ agencies are of special interest to the company and so the evaluation of the TLM is done on only holdout samples of ‘Type 1’, whereas the training is done on agencies of all types. This is intended to demonstrate the robustness properties of the various methods. Models are fit to four states labelled State 2, 15, 27, and 36, with  $n = 222, 40, 117$ , and  $46$ , representing a range of sample sizes. Training sample sizes are taken to be  $.25n$  and  $0.50n$  with holdout evaluation done on the remaining (‘Type 1’) samples. The average  $TLM_b(A)$  over  $K = 50$  training/holdout samples for the four states and seven methods are shown in Figure 10 where the base model is the Student - t model and  $\alpha = 0.3$ . Similar results are observed for other base models, with this one being most advantageous to the Student - t model. The error-bars are plus/minus one standard deviation of the average  $TLM_b(A)$  over the  $K = 50$  training/holdout samples. It is clear the normal Bayesian model used as the base model (Normal) and the classical ordinary least squares fits (OLS) have poor performance, as expected, due to the significant amount of outlier contamination in the data. In comparing restricted methods to their corresponding classical methods, there is small, but consistent improvement across the states and training sample size. For state 2, the largest state with  $n = 222$ , the restricted and classical robust methods have similar performance especially for larger training sample size. This reflects the diminishing effect of the prior as the sample size grows. Notably, the Student - t model performs poorly in comparison for this state. The predictive distribution explicitly accounts for heavy-tailed values, resulting in poorer predictions of the ‘good’ data (i.e. the Type 1 agencies). Likewise, for

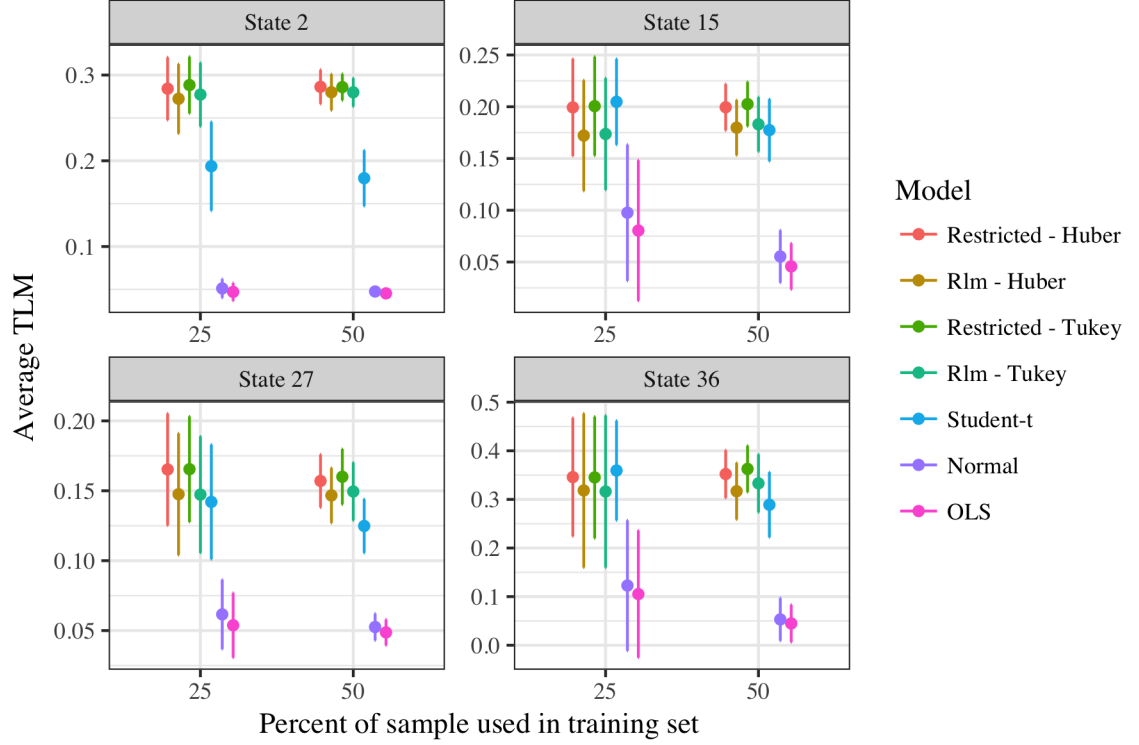


Figure 10: Average TLM plus/minus one standard deviation over  $K = 50$  splits into training and holdout samples. The panels are for the different states 2, 15, 27, and 36, with  $n = 222, 40, 117$ , and 46, respectively. The horizontal axis is the percent of  $n$  used in each training set. The color corresponds to the fitting model.

State 27, another larger state, the Student-t model is outperformed by our restricted methods. For the other states, the Student-t performs similarly to our restricted methods for the smaller states (State 15 and 36) and smaller training size (25% of the sample). However, the performance is worse for the larger training size (50% of the sample). Intuitively, as more data is available for fitting, more outliers appear and the heavy-tailed model compensates for them by assuming they come from the tails of the model; detrimental for prediction. The relative performance of the models are similar for various values  $\alpha$ . Figure 11 shows the results for one state (State 27) with training sample size  $0.5n$  as an example.

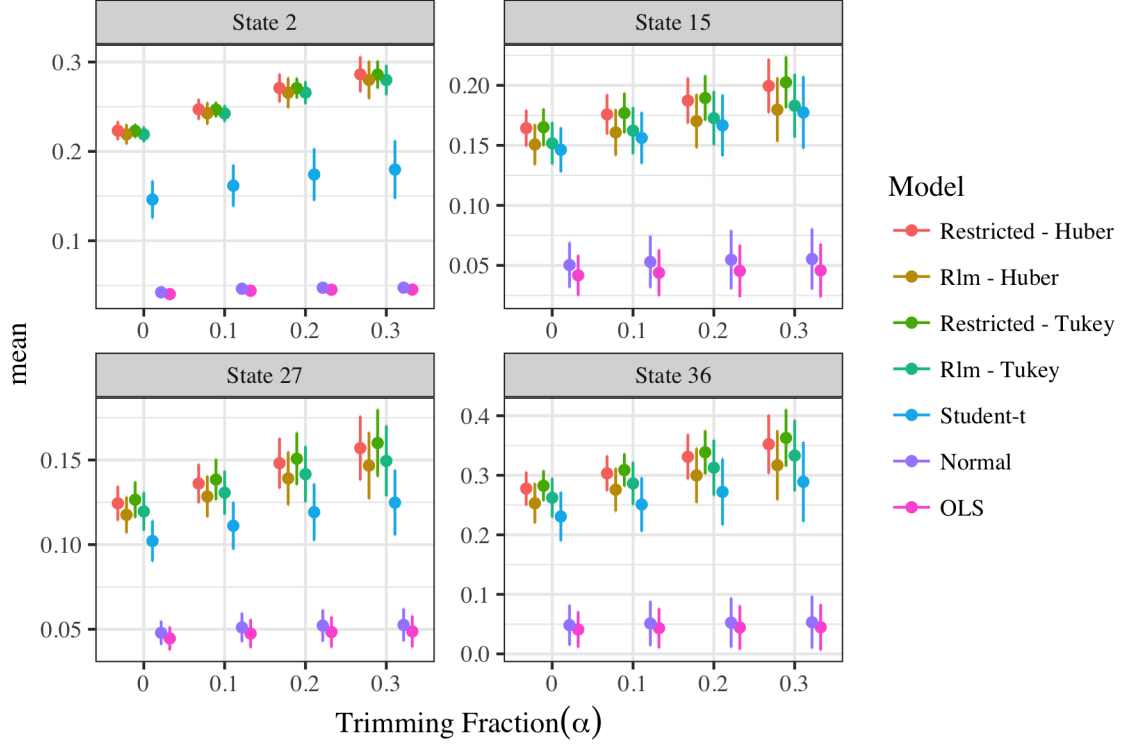


Figure 11: Average TLM plus/minus one standard deviation over  $K = 50$  splits into training and holdout samples for several values of the trimming fraction  $\alpha$ . The training sample size used is  $0.5n$ .

## 6.2 Hierarchical regression model

The previous analysis treated states independently. A natural extension is to reflect similar business environments between states using a hierarchical regression. The proposed model is:

$$\begin{aligned} \beta &\sim N_p(\mu_0, a\sigma_0^2); \quad \beta_j \stackrel{iid}{\sim} N_p(\beta, b\sigma_0^2); \quad \sigma_j^2 \sim IG(a_0, b_0); \\ y_{ij} &= x_{ij}\beta_j + \epsilon_{ij}, \quad \epsilon_{ij} \stackrel{iid}{\sim} N(0, \sigma_j^2), \quad i = 1, \dots, n_j, \quad j = 1, \dots, J \end{aligned} \quad (20)$$

where  $y_{ij}$  is the  $i^{th}$  observation of square rooted household count in 2012 in the  $j^{th}$  state, is the total number of agencies in state  $j$ , and  $J$  is the number of states.  $x_{ij}$  is the square rooted household count in 2010 and  $\beta_j$  represents the individual regression coefficient vector for state  $j$ .

We match this model to the non-hierarchical model in several ways. First,  $\mu_0$ ,  $\Sigma_0$ ,  $a_0$ , and  $b_0$  are fixed as before. We constrain  $a + b = 1$  in an attempt to partition the total variance between the individual  $\beta_j$ 's and the overall  $\beta$ . We take  $b \sim \text{beta}(v_1, v_2)$ . Using the previous data set, we assess the variation between individual estimates of the  $\beta_j$  to set  $v_1$  and  $v_2$  to allow for a reasonable amount of shrinkage. To allow for dependence across the  $\sigma_j^2$  we first take  $(z_1, \dots, z_J) \sim N_J(\mathbf{0}, \Sigma_\rho)$  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  $\Phi$  is the cdf of a standard normal. This results in the specified marginal distribution, while introducing correlation via  $\rho$ . 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  $\mu_\rho$  and  $\psi_\rho$  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  $\mu_\rho$  and  $\psi_\rho$  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 4.2 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 ?? . 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.

## 7 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 methods, 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  $T(\mathbf{y})$ ; 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 desirable inference, we recommend use of robust and relevant summary statistics in conjunction with Bayesian models.*

## 8 Appendix

### 8.1 Proofs

Proof of Theorem 4.1.

*Proof.*

$$s(X, \mathbf{y}) = s\left(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^* + X \left( \mathbf{b}(X, \mathbf{y}_{obs}) - \mathbf{b}\left(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*\right) \right)\right) \quad (21)$$

$$= \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} s(X, \mathbf{z}^*) = s(X, \mathbf{y}_{obs}), \quad \text{and} \quad (22)$$

$$\mathbf{b}(X, \mathbf{y}) = \mathbf{b}\left(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^* + X \left( \mathbf{b}(X, \mathbf{y}_{obs}) - \mathbf{b}\left(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*\right) \right)\right) \quad (23)$$



$$= \mathbf{b}(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*) + \mathbf{b}(X, \mathbf{y}_{obs}) - \mathbf{b}(X, \frac{s(X, \mathbf{y}_{obs})}{s(X, \mathbf{z}^*)} \mathbf{z}^*) \quad (24)$$

$$= \mathbf{b}(X, \mathbf{y}_{obs}) \quad (25)$$

□

Proof of Lemma 4.2.

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

$$s(X, \mathbf{y}) = s(X, Q\mathbf{y} + H\mathbf{y}) = s(X, Q\mathbf{y}). \quad (26)$$

Thus, by the chain rule  $\nabla s(X, \mathbf{y}) = Q\nabla s(X, Q\mathbf{y}) = Q\nabla s(X, \mathbf{z})$ . Hence  $X^\top \nabla s(X, \mathbf{y}) = 0$  as desired. From equation (26), all vectors  $\mathbf{z}' \in \Pi(\mathcal{A})$  satisfy  $s(X, \mathbf{z}') = s(X, \mathbf{y}) = s(X, \mathbf{y}_{obs})$ , and so all directional derivatives of  $s$  along each tangent  $\mathbf{v}$  to  $\Pi(\mathcal{A})$  in  $\mathcal{C}^\perp(X)$  at  $\mathbf{z}$  are equal to 0 (i.e.,  $\nabla s(X, \mathbf{z}) \cdot \mathbf{v} = 0$ ). Thus  $\nabla s(X, \mathbf{z})$  is orthogonal to  $\Pi(\mathcal{A})$  at  $\mathbf{z}$ . Since  $\Pi(\mathcal{A})$  has dimension  $n - p - 1$ ,  $\nabla s(X, \mathbf{z})$  gives the unique (up to scaling and reversing direction) normal in the  $n - p$  dimensional  $\mathcal{C}^\perp(X)$ . □

Proof of Lemma 4.3

*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 an 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  $s(X, \mathbf{y}) = s(X, \mathbf{y}_{obs})$ ,  $b_1(X, \mathbf{y}) = b_1(X, \mathbf{y}_{obs}), \dots, b_p(X, \mathbf{y}) = b_p(X, \mathbf{y}_{obs})$ . Consequently, the gradients are orthogonal to  $\mathcal{A}$ . Let  $\nabla \mathbf{b}(X, \mathbf{y})$  denote the  $n \times p$  matrix with columns  $\nabla b_1(X, \mathbf{y}), \dots, \nabla b_p(X, \mathbf{y})$ . We seek to show the  $n \times (p + 1)$  matrix  $[\nabla \mathbf{b}(X, \mathbf{y}), \nabla s(X, \mathbf{y})]$  has rank  $p + 1$ . Using property C5, we have that

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

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

$$[XX^\top, WW^\top]^\top [\nabla \mathbf{b}(X, \mathbf{y}), \nabla s(X, \mathbf{y})] = \begin{pmatrix} X & \mathbf{0} \\ WW^\top \nabla \mathbf{b}(X, \mathbf{y}) & \nabla s(X, \mathbf{y}) \end{pmatrix} \quad (27)$$

The last column comes from Lemma 4.2. The matrix  $[XX^\top, WW^\top]^\top$  is of full column rank (rank  $n$ ), and so the rank of  $[\nabla \mathbf{b}(X, \mathbf{y}), \nabla s(X, \mathbf{y})]$  is the same as the rank of the matrix on the right hand side of (27). This last matrix has rank  $p+1$  since  $\nabla s(X, \mathbf{y}) \neq \mathbf{0}$  by C8, and so does  $[\nabla \mathbf{b}(X, \mathbf{y}), \nabla s(X, \mathbf{y})]$ .  $\square$

Proof of Lemma 4.4

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

Proof of Corollary 4.7

*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 8.1.** (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  $\sigma_1 \geq \dots \geq \sigma_l \geq 0$  be the singular values of  $Q_M^\top Q_L$ . Then  $\cos \theta_i = \sigma_i, i = 1, \dots, l$  where  $0 \leq \theta_1 \leq \theta_2 \leq \dots \leq \theta_l \leq \frac{\pi}{2}$  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 8.2.** (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 8.1 and Theorem 8.2. Translating Miao and Ben-Israel's notation, we have  $M = \mathcal{C}^\perp(X)$ ,  $Q_M = W$ ,  $L = \mathcal{T}_y(\mathcal{A})$ , and  $Q_L = A$ . By Theorem 8.2, the

nonzero principal angles between  $\mathcal{T}_{\mathbf{y}}(\mathcal{A})$  and  $\mathcal{C}^\perp(X)$  are the same as the nonzero principal angles between  $\mathcal{T}_{\mathbf{y}}^\perp(\mathcal{A})$  and  $\mathcal{C}(X)$ . By 8.1, the non-unit singular values of  $W^\top A$  are the same as the non-unit singular values of  $U^\top B$ .  $\square$

## 8.2 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 6.1) and several heuristic arguments. While the analyses in Section 6.2 set the hyperparameters 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  $\hat{\beta}_1, \dots, \hat{\beta}_J, \hat{\sigma}_1, \dots, \hat{\sigma}_J$  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 (20),  $b = 0$  implies all the  $\beta'_j$ s are equal (no variation between states) and  $b = 1$  implies the  $\beta'_j$ s vary about  $\mu_0$  according to  $\Sigma_0 = n \cdot \text{var}(\hat{\beta})$  (see Section 6.1). We seek a prior measure for what we think  $b$  should be. In other words, how much prior uncertainty should we allow in  $\beta$  as opposed to the uncertainty amongst the  $\beta'_j$ s? Using the prior fit, a measure for uncertainty for  $\beta$  is  $\Sigma_{\hat{\beta}} = \text{var}(\hat{\beta})$ , the estimate of the covariance from the single regression. For the  $\beta'_j$ 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  $\beta'_j$ s to the amount of uncertainty in  $\beta$ . Now in the prior, we heuristically set the uncertainty in the  $\beta'_j$ 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  $\mu_\rho$  and gamma prior on  $\psi_\rho$  we first take  $\hat{z}_j = \Phi^{-1}(H(\hat{\sigma}_j^2))$ . As in the prior we assume  $(\hat{z}_1, \dots, \hat{z}_J) \sim N_J(\mathbf{0}, \Sigma_\rho)$  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  $\mu_\rho$  is set to  $\hat{\rho}_{mle}$ . Its variance is inflated somewhat and set to  $2I^{-1}(\hat{\rho}_{mle})$ . Since  $\text{var}(\rho|\mu_\rho, \psi_\rho) = \mu_\rho(1 - \mu_\rho)/(\psi_\rho + 1)$  we replace  $\mu_\rho$  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  $\psi_\rho$  equal to  $\hat{\rho}_{mle}(1 - \hat{\rho}_{mle})/(2I^{-1}(\hat{\rho}_{mle})) - 1$ . Finally, we set the rate parameter to 1 implying the variance of the gamma prior is equal to its the mean.

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