Improving Convergence Diagnostics of Iterative Algorithms

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Abstract

Abstract

1 Introduction

Iterative simulation, particularly Markov chain Monte Carlo (MCMC), is increasingly popular in statistics (Brooks and Gelman, 1998), especially in Bayesian applications where the goal is to represent posterior inference using a sample of posterior draws. Iterative simulation algorithms in common use typically can be proven to converge to the target distribution as the number of draws approaches infinity, but convergence is only approximate for any finite number of draws.

In practice we have two concerns:

1. The M chains may not have not mixed well, so that the simulations do not represent the target distribution because they still retain the influence of their history.
2. The effective sample size (number of effective simulation draws) is low, possibly much less than the total number of draws across chains, because of dependence (autocorrelation) within each chain.

These two issues are related. It is only possible to have a large number of effective draws if the chains have mixed well. Figure 1 illustrates two ways in which sequences of iterative simulations can fail to mix. In the first example, two chains are in different parts of the target distribution, in the second example, the chains move but have not attained stationarity. This situation may arise due to multimodal posteriors or because one chain is stuck in a region of high curvature with a step size too high to make an acceptable proposal. These two examples make it clear that any method for assessing mixing and effective sample size should use information between and within chains.

The other relevant point is that we are often fitting models with large numbers of parameters, so that it is not realistic to expect to make trace plots such as in Figure 1 for all quantities of interest. We need numerical summaries that can flag potential problems. However, as we will show in this paper, the currently existing and widely applied convergence diagnostics have serious flaws under some conditions. We will thus propose improvements to these diagnostics.

2 Convergence diagnostics for iterative algorithms

The Split-$\widehat{R}$ statistic and the *effective sample size* (ESS) are routinely used to monitor the convergence of iterative simulations, which are omnipresent in Bayesian statistics in the form of Markov-Chain Monte-Carlo samples. The original $\widehat{R}$ statistic (Gelman and Rubin, 1992; Brooks and Gelman, 1998) and *split*-$\widehat{R}$ (Gelman et al., 2013) are both based on the ratio of between and within-chain marginal variances of the simulations, while the latter is computed from split chains (hence the name).

2.1 *Split*-$\widehat{R}$

Below, we present the computation of *Split*-$\widehat{R}$ following Gelman et al. (2013), but using the notation style of Stan Development Team (2018c). These implementations represent the current de facto standard of

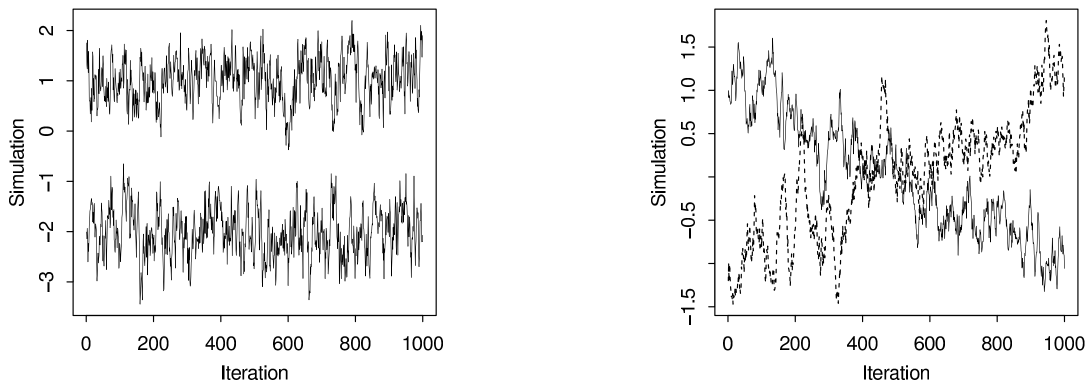


Figure 1: *Examples of two challenges in assessing convergence of iterative simulations. (a) In the left plot, either sequence alone looks stable, but the juxtaposition makes it clear that they have not converged to a common distribution. (b) In the right plot, the two sequences happen to cover a common distribution but neither sequence appears stationary. These graphs demonstrate the need to use between-sequence and also within-sequence information when assessing convergence. From Gelman et al. (2013).*

convergence diagnostics for iterative simulations. In the equations below, N is the number of draws per chain, M is the number of chains, and $S = MN$ is the total number of draws from all chains. For each scalar summary of interest θ, we compute B and W, the between- and within-chain variances:

$$B = \frac{N}{M-1}\sum_{m=1}^{M}(\overline{\theta}^{(.m)} - \overline{\theta}^{(..)})^2, \quad \text{where} \quad \overline{\theta}^{(.m)} = \frac{1}{N}\sum_{n=1}^{N}\theta^{(nm)}, \quad \overline{\theta}^{(..)} = \frac{1}{M}\sum_{m=1}^{M}\overline{\theta}^{(.m)} \tag{1}$$

$$W = \frac{1}{M}\sum_{m=1}^{M}s_j^2, \quad \text{where} \quad s_m^2 = \frac{1}{N-1}\sum_{n=1}^{N}(\theta^{(nm)} - \overline{\theta}^{(.m)})^2. \tag{2}$$

The between-chain variance, B, also contains the factor N because it is based on the variance of the within-chain means, $\overline{\theta}^{(.m)}$, each of which is an average of N values $\theta^{(nm)}$. We can estimate $\mathrm{var}(\theta \mid y)$, the marginal posterior variance of the estimand, by a weighted average of W and B, namely

$$\widehat{\mathrm{var}}^{+}(\theta \mid y) = \frac{N-1}{N}W + \frac{1}{N}B. \tag{3}$$

This quantity *overestimates* the marginal posterior variance assuming the starting distribution of the simulations is appropriately overdispersed compared to the target distribution, but is *unbiased* under stationarity (that is, if the starting distribution equals the target distribution), or in the limit $N \to \infty$. To have an overdispersed starting distribution, independent Markov chains should be initialized with diffuse starting values for the parameters.

Meanwhile, for any finite N, the within-chain variance W should *underestimate* $\mathrm{var}(\theta \mid y)$ because the individual chains haven't had the time to explore all of the target distribution and, as a result, will have less variability. In the limit as $N \to \infty$, the expectation of W also approaches $\mathrm{var}(\theta \mid y)$.

We monitor convergence of the iterative simulations to the target distribution by estimating the factor by which the scale of the current distribution for θ might be reduced if the simulations were continued in the limit $N \to \infty$. This potential scale reduction is estimated as

$$\widehat{R} = \sqrt{\frac{\widehat{\mathrm{var}}^{+}(\theta \mid y)}{W}}, \tag{4}$$

which declines to 1 as $N \to \infty$. We call this *split*-$\widehat{R}$ because we are applying it to chains that have been split in half so that M is twice the number of actual chains. Without splitting, $\widehat{R}$ would get fooled by non-stationary chains (see section/appendix).

We note that *split*-$\widehat{R}$ is also well defined for sequences that are not Markov-chains. However, for simplicity, we always refer to 'chains' instead of more generally to 'sequences' as the former is our primary use case for $\widehat{R}$-like measures.

2.2 Effective sample size

If the N simulation draws within each chain were truly independent, the between-chain variance B would be an unbiased estimate of the posterior variance, $\mathrm{var}(\theta \mid y)$, and we would have a total of $S = MN$ independent simulations from the M chains. In general, however, the simulations of θ within each chain will be autocorrelated, and thus B will be larger than $\mathrm{var}(\theta \mid y)$, in expectation.

One way to define effective sample size for correlated simulation draws is to consider the statistical efficiency of the average of the simulations $\bar{\theta}^{(\cdot\cdot)}$ as an estimate of the posterior mean $\mathrm{E}(\theta \mid y)$. This also generalizes to posterior expectations of functionals of parameters $\mathrm{E}(g(\theta) \mid y)$ and we return later to how to estimate the effective sample size of quantiles which cannot be presented as expectations. For simplification, in this section we consider the effective sample size for the posterior mean.

The effective sample size of a chain is defined in terms of the autocorrelations within the chain at different lags. The autocorrelation ρ_t at lag $t \geq 0$ for a chain with joint probability function $p(\theta)$ with mean μ and variance σ^2 is defined to be

$$\rho_t = \frac{1}{\sigma^2} \int_\Theta (\theta^{(n)} - \mu)(\theta^{(n+t)} - \mu)\, p(\theta)\, d\theta. \tag{5}$$

This is just the correlation between the two chains offset by t positions. Because we know $\theta^{(n)}$ and $\theta^{(n+t)}$ have the same marginal distribution in an MCMC setting, multiplying the two difference terms and reducing yields

$$\rho_t = \frac{1}{\sigma^2} \int_\Theta \theta^{(n)}\, \theta^{(n+t)}\, p(\theta)\, d\theta. \tag{6}$$

The effective sample size of one chain generated by a process with autocorrelations ρ_t is defined by

$$N_{\mathrm{eff}} \;=\; \frac{N}{\sum_{t=-\infty}^{\infty} \rho_t} \;=\; \frac{N}{1 + 2\sum_{t=1}^{\infty} \rho_t}. \tag{7}$$

Effective sample size N_{eff} can be larger than N in case of antithetic Markov chains, which have negative autocorrelations on odd lags. The Dynamic Hamiltonian Monte-Carlo algorithms used in Stan (Hoffman and Gelman, 2014; Betancourt, 2017) can produce $N_{\mathrm{eff}} > N$ for parameters with a close to Gaussian posterior (in the unconstrained space) and low dependency on other parameters.

In practice, the probability function in question cannot be tractably integrated and thus neither autocorrelation nor the effective sample size can be calculated. Instead, these quantities must be estimated from the samples themselves. The rest of this section describes an autocorrelation and split-$\widehat{R}$ based effective sample size estimator, based on multiple split chains. For simplicity, each chain will be assumed to be of the same length N.

Computations of autocorrelations for all lags simultaneously can be done via the fast Fourier transform algorithm (FFT; see Geyer, 2011, for more details). The autocorrelation estimates $\hat{\rho}_{t,m}$ at lag t from multiple chains $m \in (1, \ldots, M)$ are combined with the within-chain variance estimate W and the multi-chain variance estimate $\widehat{\mathrm{var}}^{+}$ introduced above to compute the combined autocorrelation at lag t as

$$\hat{\rho}_t = 1 - \frac{W - \frac{1}{M}\sum_{m=1}^{M}\hat{\rho}_{t,j}}{\widehat{\text{var}}^{+}}. \tag{8}$$

If the chains have not converged, the variance estimator $\widehat{\text{var}}^{+}$ will overestimate the true marginal variance which leads to an overestimation of the autocorrelation and an underestimation of the effective sample size.

Because of noise in the correlation estimates $\hat{\rho}_t$ increases as t increases, typically the truncated sum of $\hat{\rho}_t$ is used. Negative autocorrelations can happen only on odd lags and by summing over pairs starting from lag $t = 0$, the paired autocorrelation is guaranteed to be positive, monotone and convex modulo estimator noise (Geyer, 1992, 2011). The effective sample size of combined chains is then defined as

$$S_{\text{eff}} = \frac{N\,M}{\hat{\tau}}, \tag{9}$$

where

$$\hat{\tau} = 1 + 2\sum_{t=1}^{2k+1}\hat{\rho}_t = -1 + 2\sum_{t'=0}^{k}\hat{P}_{t'}, \tag{10}$$

and $\hat{P}_{t'} = \hat{\rho}_{2t'} + \hat{\rho}_{2t'+1}$. The initial positive sequence estimator is obtained by choosing the largest k such that $\hat{P}_{t'} > 0$ for all $t' = 1, \ldots, k$. The initial monotone sequence estimator is obtained by further reducing $\hat{P}_{t'}$ to the minimum of the preceding values so that the estimated sequence becomes monotone.

The effective sample size S_{eff} described here is different from similar formulas in the literature in that we use multiple chains and between-chain variance in the computation, which typically gives us more conservative claims (lower values of S_{eff}) compared to single chain estimates, especially when mixing of the chains is poor. If the chains are not mixing at all (e.g., the posterior is multimodal and the chains are stuck in different modes), then our S_{eff} is close to the number of chains.

2.3 Problems of current diagnostics

split-$\widehat{R}$, and S_{eff} are well defined only if the marginal posteriors have finite mean and variance, which is not always the case. *split*-$\widehat{R}$, and S_{eff} can also be unstable even if the mean and variance are finite, if the marginal distribution has thick tails. Usually *split*-$\widehat{R}$, and S_{eff} are computed only for the posterior mean, which can miss convergence and sampling efficiency problems in tails which affect, for example, the posterior interval estimates.

3 Improving convergence diagnostics

In this section, we discuss several measures that, together, can solve the problems of the current divergence diagnostics we identified above.

3.1 Rank normalization

As *split*-$\widehat{R}$, and S_{eff} are well defined only if the marginal posteriors have finite mean and variance, we propose to use rank normalized parameter values instead of the actual parameter values for the purpose of diagnosing convergence.

Rank normalized *split*-$\widehat{R}$ and S_{eff} are computed using the equations in Section 2, but replacing the original parameter values $\theta^{(nm)}$ with their corresponding rank normalized values denoted as $z^{(nm)}$. Rank normalization is done a follows: First, replace each value $\theta^{(nm)}$ by its rank $r^{(nm)}$. Average rank for ties are used to conserve the number of unique values of discrete quantities. Ranks are computed jointly for all draws from all chains. Second, normalize ranks via the inverse normal transformation

$$z^{(nm)} = \phi^{-1}((r^{(nm)} - 1/2)/S). \tag{11}$$

For continuous variables and $S \to \infty$, the rank normalized values are normally distributed. Using normalized ranks $z^{(nm)}$ instead of ranks $r^{(nm)}$ themselves has the additional benefit that the behavior of $\widehat{R}$ and S_{eff} do not change for normally distributed parameters.

We will use the term *bulk effective sample size* (bulk-ESS or bulk-S_{eff}) to refer to the effective sample size based on the rank normalized draws. Bulk-ESS is useful for diagnosing problems due to trends or different locations of the chains (see section/appendix). Further, it is well defined even for distributions with infinite mean or variance, a case where previous ESS estimates fail. However, due to the rank normalization, Bulk-ESS is no longer directly applicable to estimate the Monte Carlo standard error of the posterior mean. We will come back to the issue of computing Monte Carlo standard errors for relevant quantities in Section 3.6.

3.2 Diagnostics for folded draws

Both original and rank-normalized *split*-$\widehat{R}$ can be fooled if the chains have different scales but the same location as shown in (see section/appendix). To alleviate this problem, we propose to compute a rank normalized *split*-$\widehat{R}$ statistic not only for the original draws $\theta^{(nm)}$, but also for the corresponding folded draws $\zeta^{(mn)}$, that is the absolute deviations from the median

$$\zeta^{(mn)} = \text{abs}(\theta^{(nm)} - \text{median}(\theta)). \tag{12}$$

The rank-normalized *split*-$\widehat{R}$ measure computed on the basis of $\zeta^{(mn)}$ will be called rank-normalized *folded-split*-$\widehat{R}$. It measures convergence in the tails rather than in the bulk of the distribution. To obtain a single conservative $\widehat{R}$ estimate, we propose to report the maximum of rank normalized *split*-$\widehat{R}$ and rank normalized *folded-split*-$\widehat{R}$ for each parameter.

3.3 Convergence diagnostics for quantiles

The new $\widehat{R}$ and bulk-ESS introduced above are useful as overall efficiency measures. Next we introduce convergence diagnostics for quantiles and related quantities, which are more focused measures and help to diagnose reliability of often reported posterior intervals. Estimating the efficiency of quantile estimates has a high practical relevance in particular as we observe the efficiency for tail quantiles to often be lower than for the mean or median.

The α-quantile is defined as the parameter value θ_α for which $p(\theta \leq \theta_\alpha) = \alpha$. An estimate $\hat{\theta}_\alpha$ of θ_α can thus be obtained by finding the α-quantile of the empirical CDF (ECDF) of the posterior draws $\theta^{(s)}$. However, quantiles cannot be written as an expectation, and thus the above equations for $\widehat{R}$ and S_{eff} are not directly applicable. Thus, we first focus on the efficiency estimate for the cumulative probability $p(\theta \leq \theta_\alpha)$ for different values of θ_α.

For any θ_α, the ECDF gives an estimate of the cumulative probability

$$p(\theta \leq \theta_\alpha) \approx \bar{I}_\alpha = \frac{1}{S}\sum_{s=1}^{S} I(\theta^{(s)} \leq \theta_\alpha), \tag{13}$$

where $I()$ is the indicator function. The indicator function transforms simulation draws to 0's and 1's, and thus the subsequent computations are bijectively invariant. Efficiency estimates of the ECDF at any θ_α can now be obtained by applying rank-normalizing and subsequent computations directly on the indicator function's results.

Assuming that we know the CDF to be a certain continuous function F which is smooth near an α-quantile of interest, we could use the delta method to compute a variance estimate for $F^{-1}(\bar{I}_\alpha)$. Although we don't usually know F, the delta method approach reveals that the variance of $\bar{I}_\alpha$ for some θ_α is scaled by the (usually unknown) density $f(\theta_\alpha)$, but the efficiency depends only on the efficiency of $\bar{I}_\alpha$. Thus, we can use the effective sample size for the ECDF (we computed using the indicator function $I(\theta^{(s)} \leq \theta_\alpha)$) also for the corresponding quantile estimates.

To get a better sense of the efficiency of the chains in the distributions' tails, we propose to compute the minimum of the effective sample sizes of the 5% and 95% quantiles, which we will call *tail effective sample size* (tail-ESS or tail-S_{eff}). Tail-ESS can help diagnosing problems due to different scales of the chains (see section/appendix).

3.4 Efficiency estimates for the median absolute deviation

Since the marginal posterior distributions might not have finite mean and variance, by default RStan (Stan Development Team, 2018a) and RStanARM (Stan Development Team, 2018b) report median and median absolute deviation (MAD) instead of mean and standard error (SE). Median and MAD are well defined even when the marginal distribution does not have finite mean and variance. Since the median is just 50%-quantile, we can get an efficiency estimate for it as for any other quantile.

Further, we can also compute an efficiency estimate for the median absolute deviation (MAD) by computing the efficiency estimate of an indicator function based on the folded parameter values ζ (see Equation (12)):

$$p(\zeta \leq \zeta_{0.5}) \approx \bar{I}_{\zeta,0.5} = \frac{1}{S}\sum_{s=1}^{S} I(\zeta^{(s)} \leq \zeta_{0.5}), \tag{14}$$

where $\zeta_{0.5}$ is the median of the folded values. We see that the efficiency estimate for the MAD is obtained by applying the same approach as for the median (and other quantiles) but with the folded parameters values also used in the computation of the tail-ESS.

3.5 Efficiency estimates for small interval probability estimates

We can get more local efficiency estimates by considering small probability intervals. We propose to compute the efficiency estimates for

$$\bar{I}_{\alpha,\delta} = p(\hat{Q}_\alpha < \theta \leq \hat{Q}_{\alpha+\delta}), \tag{15}$$

where $\hat{Q}_\alpha$ is an empirical α-quantile, $\delta = 1/k$ is the length of the interval with some positive integer k, and $\alpha \in (0, \delta, \ldots, 1-\delta)$ changes in steps of δ. Each interval has S/k draws, and the efficiency measures the autocorrelation of an indicator function which is 1 when the values are inside the specific interval and 0 otherwise. This gives us a local efficiency measure which does not depend on the shape of the distribution.

3.6 Monte Carlo error estimates for quantiles

It is common practice to only report the Monte Carlo error of the mean, but not of quantiles and related quantities. As the delta method for computing the variance would require explicit knowledge of the normalized posterior density, which we don't have in most non-trivial cases, we propose the following alternative approach to compute Montor Carlo standard errors of quantiles:

1. Compute quantiles of the Beta distribution with shape parameters

$$\beta_1 = S_{\text{eff}}/S \times \bar{I}_\alpha + 1 \quad \text{and} \quad \beta_2 = S_{\text{eff}}/S \times (1 - \bar{I}_\alpha) + 1. \tag{16}$$

   Including S_{eff}/S takes into account the efficiency of the posterior draws.

2. Find indices in $s \in \{1, \dots, S\}$ closest to the ranks of these quantiles. For example, for quantile Q, find $s = \mathrm{round}(Q \times S)$.
3. Use the corresponding $\theta^{(s)}$ from the list of sorted posterior draws as quantiles from the error distribution. These quantiles can be used to approximate the Monte Carlo standard error.

3.7 Warning thresholds

Based on the experiments presented in Appendices D-F, more strict convergence diagnostics and effective sample size warning limits could be used. We propose the following warning thresholds although additional experiments would be useful:

- Rhat > 1.01
- ESS < 400

In case of running 4 chains, an effective sample size of 400 corresponds to having an effective sample size of 50 for each 8 split chains, which we consider to be minimum for reliable mean, variance and autocorrelation estimates needed for the convergence diagnostic. We recommend running at least 4 chains to get reliable between chain variances for the convergence diagnostics.

3.8 Diagnostic visualizations

In order to intuitively grasp convergence of iterative algorithms, we propose several new diagnostic visualizations in addition to the numeric convergence diagnostics discussed above. We will illustrate the usage of these visualizations by means of several examples in Section **??**.

3.8.1 Rank plots

Extending the idea of using ranks instead of the original parameter values, we propose to use rank plots for each chain instead of trace plots. Rank plots are nothing else than histograms of the ranked posterior samples (ranked over all chains) plotted separately for each chain. If rank plots of all chains look similar, this indicates good mixing of the chains. As compared to trace plots, rank plots don't tend to squeeze to a fuzzy mess in case of long chains.

3.8.2 Quantile and small interval plots

The efficiency of quantiles or small interval probabilities may vary drastistically across different quantiles and small interval positions, respectively. We thus propose to use diagnostic plots that display efficiency of quanilites or small interval probabilities across their whole range to better diagnose areas of the distributions that the iterative algorithm fails to explore efficiently.

3.8.3 Efficiency per iteration plots

For a well explored distribution, we expect the ESS measures to grow linearly with the total number of draws S, or, equivalently, that the relative efficiency (ESS divided S) is approximately constant for different values of S. For small number of draws, both bulk and tail-ESS may be unreliable and cannot necessarily detect convergence problems (see section/appendix). As a result, some convergence problems may only be detectable as S increases, which then implies the ESS to grow slower then linear or even decrease with increasing S. Equivalently, in such a case, we would expect to see a relatively sharp drop in the relative efficiency measures. We therefore propose to plot the change of both bulk and tail ESS with increasing S. This can be done based on a single model without a need to refit, as we can just extract initial sequences of certain length from the original chains. However, it should be noted that some convergence problems only occur at relatively high S and may thus not be detectable if the total number of draws is too small.

4 Examples

In this section, we will go through some examples to demonstrate the usefulness of our proposed methods as well as the associated workflow in determining convergence. Appendices D-G contain more detailed analysis of different algorithm variants and further examples.

4.1 Cauchy: A distribution with infinite mean and variance

The classic *split*-$\widehat{R}$ is based on calculating within and between chain variances. If the marginal distribution of a chain is such that the variance is not defined (i.e., infinite), the classic *split*-$\widehat{R}$ is not well justified. In this section, we will use the Cauchy distribution as an example of such a distribution. Appendix E contains more detailed analysis of different algorithm variants and further Cauchy examples.

The following Cauchy models are from Michael Betancourt's case study Fitting The Cauchy Distribution

4.1.1 Nominal parameterization of Cauchy

The nominal Cauchy model with direct parameterization is as follows:

```
parameters {
  vector[50] x;
}

model {
  x ~ cauchy(0, 1);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

4.1.1.1 Default Stan options

Run the nominal model:

Treedepth exceedence and Bayesian fraction of missing information are dynamic HMC specific diagnostics (Betancourt, 2017). We get warnings about a very large number of transitions after warmup that exceeded the maximum treedepth, which is likely due to very long tails of the Cauchy distribution. All chains have low estimated Bayesian fraction of missing information also indicating slow mixing.

```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

         Q5    Q50    Q95   Mean     SD  Rhat Bulk_ESS Tail_ESS
x[1]  -5.74  -0.01   6.31   2.50  36.40  1.03     1181      393
x[2]  -5.83  -0.01   6.07   0.65  16.20  1.01     2645      502
x[3]  -5.23   0.01   5.73   0.58  17.70  1.01     2683      823
x[4]  -6.25  -0.02   6.90   0.16  11.50  1.01     3627      644
x[5]  -9.66  -0.05   5.11  -1.41  11.30  1.01      629      156
x[6]  -5.26   0.00   5.41   0.20   5.32  1.01     3060      883
x[7]  -6.35   0.06  10.80   4.14  32.60  1.02      607      184
```

```
x[8]    -6.45  -0.01   5.37  -0.22   7.66  1.00      2658      886
x[9]    -6.53   0.00   6.30   0.15   7.38  1.01      3128      901
x[10]   -6.12  -0.01   5.92   0.06   5.74  1.01      2421      642
x[11]   -6.73   0.00   6.15   0.03   9.68  1.01      2079      600
x[12]   -5.68  -0.03   4.88   0.19  17.50  1.00      2633      774
x[13]   -4.53  -0.06   4.27   0.09   6.28  1.00      3148      811
x[14]   -4.88   0.00   5.03  -0.02   5.93  1.00      1461      492
x[15] -14.50  -0.01  11.50  -1.41  22.70  1.03       486      160
x[16]   -7.03   0.01   6.96   0.16  15.90  1.01      2329      463
x[17]   -6.59   0.01   7.69   0.96  30.20  1.01      2292      446
x[18]   -4.51   0.05   6.92   1.10  11.90  1.01      2640      447
x[19]   -7.66  -0.05   6.08  -3.14  28.10  1.01      1147      298
x[20]   -5.78   0.03  11.30   5.78  37.00  1.03       363       80
x[21]   -4.89   0.02   5.38   0.11   5.45  1.01      3276      824
x[22]   -5.59   0.04   5.37   0.49  15.40  1.01      2121      522
x[23] -14.40   0.01   7.00  -3.10  32.00  1.01       391       89
x[24]   -5.93  -0.04   5.47  -1.01  16.60  1.02      1434      284
x[25]   -7.07  -0.02   5.94  -1.76  21.30  1.01      1544      324
x[26]   -8.96  -0.06   5.85  -1.97  17.40  1.01      1778      452
x[27]   -8.81  -0.01   8.34   0.15  18.10  1.00      1816      352
x[28]   -5.26   0.02   5.93   0.11   9.51  1.02      3776      675
x[29]   -5.88   0.00   5.90  -0.04  18.50  1.01      3642      846
x[30]   -5.57  -0.02   5.14  -0.18   6.22  1.00      4363      643
x[31]   -7.36   0.01   7.25   0.07   8.71  1.00      3384      896
x[32]   -8.85  -0.04   6.50 -10.20  81.20  1.01       561      141
x[33]   -4.79   0.03   4.96  -0.35   8.61  1.01      2626      735
x[34]   -5.91  -0.03   5.37  -0.11   5.96  1.01      2408      634
x[35]   -6.10   0.02   6.79  -0.33  14.60  1.01      2654      630
x[36]   -4.86   0.10  15.60  19.30 108.00  1.04       155       34
x[37]   -8.93   0.00   7.86  -0.09  13.30  1.01      1155      427
x[38]   -5.54  -0.02   4.83  -0.33   5.95  1.00      3353      576
x[39]   -5.89  -0.03   5.84   0.11   7.29  1.02      4493      724
x[40]   -8.71   0.01   6.71  -1.98  19.80  1.00       877      148
x[41]   -6.88  -0.03   7.55  -0.27  11.30  1.00      1726      512
x[42]   -6.15   0.01   6.48   0.09  15.50  1.01      1519      448
x[43]   -6.38   0.00   7.39   0.11  12.10  1.01      2746      483
x[44]   -7.84   0.00   7.99   0.41  11.50  1.01      2999      659
x[45]   -4.77  -0.02   4.66   0.04   6.73  1.01      2904     1014
x[46]   -4.84   0.00   5.99   1.16  22.10  1.00       955      338
x[47]   -8.51   0.03  24.30   0.80  37.10  1.07       231       56
x[48]   -6.73   0.00   5.33  -0.72  10.40  1.01      1907      469
x[49]   -6.27   0.04   6.92   0.73  12.40  1.00      1490      390
x[50]   -5.21   0.00   4.65  -0.22   7.08  1.00      3109      680
I        0.00   0.50   1.00   0.50   0.50  1.00       390     4000
lp__   -92.70 -69.20 -49.00 -69.50  13.40  1.05       117      323

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

Several Rhat > 1.01 and some ESS < 400 indicate also that the results should not be trusted. The Appendix E has more results with longer chains as well.

We can further analyze potential problems using local efficiency and rank plots. We specifically investigate

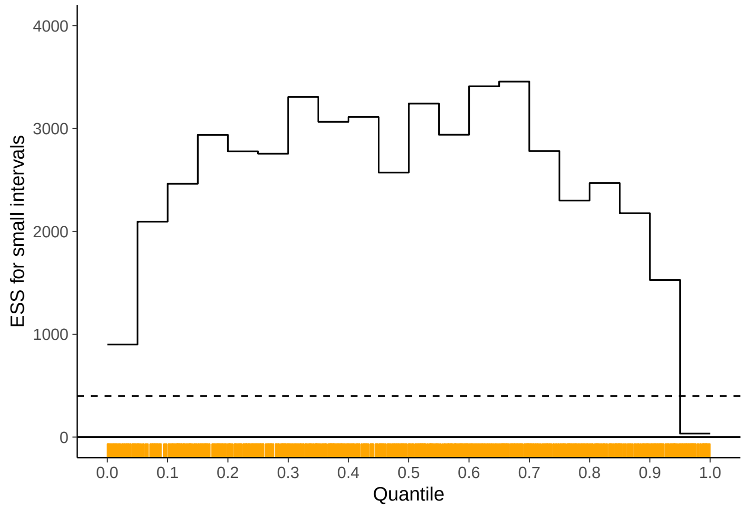


Figure 2: The local efficiency of small interval probability estimates for Cauchy model with nominal parameterization.

x[36], which has the smallest taill-ESS of 34.

We examine the sampling efficiency in different parts of the posterior by computing the efficiency of small interval probability estimates (see Section Efficiency estimate for small interval probability estimates). Each interval contains $1/k$ of the draws (e.g., 5% each, if $k = 20$). The small interval efficiency measures mixing of an function which indicates when the values are inside or outside the specific small interval. As detailed above, this gives us a local efficiency measure which does not depend on the shape of the distribution.

We see that the efficiency of our posterior draws is worryingly low in the tails (which is caused by slow mixing in long tails of Cauchy). Orange ticks show iterations that exceeded the maximum treedepth.

An alternative way to examine the efficiency in different parts of the posterior is to compute efficiencies estimates for quantiles (see Section Efficiency for quantiles). Each interval has a specified proportion of draws, and the efficiency measures mixing of a function which indicates when the values are smaller than or equal to the corresponding quantile.

Similar as above, we see that the efficiency of our posterior draws is worryingly low in the tails. Again, orange ticks show iterations that exceeded the maximum treedepth.

We may also investigate how the estimated effective sample sizes change when we use more and more draws (Brooks and Gelman (1998) proposed to use similar graph for $\widehat{R}$). If the effective sample size is highly unstable, does not increase proportionally with more draws, or even decreases, this indicates that simply running longer chains will likely not solve the convergence issues. In the plot below, we see how unstable both bulk-ESS and tail-ESS are for this example.

We can further analyze potential problems using rank plots in which we clearly see differences between chains.

4.1.2 Alternative parameterization of Cauchy

Next we examine an alternative parameterization that considers the Cauchy distribution as a scale mixture of Gaussian distributions. The model has two parameters and the Cauchy distributed x's can be computed from those. In addition to improved sampling performance, the example illustrates that focusing on diagnostics matters.

```
parameters {
  vector[50] x_a;
```

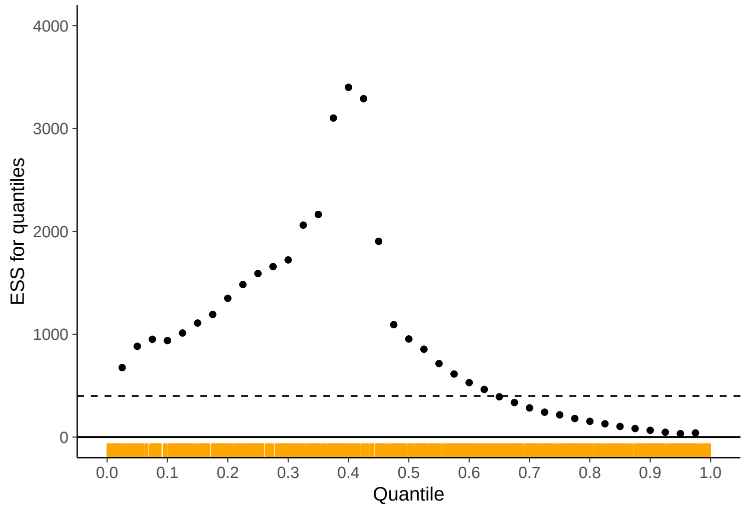


Figure 3: The efficiency of quantile estimates for Cauchy model with nominal parameterization.

```
  vector<lower=0>[50] x_b;
}

transformed parameters {
  vector[50] x = x_a ./ sqrt(x_b);
}

model {
  x_a ~ normal(0, 1);
  x_b ~ gamma(0.5, 0.5);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

Run the alternative model:

There are no warnings, and the sampling is much faster.

```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

            Q5   Q50  Q95  Mean   SD  Rhat Bulk_ESS Tail_ESS
x_a[1]   -1.65 -0.02 1.66 -0.01 0.99  1.00     4361     2961
x_a[2]   -1.67  0.00 1.63 -0.01 1.01  1.00     4015     3167
x_a[3]   -1.66 -0.03 1.62 -0.01 1.00  1.00     4190     3013
x_a[4]   -1.63 -0.01 1.69  0.01 1.01  1.00     3626     2822
x_a[5]   -1.64 -0.01 1.58 -0.01 0.98  1.00     3447     3029
x_a[6]   -1.62 -0.01 1.56 -0.01 0.97  1.00     3975     2795
x_a[7]   -1.61  0.00 1.65  0.01 1.01  1.00     3919     2271
x_a[8]   -1.67 -0.03 1.60 -0.02 1.01  1.00     3736     3040
x_a[9]   -1.63 -0.04 1.55 -0.03 0.99  1.00     3852     3075
x_a[10]  -1.66 -0.03 1.74  0.00 1.02  1.00     3457     2810
x_a[11]  -1.56 -0.02 1.55 -0.01 0.97  1.00     3532     2822
x_a[12]  -1.64  0.00 1.69  0.01 1.00  1.00     3462     3036
x_a[13]  -1.59  0.01 1.63  0.01 0.99  1.00     3479     2764
```

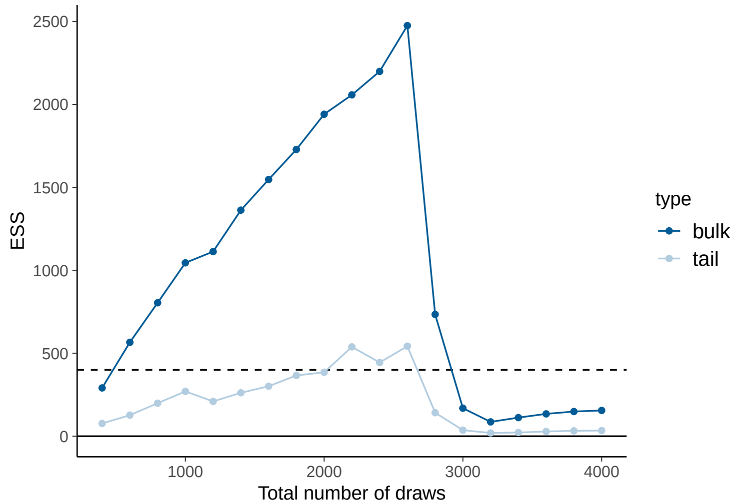


Figure 4: The estimated effective sample sizes with increasing number of iterations for Cauchy model with nominal parameterization.

x_a[14]	-1.72	-0.03	1.63	-0.03	1.01	1.00	3872	3179
x_a[15]	-1.65	0.02	1.70	0.02	1.02	1.00	3843	2855
x_a[16]	-1.67	-0.01	1.62	-0.01	1.01	1.00	3610	3047
x_a[17]	-1.63	-0.01	1.66	-0.01	0.99	1.00	4363	3076
x_a[18]	-1.65	-0.01	1.69	-0.01	1.01	1.00	4636	3088
x_a[19]	-1.61	-0.02	1.59	-0.02	0.98	1.00	4055	3037
x_a[20]	-1.64	-0.01	1.62	0.00	1.00	1.00	4340	2792
x_a[21]	-1.67	0.04	1.68	0.02	1.03	1.00	3628	2719
x_a[22]	-1.63	-0.01	1.64	-0.01	1.01	1.00	3976	2775
x_a[23]	-1.62	0.03	1.70	0.02	1.01	1.00	4266	2682
x_a[24]	-1.66	0.00	1.67	0.00	1.00	1.00	3710	2889
x_a[25]	-1.64	0.02	1.66	0.00	1.00	1.00	4408	3062
x_a[26]	-1.65	-0.02	1.61	0.00	1.00	1.00	3854	2674
x_a[27]	-1.66	0.00	1.68	0.00	1.01	1.00	3331	2944
x_a[28]	-1.69	0.02	1.68	0.02	1.01	1.00	4055	2689
x_a[29]	-1.57	0.00	1.64	0.02	0.99	1.00	4097	3213
x_a[30]	-1.61	0.00	1.64	0.01	0.99	1.00	3961	2900
x_a[31]	-1.65	0.01	1.61	0.00	0.99	1.00	4097	3088
x_a[32]	-1.59	-0.01	1.59	-0.01	0.97	1.00	4189	3171
x_a[33]	-1.69	-0.01	1.77	0.00	1.05	1.00	3853	2594
x_a[34]	-1.68	0.01	1.69	0.00	1.01	1.00	4012	2787
x_a[35]	-1.61	0.03	1.67	0.03	1.00	1.00	3920	2829
x_a[36]	-1.67	0.00	1.60	-0.01	0.99	1.00	4107	2797
x_a[37]	-1.69	-0.03	1.59	-0.02	1.00	1.00	3956	2942
x_a[38]	-1.67	-0.02	1.64	-0.02	1.02	1.00	4210	2919
x_a[39]	-1.66	-0.02	1.65	-0.02	1.02	1.00	4482	2869
x_a[40]	-1.63	0.00	1.62	0.00	1.00	1.00	4139	2848
x_a[41]	-1.68	0.02	1.61	0.00	0.99	1.00	3963	2962
x_a[42]	-1.64	0.03	1.64	0.02	1.00	1.00	4161	3077
x_a[43]	-1.64	-0.03	1.63	-0.02	1.01	1.00	3808	2849
x_a[44]	-1.66	-0.03	1.63	-0.02	1.00	1.00	3743	2865
x_a[45]	-1.68	0.02	1.73	0.01	1.02	1.00	3783	2546
x_a[46]	-1.56	0.04	1.66	0.05	0.97	1.00	4340	3277

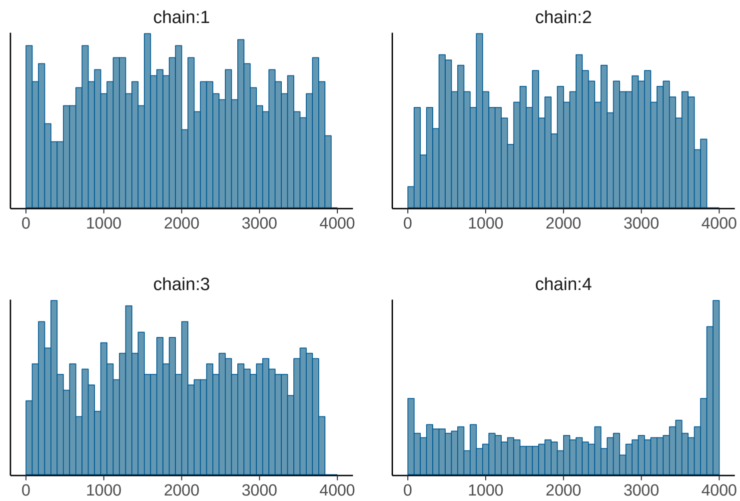


Figure 5: Rank plots of posterior draws from four chains for Cauchy model with nominal parameterization.

x_a[47]	-1.66	0.02	1.58	0.00	1.00	1.00	4283	2946
x_a[48]	-1.61	0.00	1.66	0.00	0.98	1.00	4001	2779
x_a[49]	-1.62	0.00	1.64	0.00	1.00	1.00	3906	3099
x_a[50]	-1.62	-0.01	1.58	0.00	0.99	1.00	3794	2962
x_b[1]	0.00	0.44	4.00	1.00	1.44	1.00	2268	1264
x_b[2]	0.00	0.46	3.75	1.00	1.38	1.00	2444	1428
x_b[3]	0.00	0.47	3.89	1.03	1.46	1.00	3578	1950
x_b[4]	0.00	0.46	3.83	1.01	1.41	1.00	2693	1342
x_b[5]	0.00	0.45	3.95	1.03	1.46	1.00	3056	1731
x_b[6]	0.00	0.44	3.80	1.00	1.41	1.00	3264	1786
x_b[7]	0.01	0.43	3.62	0.95	1.32	1.00	2888	1907
x_b[8]	0.00	0.44	3.79	1.01	1.40	1.00	2876	1578
x_b[9]	0.00	0.50	3.67	1.00	1.36	1.00	2820	1535
x_b[10]	0.00	0.44	3.79	0.99	1.39	1.00	2534	1699
x_b[11]	0.01	0.49	3.90	1.03	1.44	1.00	3595	2032
x_b[12]	0.00	0.44	3.82	0.99	1.40	1.00	2405	1200
x_b[13]	0.00	0.46	3.97	1.03	1.45	1.00	2045	1073
x_b[14]	0.00	0.44	3.97	1.03	1.49	1.00	2829	1443
x_b[15]	0.01	0.45	3.77	1.01	1.41	1.00	2853	1447
x_b[16]	0.00	0.48	3.79	1.01	1.43	1.00	2661	1604
x_b[17]	0.01	0.46	3.93	1.02	1.42	1.00	2775	1477
x_b[18]	0.01	0.50	4.11	1.06	1.53	1.00	2689	1170
x_b[19]	0.00	0.45	3.92	1.00	1.41	1.00	2392	1450
x_b[20]	0.00	0.42	3.96	0.99	1.42	1.00	2296	1240
x_b[21]	0.01	0.49	3.94	1.04	1.43	1.00	3069	1848
x_b[22]	0.00	0.45	3.95	1.02	1.46	1.00	3012	1733
x_b[23]	0.00	0.46	3.95	1.00	1.42	1.00	1787	1093
x_b[24]	0.00	0.44	3.86	1.00	1.43	1.00	1903	1008
x_b[25]	0.00	0.45	3.66	0.98	1.39	1.00	2348	1094
x_b[26]	0.00	0.47	4.05	1.03	1.46	1.00	2421	1549
x_b[27]	0.00	0.45	3.90	1.01	1.41	1.00	2777	1470
x_b[28]	0.00	0.46	3.79	0.98	1.37	1.00	3353	1699
x_b[29]	0.01	0.46	3.87	1.01	1.43	1.00	3428	1997
x_b[30]	0.00	0.44	3.89	1.01	1.43	1.00	2833	1554

x_b[31]	0.00	0.49	3.84	1.01	1.41	1.00	3035	1633
x_b[32]	0.00	0.43	3.75	0.97	1.36	1.00	2276	1602
x_b[33]	0.00	0.45	3.79	1.00	1.41	1.00	3093	1888
x_b[34]	0.00	0.47	3.97	1.03	1.45	1.00	3309	1650
x_b[35]	0.00	0.48	3.84	1.02	1.42	1.00	2493	1588
x_b[36]	0.00	0.44	3.89	0.99	1.39	1.00	3108	1876
x_b[37]	0.00	0.46	3.70	0.98	1.35	1.00	2644	1322
x_b[38]	0.01	0.45	3.93	1.01	1.45	1.00	3155	1776
x_b[39]	0.00	0.45	3.75	0.99	1.42	1.00	2038	934
x_b[40]	0.00	0.42	3.76	0.94	1.31	1.00	2657	1403
x_b[41]	0.00	0.46	3.78	1.00	1.38	1.00	2648	1370
x_b[42]	0.00	0.45	3.89	1.00	1.43	1.00	2334	1365
x_b[43]	0.00	0.47	4.03	1.03	1.44	1.00	2967	1797
x_b[44]	0.00	0.43	3.69	0.97	1.37	1.00	2557	1591
x_b[45]	0.00	0.44	3.66	0.96	1.30	1.00	2731	1785
x_b[46]	0.00	0.46	3.74	1.01	1.40	1.00	2538	1183
x_b[47]	0.01	0.47	3.83	1.01	1.39	1.00	3948	2071
x_b[48]	0.01	0.48	3.89	1.02	1.39	1.00	3207	1917
x_b[49]	0.00	0.47	3.74	1.00	1.35	1.00	2550	1533
x_b[50]	0.00	0.46	4.01	1.00	1.48	1.00	2881	1395
x[1]	-6.47	-0.02	6.52	0.01	34.90	1.01	3901	2122
x[2]	-6.52	0.00	6.50	3.39	146.00	1.00	3767	1947
x[3]	-6.31	-0.03	5.95	-0.08	16.20	1.00	3681	2514
x[4]	-6.76	-0.01	5.86	-1.26	50.70	1.00	3244	2159
x[5]	-6.67	-0.01	5.75	-0.31	30.30	1.00	3355	2430
x[6]	-5.64	-0.01	6.48	-146.00	6460.00	1.00	3802	2536
x[7]	-6.59	0.00	6.37	-0.58	22.60	1.00	3480	2508
x[8]	-6.50	-0.04	6.29	-0.04	20.60	1.00	3474	2374
x[9]	-5.73	-0.04	5.96	-0.92	55.60	1.00	3493	2262
x[10]	-6.37	-0.04	6.43	-0.20	25.20	1.00	2871	2286
x[11]	-5.61	-0.02	5.55	0.12	12.40	1.00	3423	2587
x[12]	-7.12	0.00	6.19	0.41	91.80	1.00	3340	2329
x[13]	-6.44	0.02	6.22	-5.65	202.00	1.00	3332	2164
x[14]	-6.72	-0.04	6.56	-2.94	135.00	1.00	3693	2257
x[15]	-5.68	0.02	6.06	-0.86	30.40	1.00	3511	1969
x[16]	-6.99	-0.01	7.24	-0.40	24.60	1.00	3614	2406
x[17]	-5.78	-0.01	5.39	-0.06	25.10	1.00	3880	2520
x[18]	-5.45	-0.01	5.92	-0.55	259.00	1.00	4303	2254
x[19]	-7.16	-0.02	5.84	9.85	549.00	1.00	3505	1931
x[20]	-7.39	-0.01	6.68	-3.09	146.00	1.00	3411	1916
x[21]	-5.93	0.05	5.85	0.23	45.60	1.00	3419	2179
x[22]	-6.96	-0.02	6.23	-0.20	27.10	1.00	3554	2149
x[23]	-5.99	0.05	6.54	2.51	115.00	1.00	3456	2098
x[24]	-6.75	0.00	6.99	-0.67	111.00	1.00	3541	1922
x[25]	-6.33	0.02	6.40	-2.71	100.00	1.00	4036	2356
x[26]	-5.57	-0.02	6.32	0.20	14.50	1.00	3335	2319
x[27]	-6.40	0.00	6.17	-0.78	52.60	1.00	3377	2400
x[28]	-5.70	0.02	6.49	3.10	105.00	1.00	3446	2121
x[29]	-5.40	0.00	5.67	-0.12	18.10	1.00	3918	2430
x[30]	-5.83	-0.01	6.45	1.00	51.20	1.00	3642	2138
x[31]	-5.85	0.02	5.66	0.86	26.30	1.00	3595	2271
x[32]	-6.49	-0.01	6.18	0.11	50.70	1.00	4227	2731
x[33]	-7.08	-0.01	6.34	-0.41	23.50	1.00	3807	2376
x[34]	-6.59	0.01	6.05	0.95	48.20	1.00	4084	2358

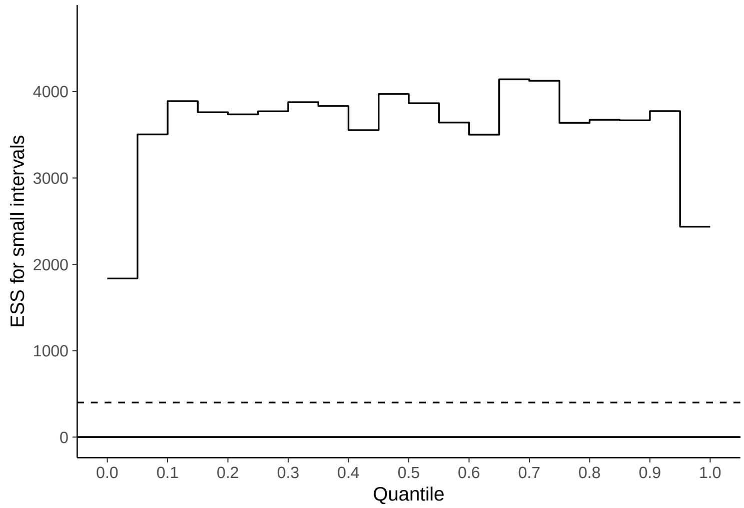


Figure 6: The local efficiency of small interval probability estimates for Cauchy model with alternative parameterization.

```
x[35]    -5.44   0.03   6.13    0.32   48.40  1.00      3756      2247
x[36]    -6.15   0.00   6.11   -0.06   28.40  1.00      3600      2386
x[37]    -6.08  -0.03   5.34    0.70   59.90  1.00      3623      2005
x[38]    -5.74  -0.02   5.77    0.20   13.20  1.00      3820      2536
x[39]    -6.73  -0.03   5.84    2.77  285.00  1.00      4121      1944
x[40]    -6.39   0.01   6.52   -2.75  103.00  1.00      3612      1823
x[41]    -6.01   0.02   5.92   -0.42   35.70  1.00      3492      2222
x[42]    -7.39   0.05   6.86    0.49   22.50  1.00      3558      1949
x[43]    -5.98  -0.03   6.69   14.40  626.00  1.00      3823      2516
x[44]    -7.04  -0.04   6.17    1.55  106.00  1.00      3310      2239
x[45]    -5.75   0.02   6.23   -0.43   32.30  1.00      3752      2437
x[46]    -5.59   0.06   6.33   -0.32   76.00  1.00      3898      1976
x[47]    -5.49   0.03   5.43   -0.02   12.10  1.00      3893      2659
x[48]    -5.96   0.00   4.85   -0.01   21.00  1.00      3674      2274
x[49]    -6.55   0.00   5.25   -1.24  129.00  1.00      3576      2243
x[50]    -6.74  -0.01   6.90   -1.06  147.00  1.00      3437      2486
I         0.00   0.00   1.00    0.50    0.50  1.00      2648      4000
lp__    -95.20 -81.00 -68.70  -81.30    8.08  1.00      1310      1928

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

All Rhat < 1.01 and ESS > 400 indicate the sampling worked much better with the alternative parameterization. Appendix E has more results using other alternative parameterizations. The `x_a` and `x_b` used to form the Cauchy distributed `x` have stable quantile, mean and sd values. As `x` is Cauchy distributed it has only stable quantiles, but wildly varying mean and sd estimates as the true values are not finite.

We can further analyze potential problems using local efficiency estimates and rank plots. We take a detailed look at x[40], which has the smallest bulk-ESS of 2848.

We examine the sampling efficiency in different parts of the posterior by computing the efficiency estimates for small interval probability estimates.

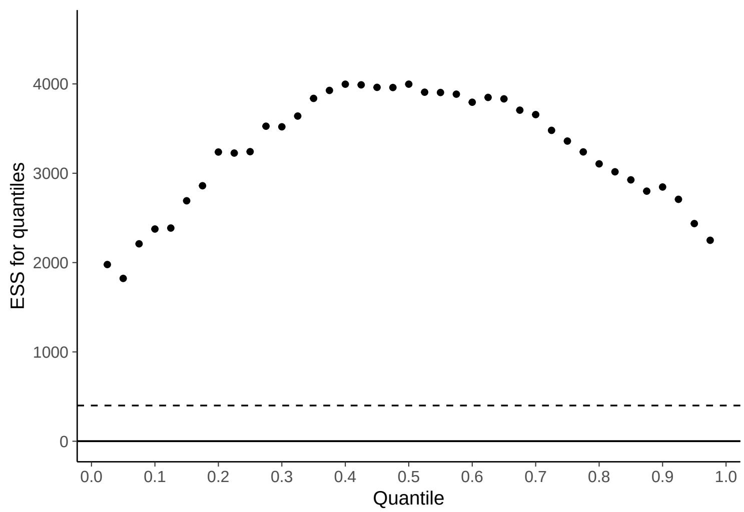


Figure 7: The efficiency of quantile estimates for Cauchy model with alternative parameterization.

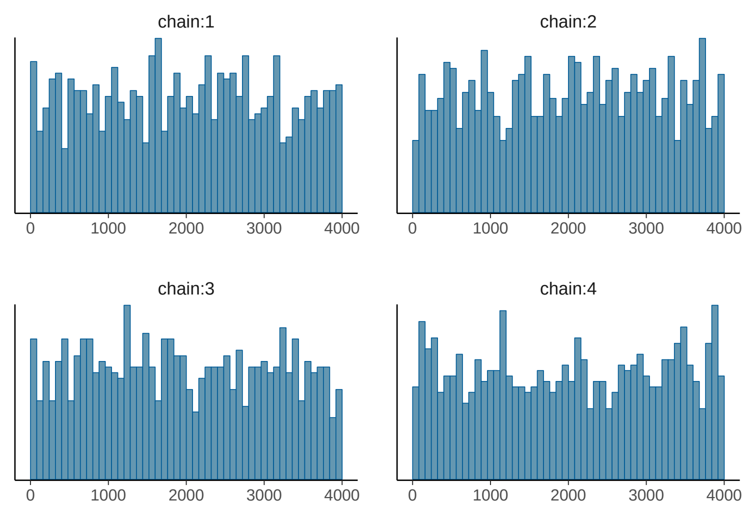


Figure 8: Rank plots of posterior draws from four chains for Cauchy model with alternative parameterization.

The efficiency estimate is good in all parts of the posterior. Further, we examine the sampling efficiency of different quantile estimates.

Rank plots also look rather similar across chains.

In summary, the alternative parameterization produces results that look much better than for the nominal parameterization. There are still some differences in the tails, which we also identified via the tail-ESS.

4.1.3 Half-Cauchy with nominal parameterization

Half-Cauchy priors are common and, for example, in Stan usually set using the nominal parameterization. However, when the constraint `<lower=0>` is used, Stan does the sampling automatically in the unconstrained `log(x)` space, which changes the geometry crucially.

```
parameters {
  vector<lower=0>[50] x;
```

```
}

model {
  x ~ cauchy(0, 1);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

Run the half-Cauchy with nominal parameterization (and positive constraint):

There are no warnings, and the sampling is much faster than for the Cauchy nominal model.

```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

         Q5   Q50  Q95  Mean      SD  Rhat Bulk_ESS Tail_ESS
x[1]   0.08  1.03 13.6 11.10  388.00     1     8077     2223
x[2]   0.10  1.02 10.8 11.60  482.00     1     9868     2612
x[3]   0.06  1.00 12.9  5.40   71.60     1     7895     2097
x[4]   0.09  0.98 11.5  4.41   29.50     1     7596     2347
x[5]   0.08  1.03 14.0  4.52   19.80     1     7495     2230
x[6]   0.08  0.99 11.7 12.50  380.00     1     7948     2145
x[7]   0.07  0.98 12.0  9.23  281.00     1     8336     2117
x[8]   0.09  0.99 10.8  4.61   40.80     1     8194     2165
x[9]   0.09  1.02 11.6 11.70  483.00     1     8464     2127
x[10]  0.07  1.03 14.9  6.01   51.00     1     7963     2399
x[11]  0.08  0.97 12.5 15.60  532.00     1     6980     1788
x[12]  0.07  1.03 13.3  4.10   17.50     1     8226     2029
x[13]  0.08  1.01 14.1  8.88  120.00     1     8077     2032
x[14]  0.07  0.96 13.5  6.91   71.50     1     7455     2261
x[15]  0.07  1.00 14.4  8.66   95.80     1     6766     2246
x[16]  0.08  0.99 14.1  5.55   38.40     1     7396     2174
x[17]  0.08  0.99 11.7  8.70  300.00     1     7144     2260
x[18]  0.09  0.98 11.6 14.40  398.00     1     7614     2035
x[19]  0.07  0.99 14.3  6.33   69.10     1     7823     1825
x[20]  0.09  1.00 11.2  6.40  160.00     1     7905     2355
x[21]  0.07  1.00 12.0  7.03  144.00     1     7843     2078
x[22]  0.09  1.02 12.7 32.20 1730.00     1     7735     2043
x[23]  0.07  0.98 13.5  6.33   67.30     1     7119     2142
x[24]  0.07  1.00 12.3  4.99   41.60     1     6893     1982
x[25]  0.09  1.00 11.5  8.60  270.00     1     7757     2351
x[26]  0.08  0.98 10.7  6.97  119.00     1     6433     2230
x[27]  0.08  1.01 13.4  4.88   34.30     1     7005     2119
x[28]  0.08  0.97 11.4  5.76   66.70     1     9631     2228
x[29]  0.07  1.00 13.7 10.40  240.00     1     6109     2312
x[30]  0.09  1.02 11.0  7.98  206.00     1     7958     2368
x[31]  0.08  0.96 12.4  4.39   32.10     1     6493     2102
x[32]  0.10  1.01 11.5  4.99   55.40     1     7043     1742
x[33]  0.08  0.99 13.8  5.45   36.80     1     6913     2455
x[34]  0.08  0.98 12.4  5.92   78.20     1     8610     2514
x[35]  0.07  0.96 13.6  5.70   57.40     1     6406     2160
x[36]  0.06  1.00 13.5  5.36   39.60     1     7694     2031
x[37]  0.07  1.00 13.9  8.29  196.00     1     7276     2491
x[38]  0.08  1.02 12.2  6.40  119.00     1     6790     2369
```

```
x[39]    0.10   1.01  11.7   6.67   88.50     1     7739     2518
x[40]    0.09   0.96  12.1   5.16   44.40     1     7087     2349
x[41]    0.07   0.96  12.9   4.97   42.30     1     8650     2333
x[42]    0.07   1.02  13.3   7.77  132.00     1     8703     2410
x[43]    0.08   0.97  10.2  26.60 1400.00     1     8747     2194
x[44]    0.08   1.03  12.3   5.96   59.30     1     6378     2257
x[45]    0.08   0.98  12.2   7.70  123.00     1     8430     2314
x[46]    0.08   0.99  12.1   5.36   72.20     1     8185     2237
x[47]    0.08   1.01  14.5   7.00   76.70     1     9562     2265
x[48]    0.08   1.01  13.0   5.06   30.40     1     8402     2690
x[49]    0.08   1.00  12.9   7.48  100.00     1     7993     1804
x[50]    0.08   1.00  13.2   8.86  179.00     1     7523     2243
I        0.00   0.00   1.0   0.49    0.50     1     7357     4000
lp__   -80.60 -69.10 -59.3 -69.30    6.42     1     1218     2001

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

All Rhat < 1.01 and ESS > 400 indicate good performance of the sampler. We see that the Stan's automatic (and implicit) transformation of constraint parameters can have a big effect on the sampling performance. More experiments with different parameterizations of the half-Cauchy distribution can be found in Appendix E.

4.2 Hierarchical model: Eight Schools

The Eight Schools data is a classic example for hierarchical models (see Section 5.5 in Gelman et al., 2013), which despite the apparent simplicity nicely illustrates the typical problems in inference for hierarchical models. The Stan models below are from Michael Betancourt's case study on Diagnosing Biased Inference with Divergences. Appendix F contains more detailed analysis of different algorithm variants.

4.2.1 A Centered Eight Schools model

```
data {
  int<lower=0> J;
  real y[J];
  real<lower=0> sigma[J];
}

parameters {
  real mu;
  real<lower=0> tau;
  real theta[J];
}

model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 5);
  theta ~ normal(mu, tau);
  y ~ normal(theta, sigma);
}
```

4.2.1.1 Centered Eight Schools model

We directly run the centered parameterization model with an increased `adapt_delta` value to reduce the probability of getting divergent transitions.

Despite an increased `adapt_delta`, we still observe a lot of divergent transitions, which in itself is already sufficient indicator to not trust the results. We can use Rhat and ESS diagnostics to recognize problematic parts of the posterior and they could be used in cases when other MCMC algorithms than HMC is used.

```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

              Q5    Q50   Q95   Mean   SD  Rhat Bulk_ESS Tail_ESS
mu         -1.11   4.53  9.90   4.44 3.39  1.02      548      754
tau         0.39   2.85  9.61   3.62 3.10  1.07       67       82
theta[1]   -2.24   5.81 16.30   6.23 5.74  1.02      747     1294
theta[2]   -2.60   5.07 13.40   5.08 4.86  1.01      970     1240
theta[3]   -5.01   4.35 12.10   3.94 5.33  1.01      899     1147
theta[4]   -2.86   5.00 12.80   4.89 4.82  1.01      986     1059
theta[5]   -4.74   4.03 10.80   3.66 4.81  1.01      715      988
theta[6]   -4.15   4.28 11.60   4.08 4.84  1.01      833      976
theta[7]   -1.30   5.97 15.60   6.31 5.18  1.02      612     1182
theta[8]   -3.37   5.12 13.80   4.98 5.34  1.01      901     1477
lp__      -24.70 -15.00  0.37 -14.00 7.44  1.07       69       89

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

See Appendix F for results of longer chains.

Bulk-ESS and Tail-ESS for the between school standard deviation `tau` are 67 and 82 respectively. Both are less than 400, indicating we should investigate that parameter more carefully. We thus examine the sampling efficiency in different parts of the posterior by computing the efficiency estimate for small interval estimates for `tau`. These plots may either show quantiles or parameter values at the vertical axis. Red ticks show divergent transitions.

We see that the sampler has difficulties in exploring small `tau` values. As the sampling efficiency for estimating small `tau` values is practically zero, we may assume that we may miss substantial amount of posterior mass and get biased estimates. Red ticks, which show iterations with divergences, have concentrated to small `tau` values, indicate also problems exploring small values which is likely to cause bias.

We examine also the sampling efficiency of different quantile estimates. Again, these plots may either show quantiles or parameter values at the vertical axis.

Most of the quantile estimates have worryingly low effective sample size.

Let's see how the estimated effective sample size changes when we use more and more draws. Here we don't see sudden changes, but both bulk-ESS and tail-ESS are too low. See Appendix F for results of longer chains.

In lines with these findings, the rank plots of `tau` clearly show problems in the mixing of the chains.

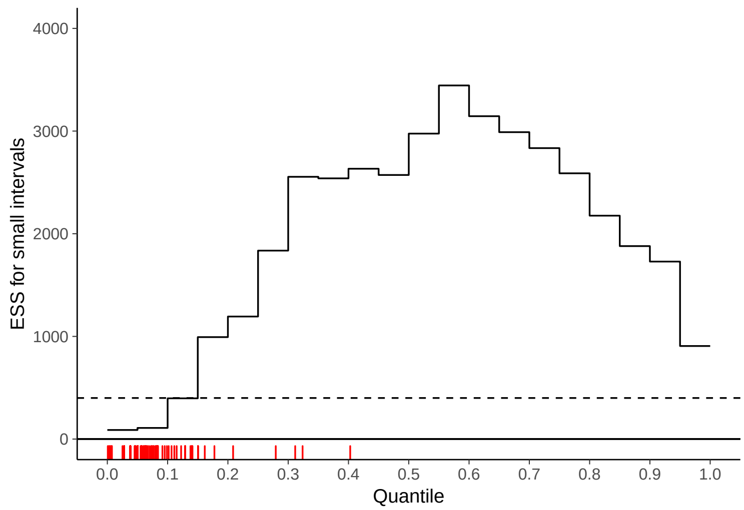


Figure 9: The local efficiency of small interval probability estimates for 8 schools model with centered parameterization.

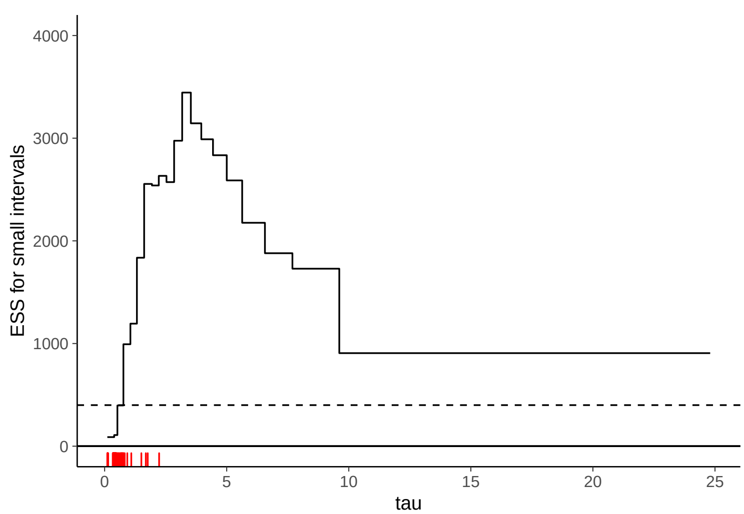


Figure 10: The local efficiency of small interval probability estimates for 8 schools model with centered parameterization. Vertical axis is instead of ranks in scale of parameter τ.

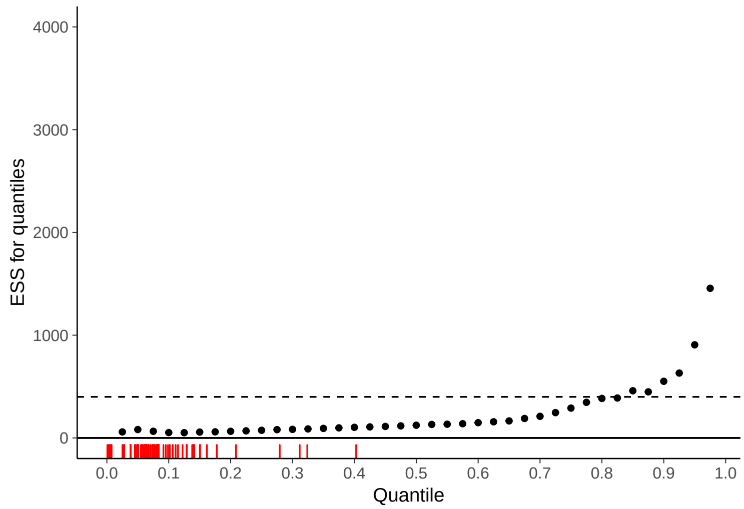


Figure 11: The efficiency of quantile estimates for 8 schools model with centered parameterization.

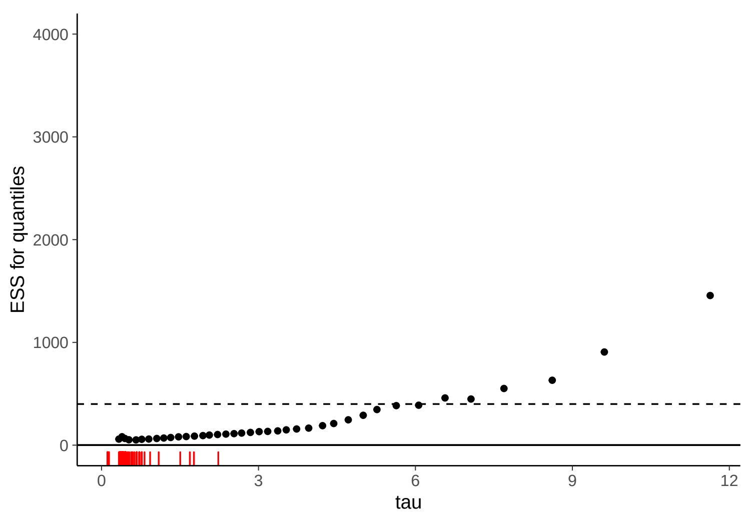


Figure 12: The efficiency of quantile estimates for 8 schools model with centered parameterization. Vertical axis is instead of ranks in scale of parameter τ.

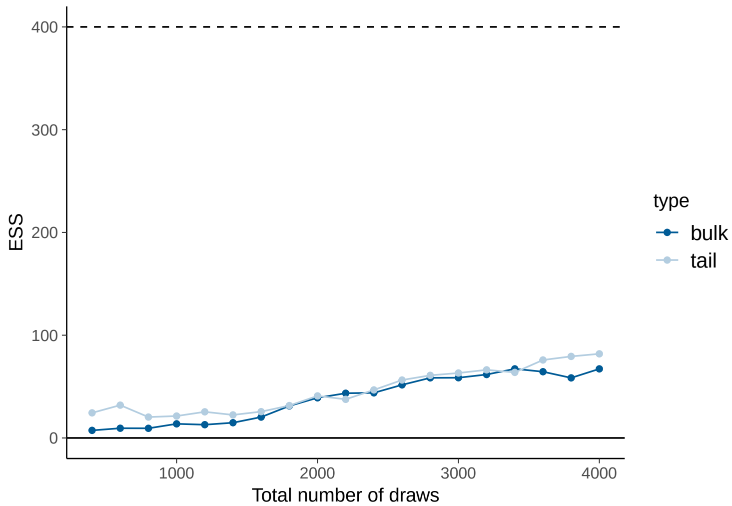


Figure 13: The estimated effective sample sizes with increasing number of iterations for 8 schools model with centered parameterization.

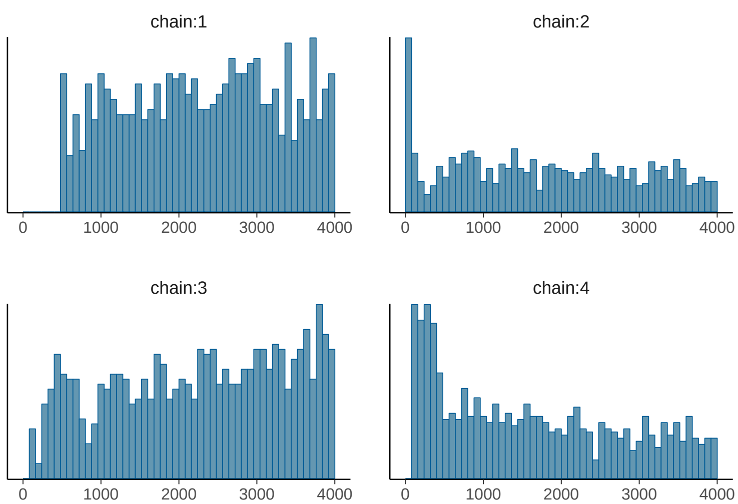


Figure 14: Rank plots of posterior draws from four chains for 8 schools model with centered parameterization.

4.2.2 Non-centered Eight Schools model

For hierarchical models, the non-centered parameterization often works better than the centered one:

```
data {
  int<lower=0> J;
  real y[J];
  real<lower=0> sigma[J];
}

parameters {
  real mu;
  real<lower=0> tau;
  real theta_tilde[J];
}

transformed parameters {
  real theta[J];
  for (j in 1:J)
    theta[j] = mu + tau * theta_tilde[j];
}

model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 5);
  theta_tilde ~ normal(0, 1);
  y ~ normal(theta, sigma);
}
```

For reasons of comparability, we also run the non-centered parameterization model with an increased `adapt_delta` value:

We get zero divergences and no other warnings which is a first good sign.

```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

                   Q5   Q50   Q95  Mean   SD  Rhat Bulk_ESS Tail_ESS
mu              -1.14  4.42  9.96  4.47 3.37     1     5531     3004
tau              0.30  2.81  9.50  3.59 3.17     1     2872     1908
theta_tilde[1]  -1.29  0.31  1.88  0.31 0.98     1     5046     2874
theta_tilde[2]  -1.44  0.11  1.62  0.10 0.94     1     4177     2735
theta_tilde[3]  -1.64 -0.08  1.48 -0.08 0.97     1     6485     2994
theta_tilde[4]  -1.51  0.08  1.62  0.06 0.95     1     6076     2514
theta_tilde[5]  -1.71 -0.17  1.39 -0.16 0.94     1     5608     3177
theta_tilde[6]  -1.64 -0.06  1.53 -0.06 0.97     1     4855     2773
theta_tilde[7]  -1.25  0.40  1.87  0.37 0.96     1     4796     2849
theta_tilde[8]  -1.54  0.07  1.66  0.06 0.96     1     6142     2972
theta[1]        -1.62  5.64 16.30  6.25 5.58     1     4907     3015
theta[2]        -2.42  4.82 13.00  5.01 4.68     1     5122     3242
theta[3]        -4.63  4.26 12.10  4.09 5.27     1     5457     3407
theta[4]        -2.73  4.75 12.50  4.82 4.78     1     4695     3130
theta[5]        -3.96  3.82 11.00  3.72 4.62     1     5346     3398
theta[6]        -3.88  4.27 11.40  4.13 4.95     1     5670     3393
theta[7]        -0.98  5.88 15.40  6.38 5.10     1     4708     3242
theta[8]        -3.23  4.78 13.10  4.87 5.17     1     4924     3037
lp__           -11.20 -6.60 -3.78 -6.92 2.31     1     1641     2344
```

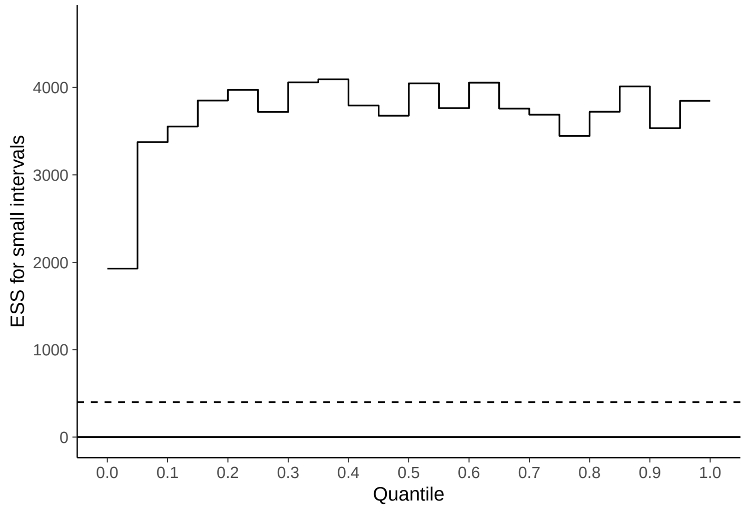


Figure 15: The local efficiency of small interval probability estimates for 8 schools model with non-centered parameterization.

```
For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

All Rhat < 1.01 and ESS > 400 indicate a much better performance of the non-centered parameterization.

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates for `tau`.

Small `tau` values are still more difficult to explore, but the relative efficiency is in a good range. We may also check this with a finer resolution:

The sampling efficiency for different quantile estimates looks good as well.

In line with these findings, the rank plots of `tau` show no substantial differences between chains.

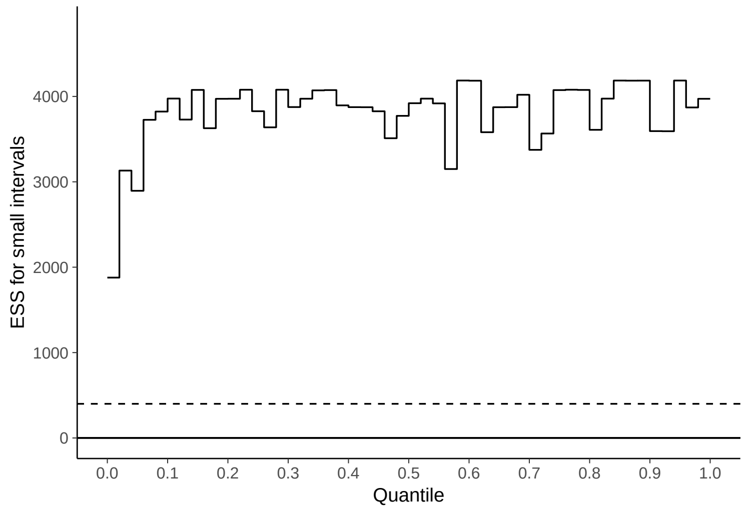


Figure 16: The local efficiency of small interval probability estimates with more fine resolution for 8 schools model with non-centered parameterization.

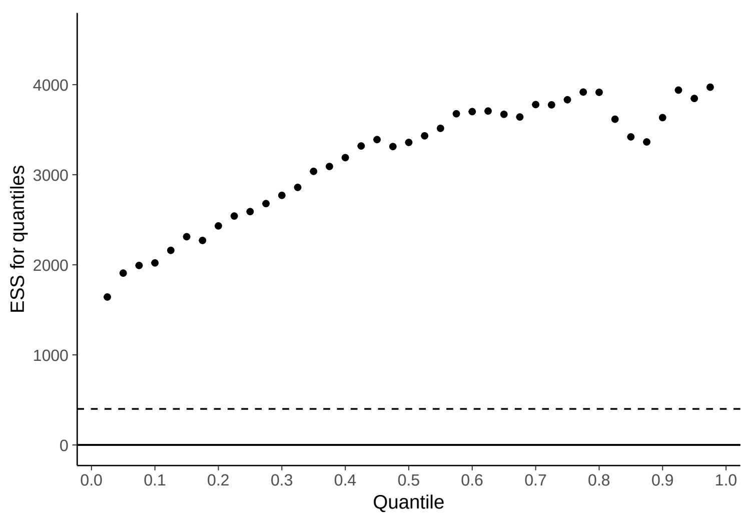


Figure 17: The efficiency of quantile estimates for 8 schools model with non-centered parameterization.

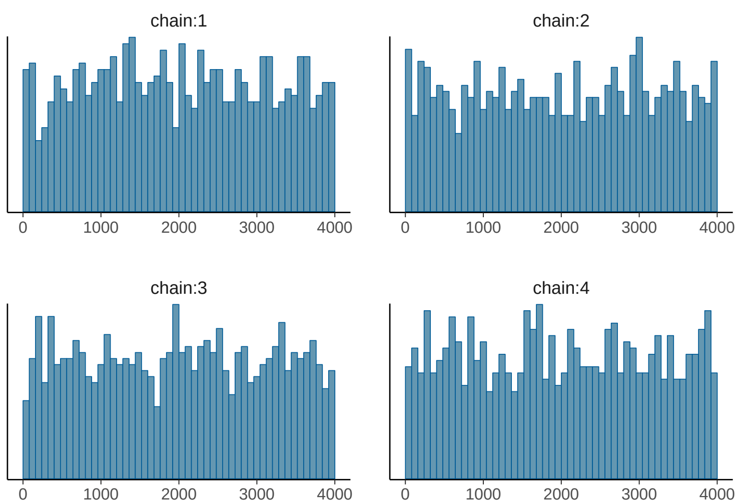


Figure 18: Rank plots of posterior draws from four chains for 8 schools model with non-centered parameterization.

References

Appendices

Appendix A: Abbreviations

The following abbreviations are used throughout the appendices:

- N = total number of draws
- Rhat = classic no-split-Rhat
- sRhat = classic split-Rhat
- zsRhat = rank-normalized split-Rhat
  - all chains are jointly ranked and z-transformed
  - can detect differences in location and trends
- zfsRhat = rank-normalized folded split-Rhat
  - all chains are jointly "folded" by computing absolute deviation from median, ranked and z-transformed
  - can detect differences in scales
- seff = no-split effective sample size
- reff = seff / N
- zsseff = rank-normalized split effective sample size
  - estimates the efficiency of mean estimate for rank normalized values
- zsreff = zsseff / N
- zfsseff = rank-normalized folded split effective sample size
  - estimates the efficiency of rank normalized *mean* absolute deviation
- zfsreff = zfsseff / N
- tailseff = minimum of rank-normalized split effective sample sizes of the 5% and 95% quantiles
- tailreff = tailseff / N
- medsseff = median split effective sample size
  - estimates the efficiency of the median
- medsreff = medsseff / N
- madsseff = mad split effective sample size
  - estimates the efficiency of the median absolute deviation
- madsreff = madsseff / N

Appendix B: Examples of rank normalization

We will illustrate the rank normalization with a few examples. First, we plot histograms, and empirical cumulative distribution functions (ECDF) with respect to the original parameter values (θ), scaled ranks (ranks divided by the maximum rank), and rank normalized values (z). We used scaled ranks to make the plots look similar for different number of draws.

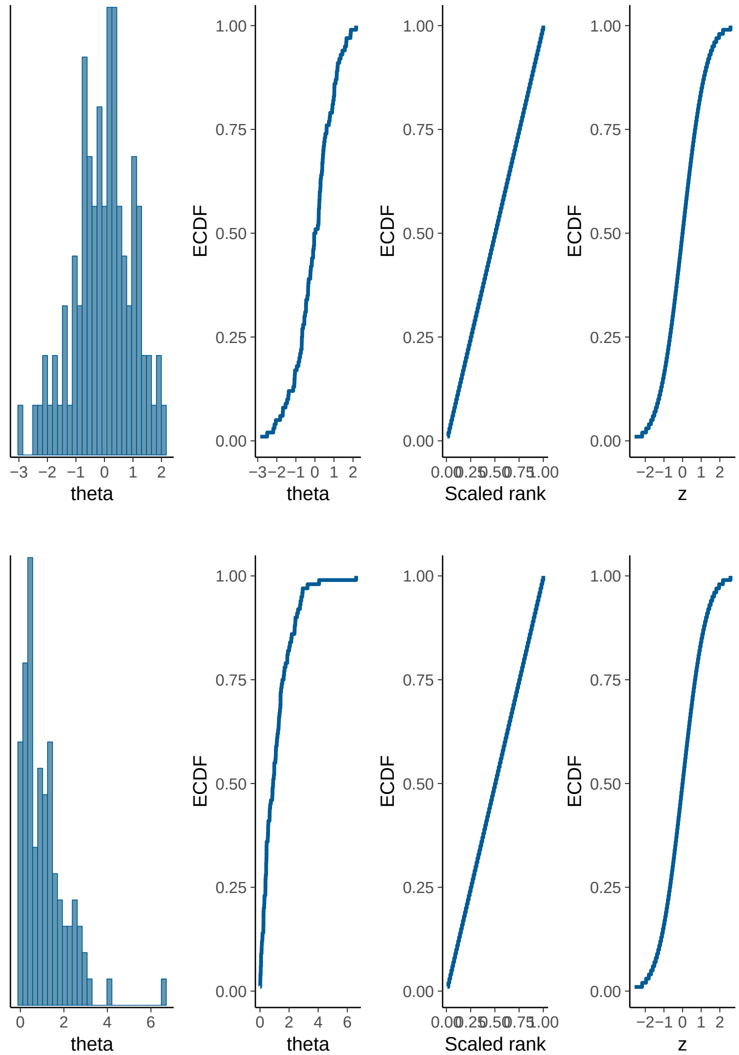
100 draws from Normal(0, 1):

100 draws from Exponential(1):

100 draws from Cauchy(0, 1):

In the above plots, the ECDF with respect to scaled rank and rank normalized z-values look exactly the same for all distributions. In *Split*-$\widehat{R}$ and effective sample size computations, we rank all draws jointly, but then compare ranks and ECDF of individual split chains. To illustrate the variation between chains, we draw 8 batches of 100 draws each from Normal(0, 1):

The variation in ECDF due to the variation ranks is now visible also in scaled ranks and rank normalized z-values from different batches (chains).



The benefit of rank normalization is more obvious for non-normal distribution such as Cauchy:

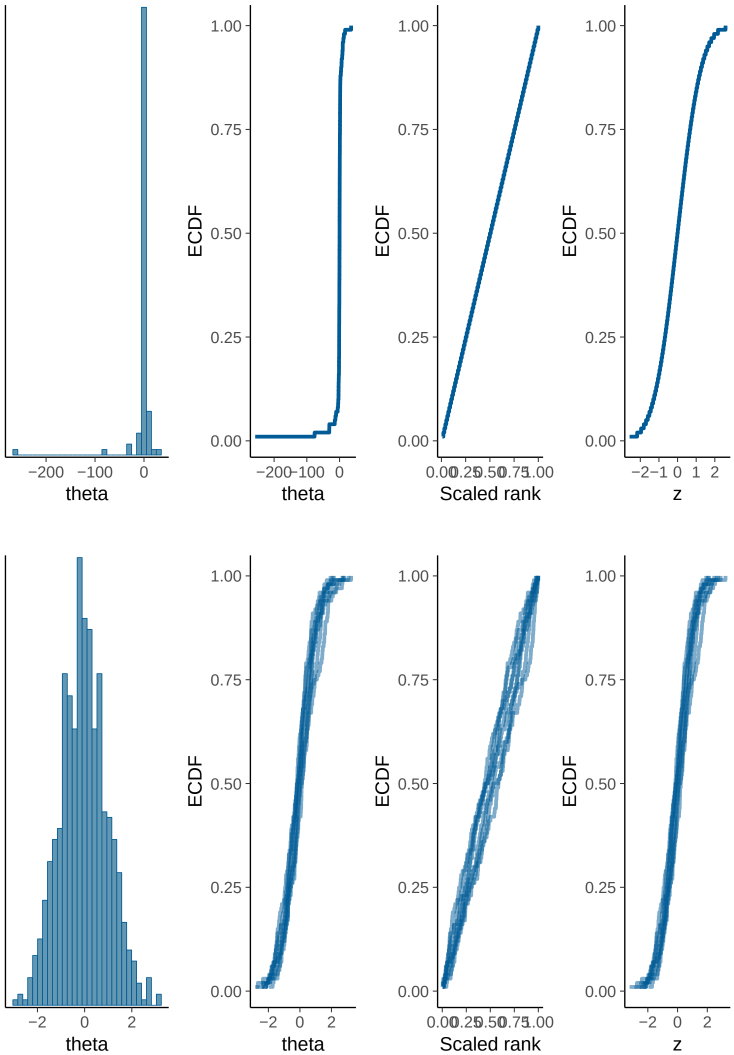
Rank normalization makes the subsequent computations well defined and invariant under bijective transformations. This means that we get the same results, for example, if we use unconstrained or constrained parameterisations in a model.

Appendix C: Variance of the cumulative distribution function

In Section 3, we had defined the empirical CDF (ECDF) for any θ_α as

$$p(\theta \leq \theta_\alpha) \approx \bar{I}_\alpha = \frac{1}{S} \sum_{s=1}^{S} I(\theta^{(s)} \leq \theta_\alpha),$$

For independent draws, $\bar{I}_\alpha$ has a $\mathrm{Beta}(\bar{I}_\alpha + 1, S - \bar{I}_\alpha + 1)$ distribution. Thus we can easily examine the variation of the ECDF for any θ_α value from a single chain. If $\bar{I}_\alpha$ is not very close to 1 or S and S is large, we can use the variance of Beta distribution

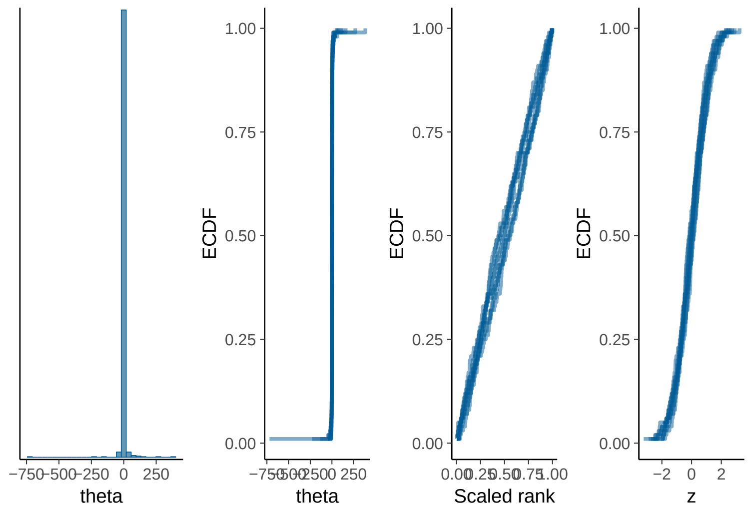


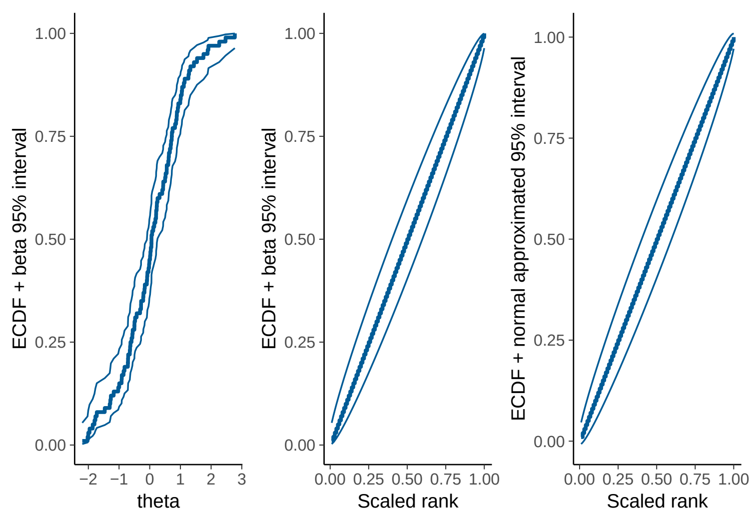
$$\mathrm{Var}[p(\theta \leq \theta_\alpha)] = \frac{(\bar{I}_\alpha + 1) * (S - \bar{I}_\alpha + 1)}{(S+2)^2(S+3)}.$$

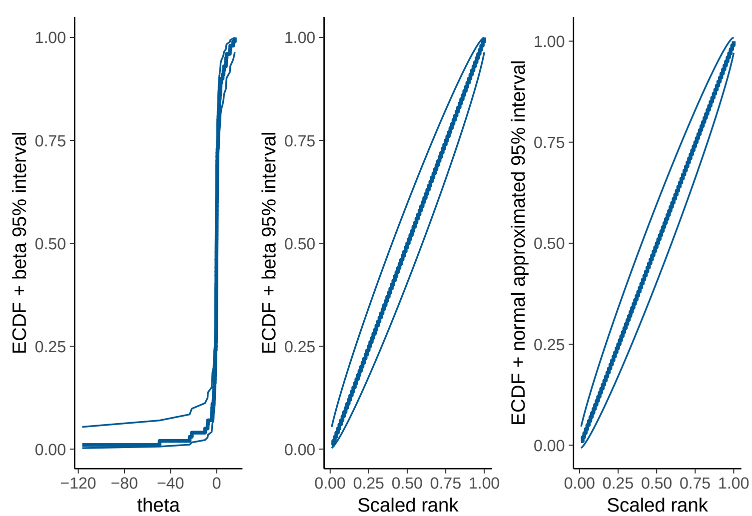
We illustrate uncertainty intervals of the Beta distribution and normal approximation of ECDF for 100 draws from Normal(0, 1):

Uncertainty intervals of ECDF for draws from Cauchy(0, 1) illustrate again the improved visual clarity in plotting when using scaled ranks:

The above plots illustrate that the normal approximation is accurate for practical purposes in MCMC diagnostics.


theta
ECDF
theta
ECDF
Scaled rank
ECDF
z


ECDF + beta 95% interval
theta
ECDF + beta 95% interval
Scaled rank
ECDF + normal approximated 95% interval
Scaled rank


ECDF + beta 95% interval
theta
ECDF + beta 95% interval
Scaled rank
ECDF + normal approximated 95% interval
Scaled rank

Appendix D: Normal distributions with additional trend, shift or scaling

This part focuses on diagnostics for

- all chains having a trend and a similar marginal distribution
- one of the chains having a different mean
- one of the chains having a lower marginal variance

To simplify, in this part, independent draws are used as a proxy for very efficient MCMC sampling. First, we sample draws from a standard-normal distribution. We will discuss the behavior for non-normal distributions later. See Appendix A for the abbreviations used.

Adding the same trend to all chains

All chains are from the same Normal(0, 1) distribution plus a linear trend added to all chains:

If we don't split chains, Rhat misses the trends if all chains still have a similar marginal distribution.

Split-Rhat can detect trends, even if the marginals of the chains are similar.

Result: Split-Rhat is useful for detecting non-stationarity (i.e., trends) in the chains. If we use a threshold of 1.01, we can detect trends which account for 2% or more of the total marginal variance. If we use a threshold of 1.1, we detect trends which account for 30% or more of the total marginal variance.

The effective sample size is based on split Rhat and within-chain autocorrelation. We plot the relative efficiency $R_{\text{eff}} = S_{\text{eff}}/S$ for easier comparison between different values of S. In the plot below, dashed lines indicate the threshold at which we would consider the effective sample size to be sufficient (i.e., $S_{\text{eff}} > 400$). Since we plot the relative efficiency instead of the effective sample size itself, this threshold is divided by S, which we compute here as the number of iterations per chain (variable `iter`) times the number of chains (4).

Result: Split-Rhat is more sensitive to trends for small sample sizes, but effective sample size becomes more sensitive for larger samples sizes (as autocorrelations can be estimated more accurately).

Advice: If in doubt, run longer chains for more accurate convergence diagnostics.

Shifting one chain

Next we investigate the sensitivity to detect if one of the chains has not converged to the same distribution as the others, but has a different mean.

Result: If we use a threshold of 1.01, we can detect shifts with a magnitude of one third or more of the marginal standard deviation. If we use a threshold of 1.1, we detect shifts with a magnitude equal to or larger than the marginal standard deviation.

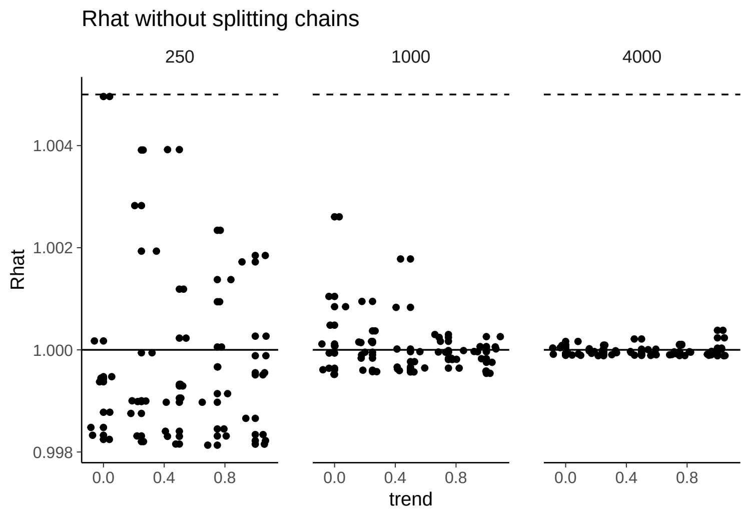
Result: The effective sample size is not as sensitive, but a shift with a magnitude of half the marginal standard deviation or more will lead to very low relative efficiency when the total number of draws increases.

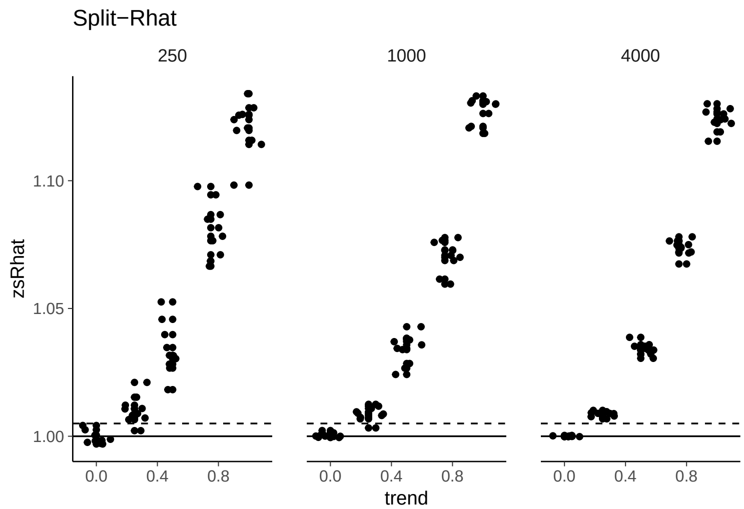
Rank plots can be used to visualize differences between chains. Here, we show rank plots for the case of 4 chains, 250 draws per chain, and a shift of 0.5.

Although, Rhat was less than 1.05 for this situation, the rank plots clearly show that the first chains behaves differently.

Scaling one chain

Next, we investigate the sensitivity to detect if one of the chains has not converged to the same distribution as the others, but has lower marginal variance.





We first look at the Rhat estimates:

Result: Split-Rhat is not able to detect scale differences between chains.

Result: Folded-Split-Rhat focuses on scales and detects scale differences.

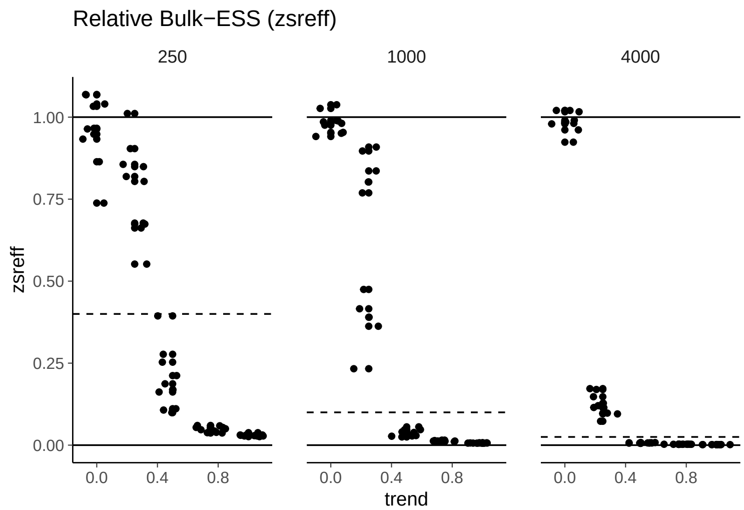
Result: If we use a threshold of 1.01, we can detect a chain with scale less than 3/4 of the standard deviation of the others. If we use threshold of 1.1, we detect a chain with standard deviation less than 1/4 of the standard deviation of the others.

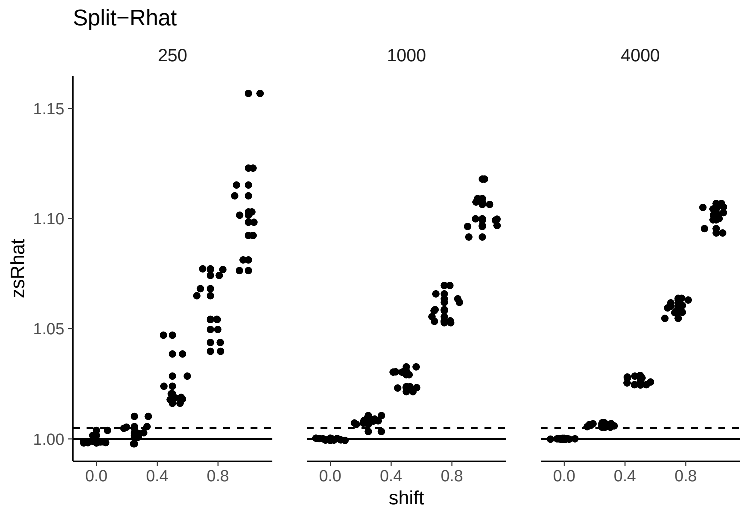
Next, we look at the effective sample size estimates:

Result: The bulk effective sample size of the mean does not see a problem as it focuses on location differences between chains.

Rank plots can be used to visualize differences between chains. Here, we show rank plots for the case of 4 chains, 250 draws per chain, and with one chain having a standard deviation of 0.75 as opposed to a standard deviation of 1 for the other chains.

Although folded Rhat is 1.06, the rank plots clearly show that the first chains behaves differently.





Appendix E: Cauchy: A distribution with infinite mean and variance

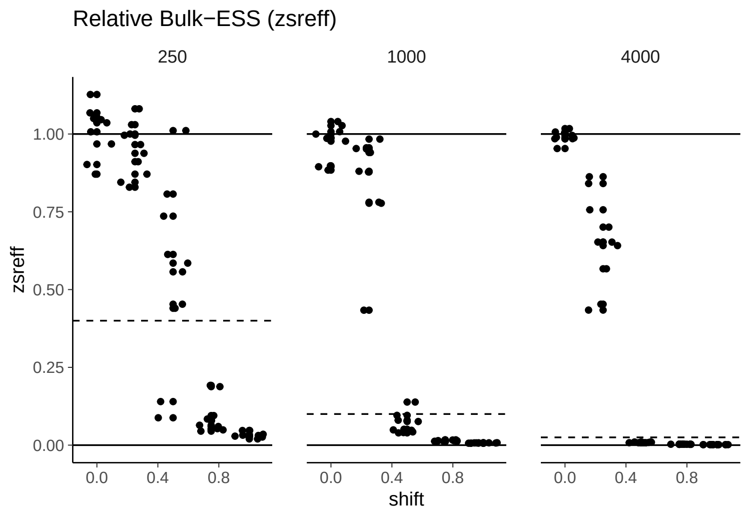
The classic split-Rhat is based on calculating within and between chain variances. If the marginal distribution of a chain is such that the variance is not defined (i.e. infinite), the classic split-Rhat is not well justified. In this section, we will use the Cauchy distribution as an example of such distribution. Also in cases where mean and variance are finite, the distribution can be far from Gaussian. Especially distributions with very long tails cause instability for variance and autocorrelation estimates. To alleviate these problems we will use Split-Rhat for rank-normalized draws.

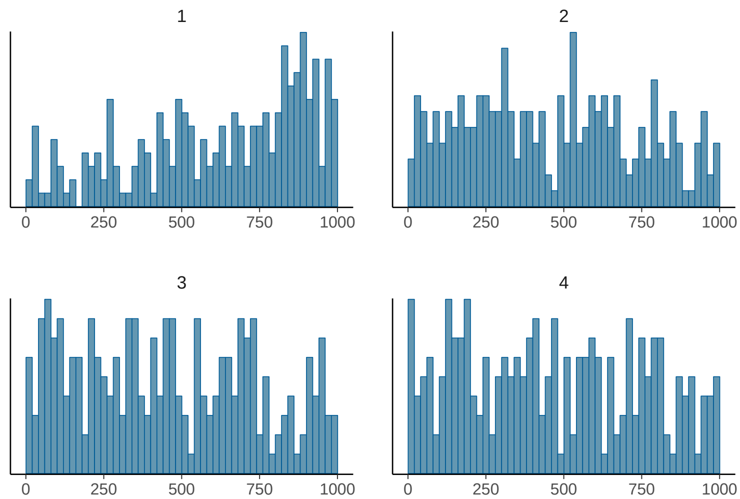
The following Cauchy models are from Michael Betancourt's case study Fitting The Cauchy Distribution

Nominal parameterization of Cauchy

We already looked at the nominal Cauchy model with direct parameterization in the main text, but for completeness, we take a closer look using different variants of the diagnostics.

```
parameters {
  vector[50] x;
}
```





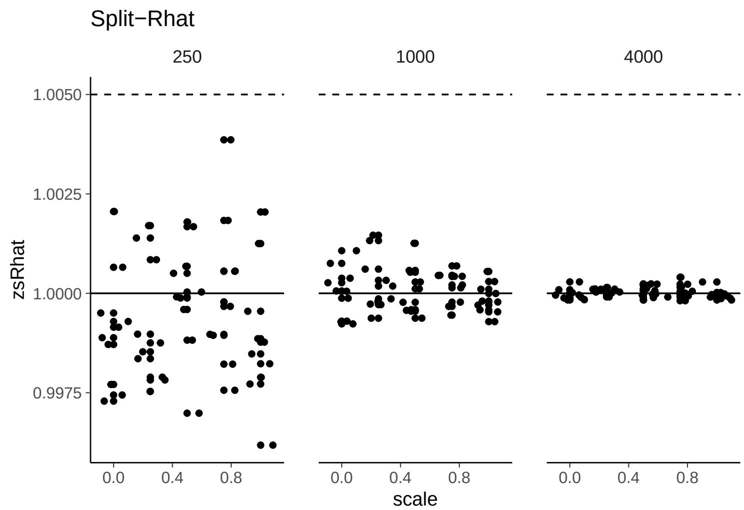

```
model {
  x ~ cauchy(0, 1);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

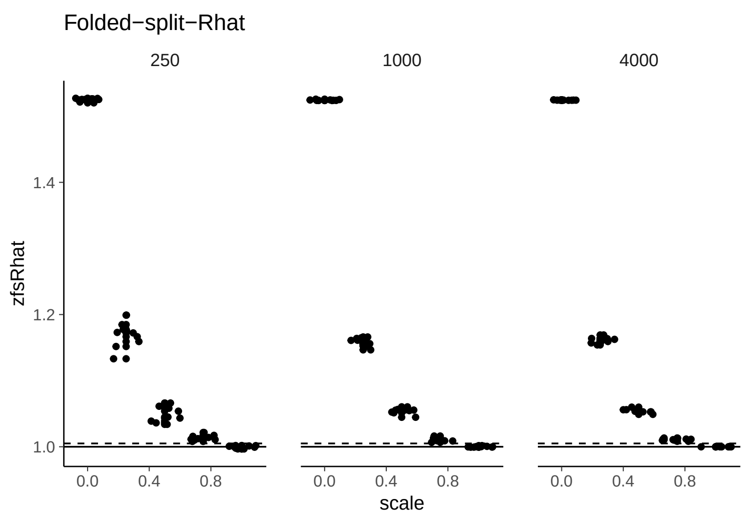
4.2.2.1 Default Stan options

Run the nominal model:

Treedepth exceedence and Bayesian Fraction of Missing Information are dynamic HMC specific diagnostics (Betancourt, 2017). We get warnings about very large number of transitions after warmup that exceeded the maximum treedepth, which is likely due to very long tails of the Cauchy distribution. All chains have low estimated Bayesian fraction of missing information also indicating slow mixing.

Trace plots for the first parameter look wild with occasional large values:





Let's check Rhat and ESS diagnostics.

For one parameter, Rhats exceed the classic threshold of 1.1. Depending on the Rhat estimate, a few others also exceed the threshold of 1.01. The rank normalized split-Rhat has several values over 1.01. Please note that the classic split-Rhat is not well defined in this example, because mean and variance of the Cauchy distribution are not finite.

Both classic and new effective sample size estimates have several very small values, and so the overall sample shouldn't be trusted.

Result: Effective sample size is more sensitive than (rank-normalized) split-Rhat to detect problems of slow mixing.

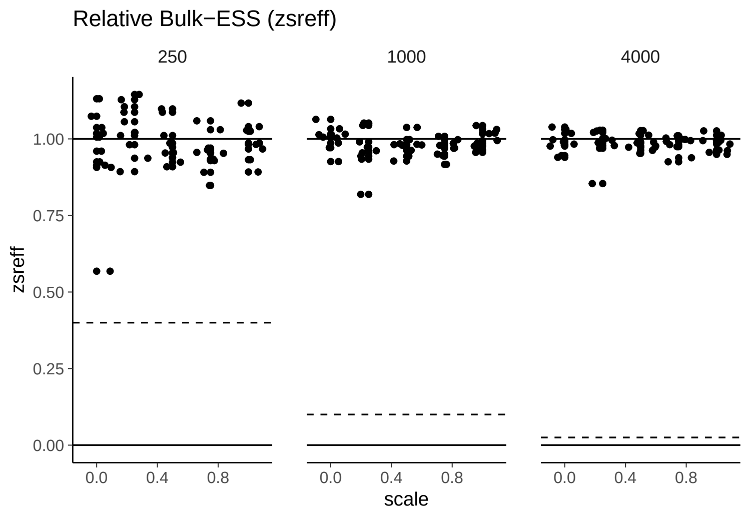
We also check the log posterior value `lp__` and find out that the effective sample size is worryingly low.

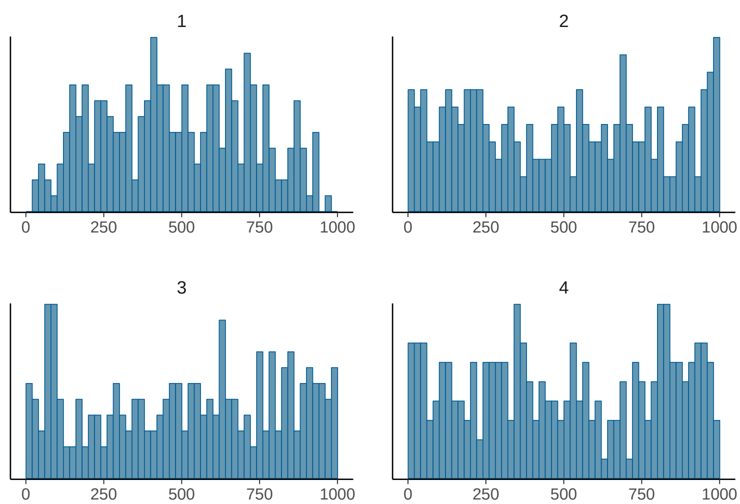
```
lp__: Bulk-ESS =  117
```

```
lp__: Tail-ESS =  323
```

We can further analyze potential problems using local effective sample size and rank plots. We examine x[36], which has the smallest tail-ESS of 117.

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size





for small interval probability estimates (see Section Efficiency for small interval probability estimates). Each interval contains $1/k$ of the draws (e.g., with $k = 20$). The small interval efficiency measures mixing of an indicator function which indicates when the values are inside the specific small interval. This gives us a local efficiency measure which does not depend on the shape of the distribution.

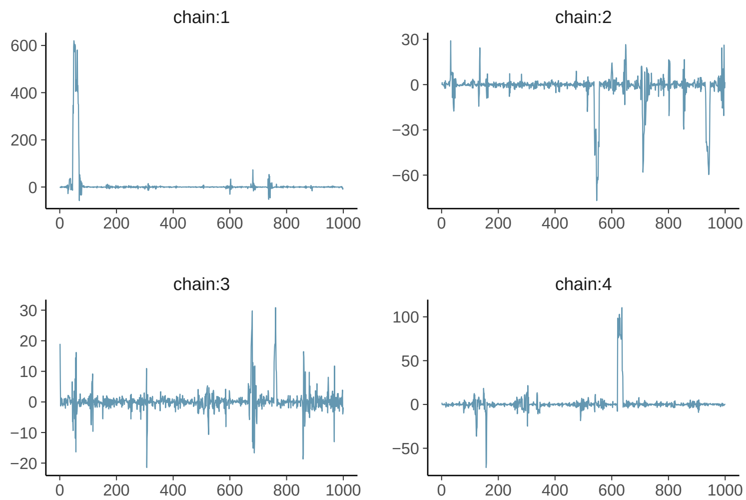
We see that the efficiency is worryingly low in the tails (which is caused by slow mixing in long tails of Cauchy). Orange ticks show draws that exceeded the maximum treedepth.

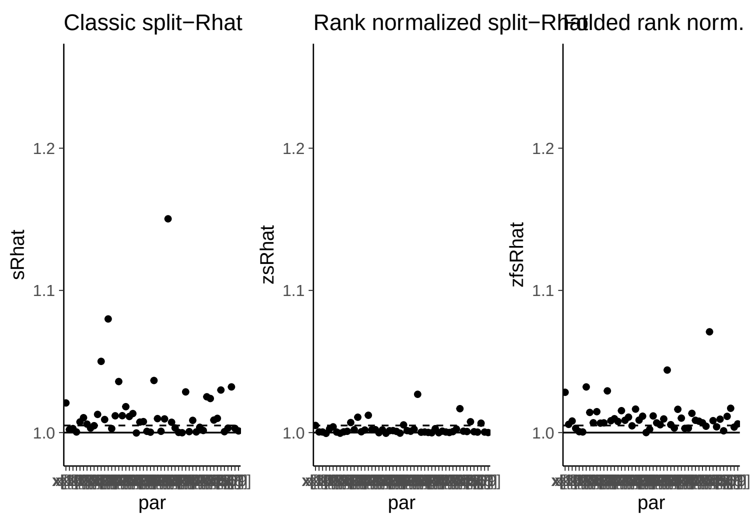
An alternative way to examine the effective sample size in different parts of the posterior is to compute effective sample size for quantiles (see Section Efficiency for quantiles). Each interval has a specified proportion of draws, and the efficiency measures mixing of an indicator function's results which indicate when the values are inside the specific interval.

We see that the efficiency is worryingly low in the tails (which is caused by slow mixing in long tails of Cauchy). Orange ticks show draws that exceeded the maximum treedepth.

We can further analyze potential problems using rank plots, from which we clearly see differences between chains.

4.2.2.2 Default Stan options + increased maximum treedepth





We can try to improve the performance by increasing `max_treedepth` to 20:

Trace plots for the first parameter still look wild with occasional large values.

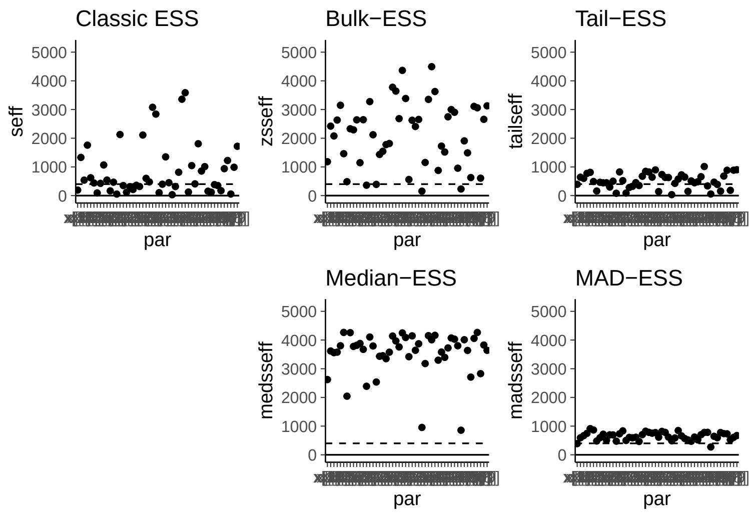
We check the diagnostics for all x.

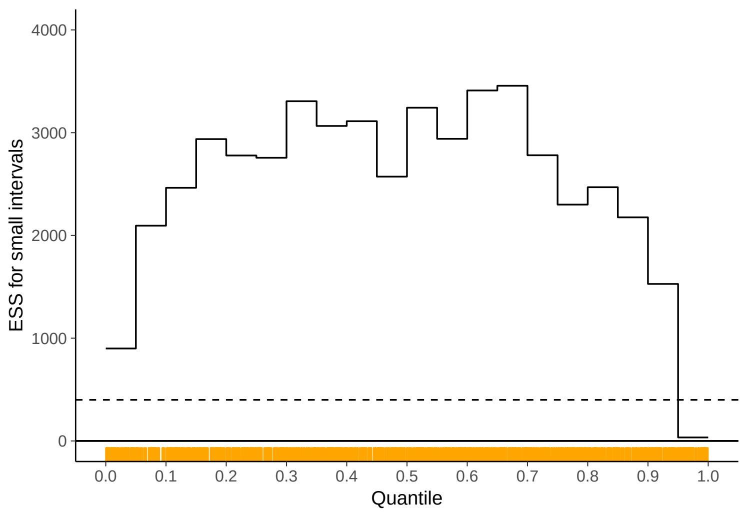
All Rhats are below 1.1, but many are over 1.01. Classic split-Rhat has more variation than the rank normalized Rhat (note that the former is not well defined). The folded rank normalized Rhat shows that there is still more variation in the scale than in the location between different chains.

Some classic effective sample sizes are very small. If we wouldn't realize that the variance is infinite, we might try to run longer chains, but in case of an infinite variance, zero relative efficiency (ESS/S) is the truth and longer chains won't help with that. However other quantities can be well defined, and that's why it is useful to also look at the rank normalized version as a generic transformation to achieve finite mean and variance. The smallest bulk-ESS is less than 1000, which is not that bad. The smallest median-ESS is larger than 2500, that is we are able to estimate the median efficiently. However, many tail-ESS's are less than 400 indicating problems for estimating the scale of the posterior.

Result: The rank normalized effective sample size is more stable than classic effective sample size, which is not well defined for the Cauchy distribution.

Result: It is useful to look at both bulk- and tail-ESS.





We check also `lp__`. Although increasing `max_treedepth` improved bulk-ESS of `x`, the efficiency for `lp__` didn't change.

`lp__: Bulk-ESS = 240`

`lp__: Tail-ESS = 587`

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.

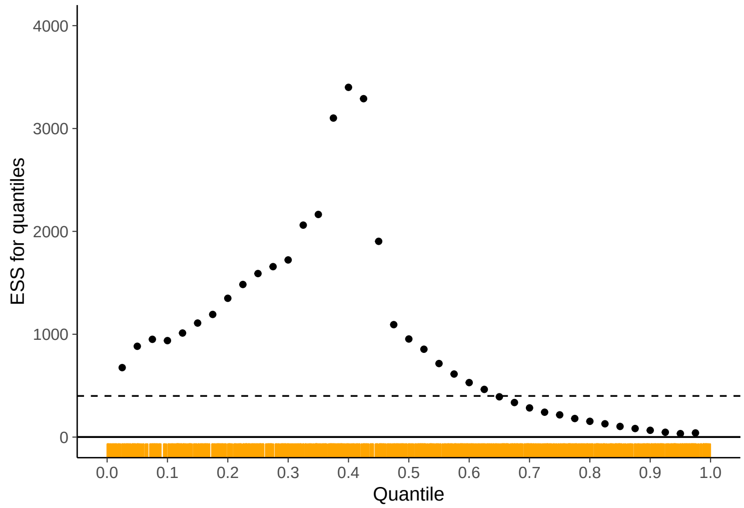
It seems that increasing `max_treedepth` has not much improved the efficiency in the tails. We also examine the effective sample size of different quantile estimates.

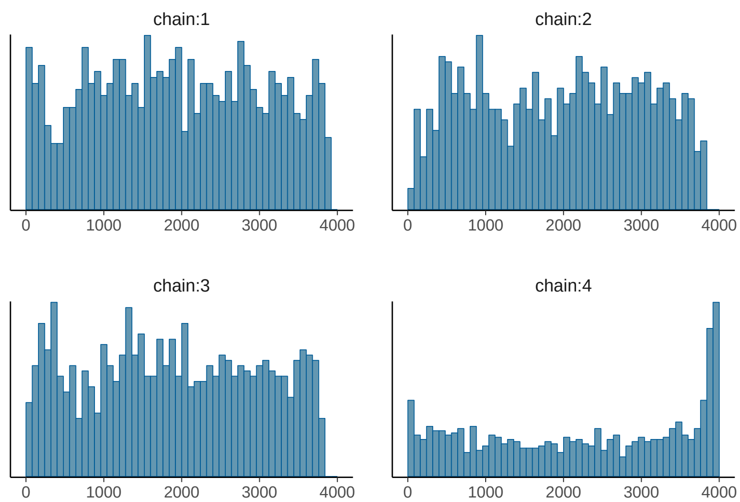
The rank plot visualisation of x[11], which has the smallest tail-ESS of NaN among the x, indicates clear convergence problems.

The rank plot visualisation of `lp__`, which has an effective sample size 240, doesn't look so good either.

4.2.2.3 Default Stan options + increased maximum treedepth + longer chains

Let's try running 8 times longer chains.





Trace plots for the first parameter still look wild with occasional large values.

Let's check the diagnostics for all x.

All Rhats are below 1.01. The classic split-Rhat has more variation than the rank normalized Rhat (note that the former is not well defined in this case).

Most classic ESS's are close to zero. Running longer chains just made most classic ESS's even smaller.

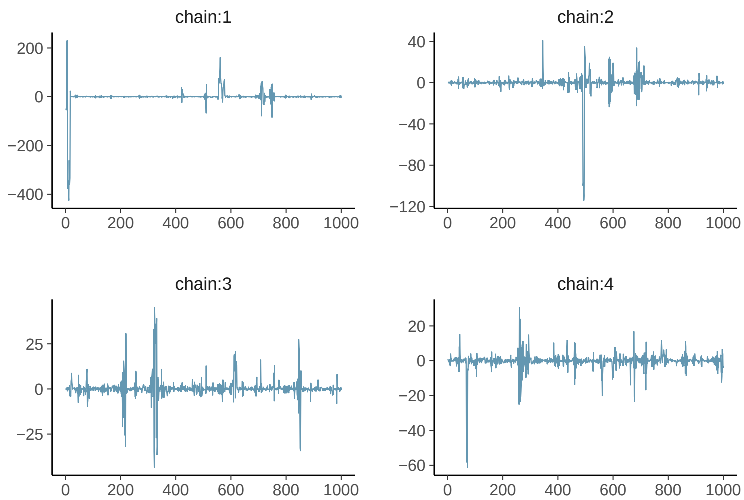
The smallest bulk-ESS are around 5000, which is not that bad. The smallest median-ESS's are larger than 25000, that is we are able to estimate the median efficiently. However, the smallest tail-ESS is 919 indicating problems for estimating the scale of the posterior.

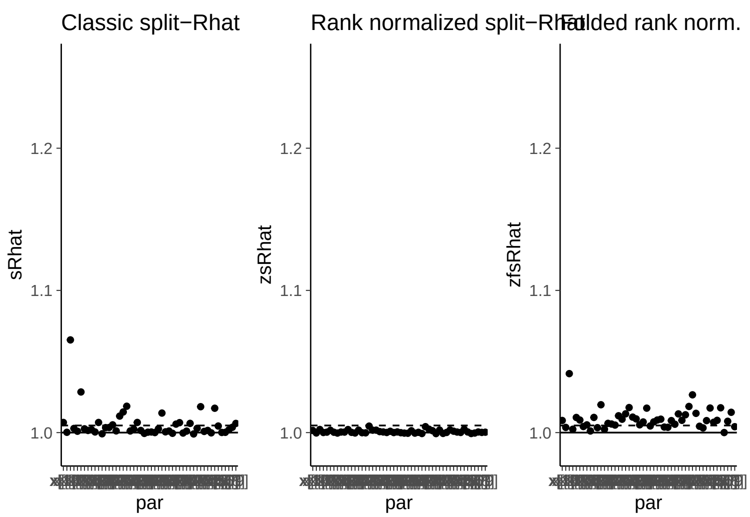
Result: The rank normalized effective sample size is more stable than classic effective sample size even for very long chains.

Result: It is useful to look at both bulk- and tail-ESS.

We also check `lp__`. Although increasing the number of iterations improved bulk-ESS of the x, the relative efficiency for `lp__` didn't change.

```
lp__: Bulk-ESS = 1289
```





`lp__: Tail-ESS = 1887`

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.

Increasing the chain length did not seem to change the relative efficiency. With more draws from the longer chains we can use a finer resolution for the local efficiency estimates.

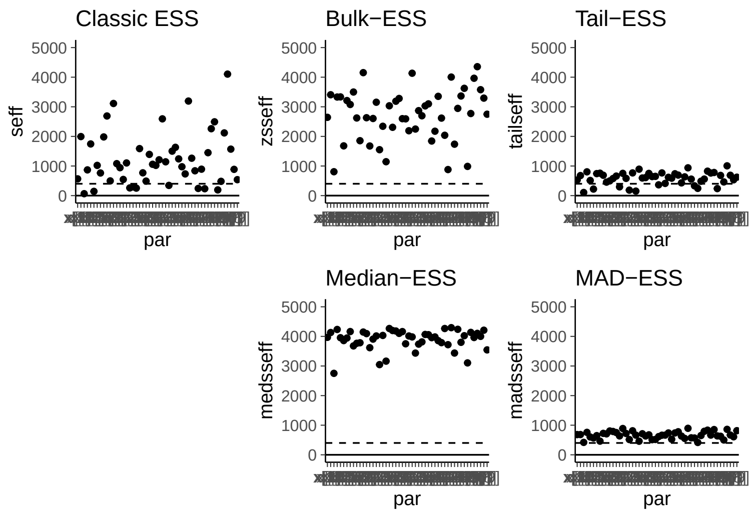
The sampling efficiency far in the tails is worryingly low. This was more difficult to see previously with less draws from the tails. We see similar problems in the plot of effective sample size for quantiles.

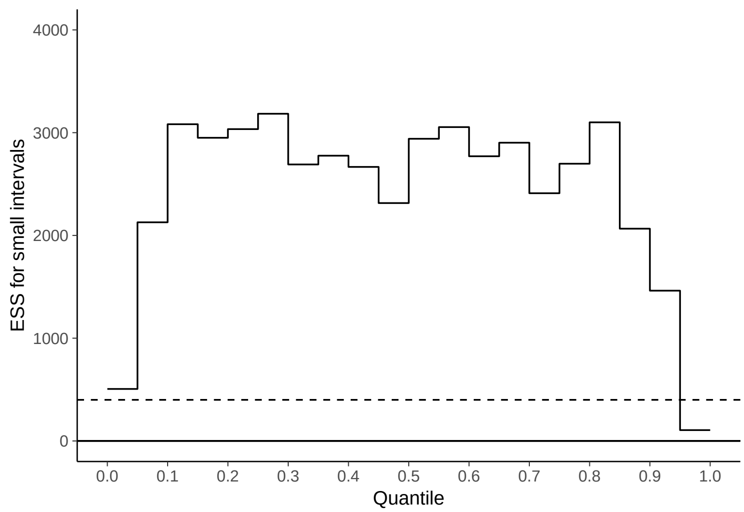
Let's look at the rank plot visualisation of x[39], which has the smallest tail-ESS NaN among the x.

Increasing the number of iterations couldn't remove the mixing problems at the tails. The mixing problem is inherent to the nominal parameterization of Cauchy distribution.

First alternative parameterization of the Cauchy distribution

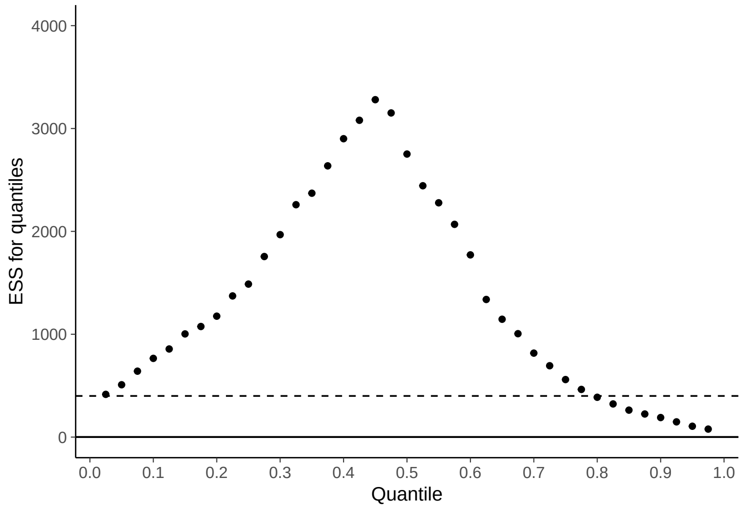
Next, we examine an alternative parameterization and consider the Cauchy distribution as a scale mixture of Gaussian distributions. The model has two parameters and the Cauchy distributed x can be computed from

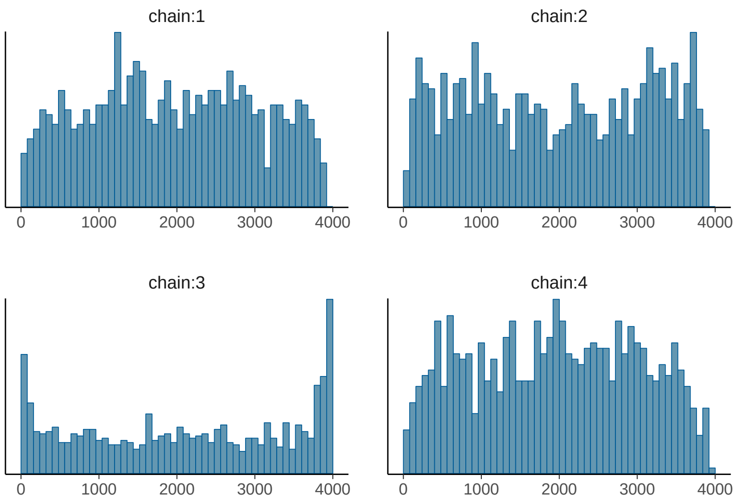




those. In addition to improved sampling performance, the example illustrates that focusing on diagnostics matters.

```
parameters {
  vector[50] x_a;
  vector<lower=0>[50] x_b;
}

transformed parameters {
  vector[50] x = x_a ./ sqrt(x_b);
}

model {
  x_a ~ normal(0, 1);
  x_b ~ gamma(0.5, 0.5);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
```





}

We run the alternative model:

There are no warnings and the sampling is much faster.

All Rhats are below 1.01. Classic split-Rhats also look good even though they are not well defined for the Cauchy distribution.

Result: Rank normalized ESS's have less variation than classic one which is not well defined for Cauchy.

We check `lp__`:

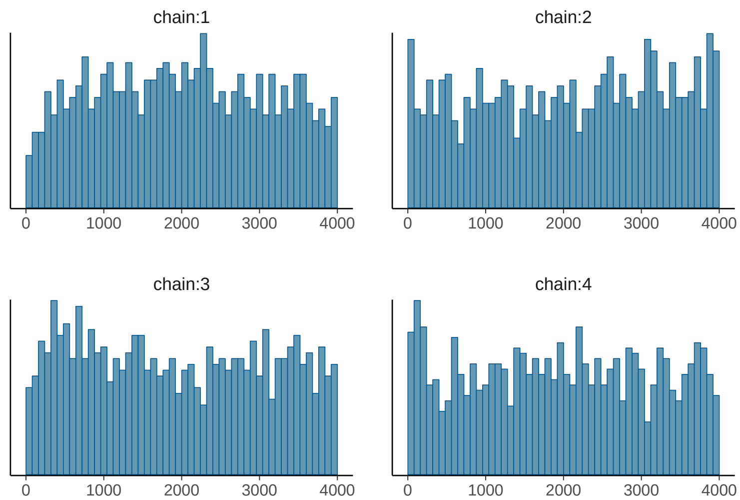
`lp__: Bulk-ESS = 1310`

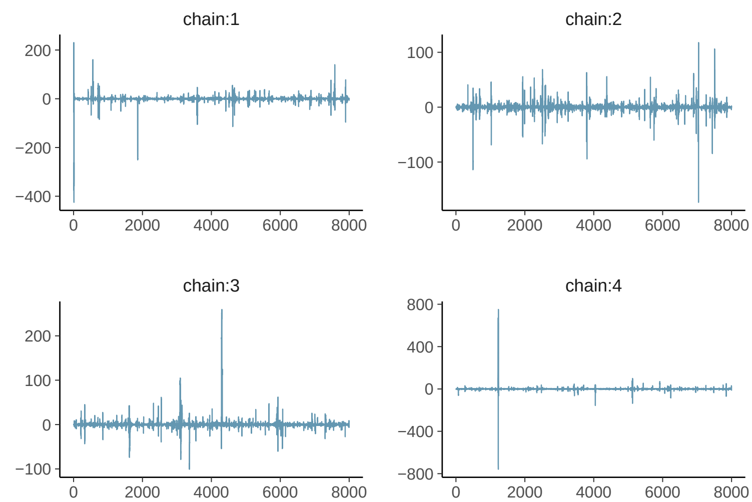
`lp__: Tail-ESS = 1928`

The relative efficiencies for `lp__` are also much better than with the nominal parameterization.

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.

The effective sample size is good in all parts of the posterior. We also examine the effective sample size of different quantile estimates.





We compare the mean relative efficiencies of the underlying parameters in the new parameterization and the actual x we are interested in.

```
Mean Bulk-ESS for x = 3629.24
```

```
Mean Tail-ESS for x = 2265.22
```

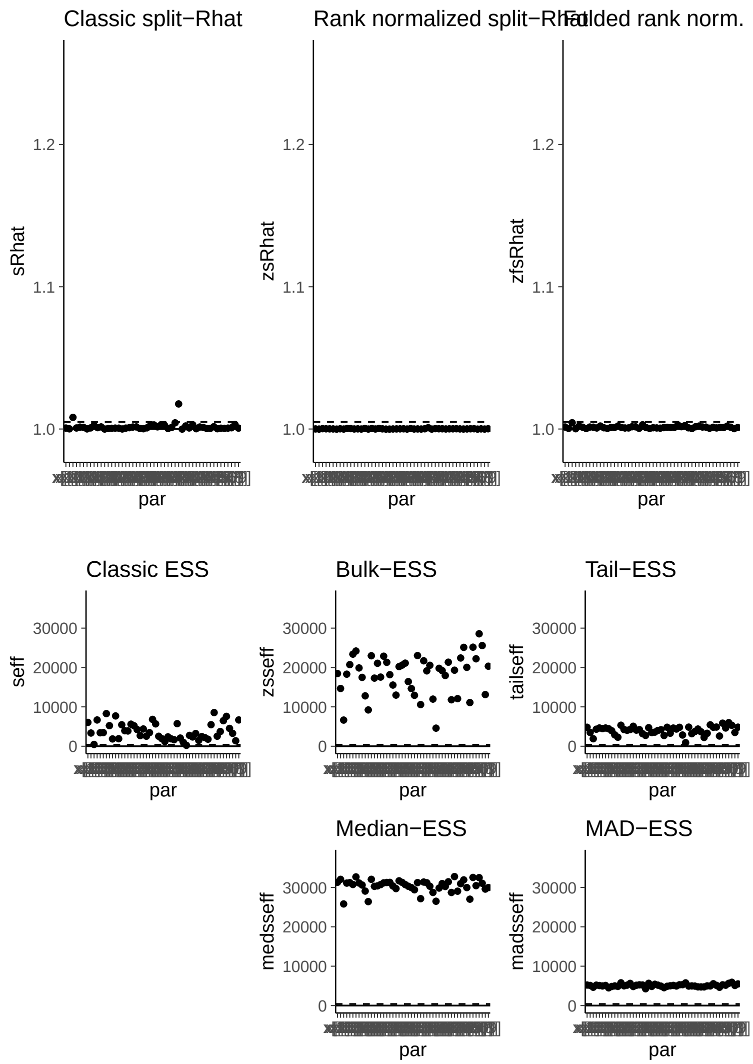
```
Mean Bulk-ESS for x_a = 3956.06
```

```
Mean Bulk-ESS for x_b = 2761.22
```

Result: We see that the effective sample size of the interesting x can be different from the effective sample size of the parameters x_a and x_b that we used to compute it.

The rank plot visualisation of x[40], which has the smallest tail-ESS of 1823 among the x looks better than for the nominal parameterization.

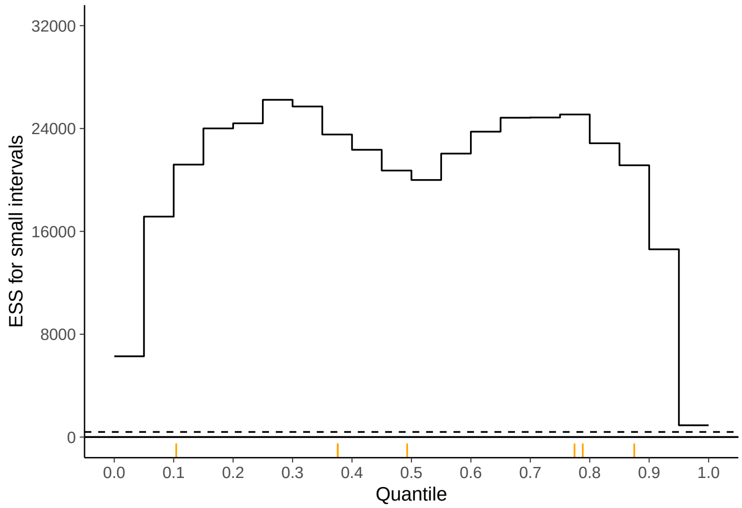
Similarly, the rank plot visualisation of `lp__`, which has a relative efficiency of -81.34, 0.23, 8.08, -95.19, -80.99, -68.66, 1288, 0.32, 1303, 1296, 1310, 0.33, 1, 1, 1, 1, 1, 2366, 0.59, 1928, 0.48, 1708, 0.43, 2912, 0.73 looks better than for the nominal parameterization.

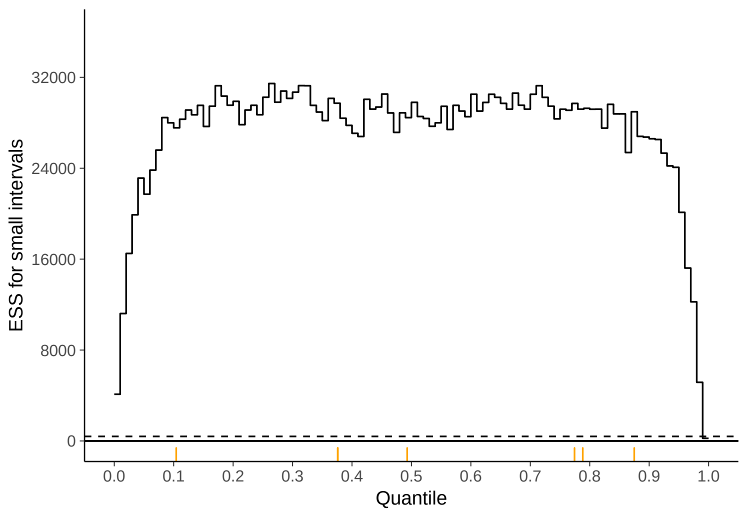


Another alternative parameterization of the Cauchy distribution

Another alternative parameterization is obtained by a univariate transformation as shown in the following code (see also the 3rd alternative in Michael Betancourt's case study).

```
parameters {
  vector<lower=0, upper=1>[50] x_tilde;
}

transformed parameters {
vector[50] x = tan(pi() * (x_tilde - 0.5));
}

model {
  // Implicit uniform prior on x_tilde
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
```






```
}
```

We run the alternative model:

There are no warnings, and the sampling is much faster than for the nominal model.

All Rhats except some folded Rhats are below 1.01. Classic split-Rhat's look also good even though it is not well defined for the Cauchy distribution.

Result: Rank normalized relative efficiencies have less variation than classic ones. Bulk-ESS and median-ESS are slightly larger than 1, which is possible for antithetic Markov chains which have negative correlation for odd lags.

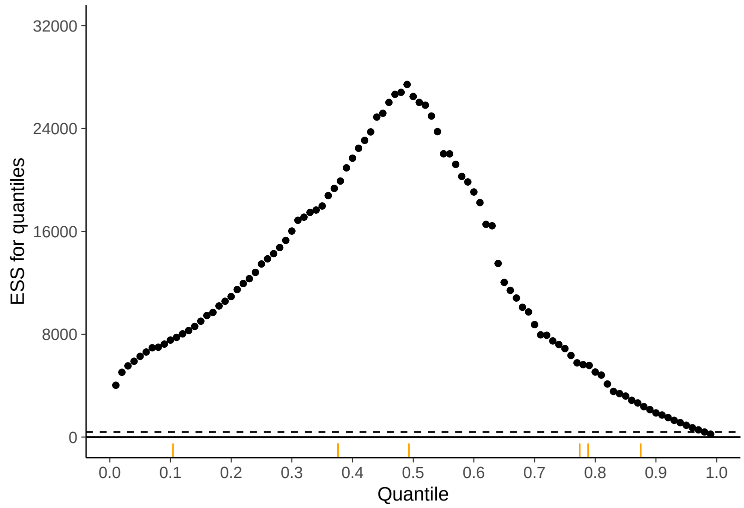
We also take a closer look at the `lp__` value:

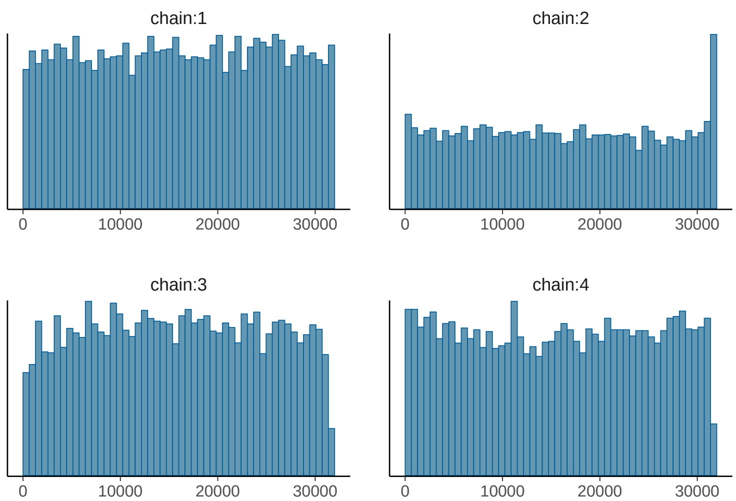
`lp__: Bulk-ESS = 1494`

`lp__: Tail-ESS = 1884`

The effective sample size for these are also much better than with the nominal parameterization.

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.





We examine also the sampling efficiency of different quantile estimates.

The effective sample size in tails is worse than for the first alternative parameterization, although it's still better than for the nominal parameterization.

We compare the mean effective sample size of the underlying parameter in the new parameterization and the actually Cauchy distributed x we are interested in.

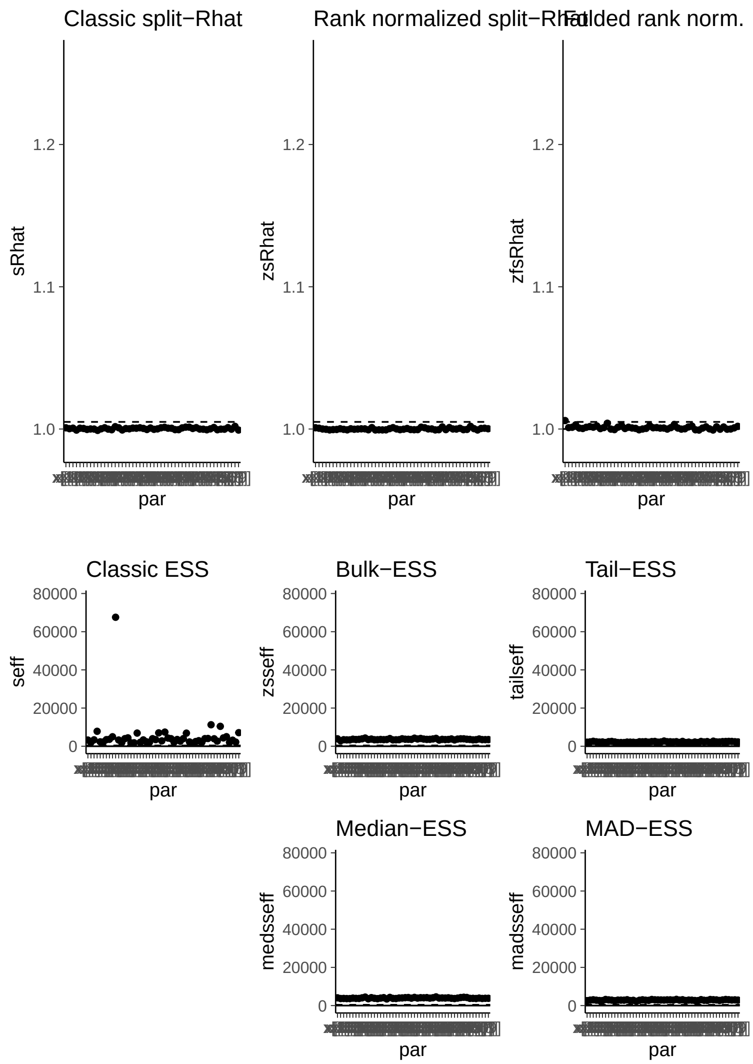
```
Mean bulk-seff for x = 4702.98
```

```
Mean tail-seff for x = 1602.7
```

```
Mean bulk-seff for x_tilde = 4702.98
```

```
Mean tail-seff for x_tilde = 1612.14
```

The Rank plot visualisation of x[5], which has the smallest tail-ESS of 1891 among the x reveals shows good efficiency, similar to the results for `lp__`.

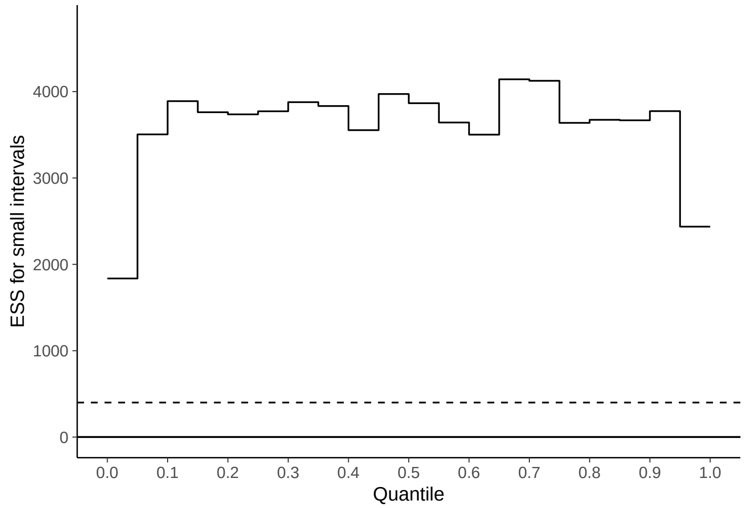


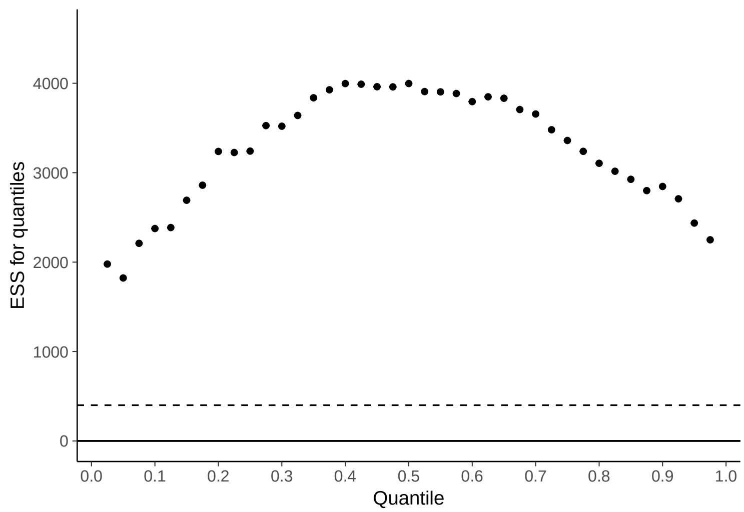
Half-Cauchy distribution with nominal parameterization

Half-Cauchy priors are common and, for example, in Stan usually set using the nominal parameterization. However, when the constraint `<lower=0>` is used, Stan does the sampling automatically in the unconstrained `log(x)` space, which changes the geometry crucially.

```
parameters {
  vector<lower=0>[50] x;
}

model {
  x ~ cauchy(0, 1);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

We run the half-Cauchy model with nominal parameterization (and positive constraint).





There are no warnings and the sampling is much faster than for the full Cauchy distribution with nominal parameterization.

All Rhats are below 1.01. Classic split-Rhats also look good even though they are not well defined for the half-Cauchy distribution.

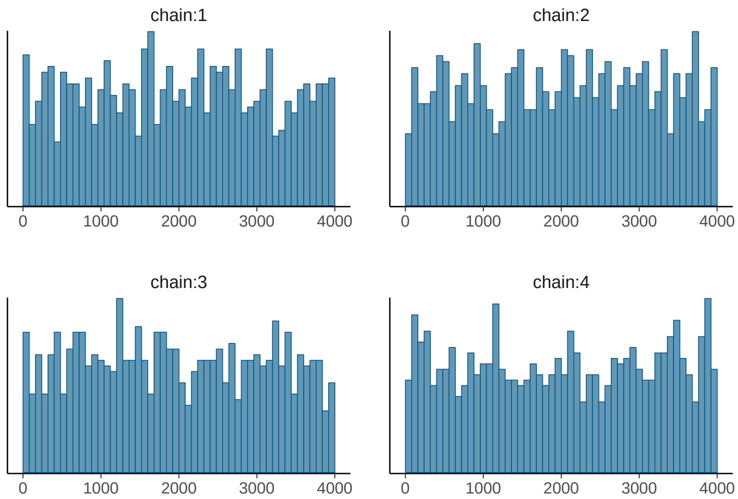
Result: Rank normalized effective sample size have less variation than classic ones. Some Bulk-ESS and median-ESS are larger than 1, which is possible for antithetic Markov chains which have negative correlation for odd lags.

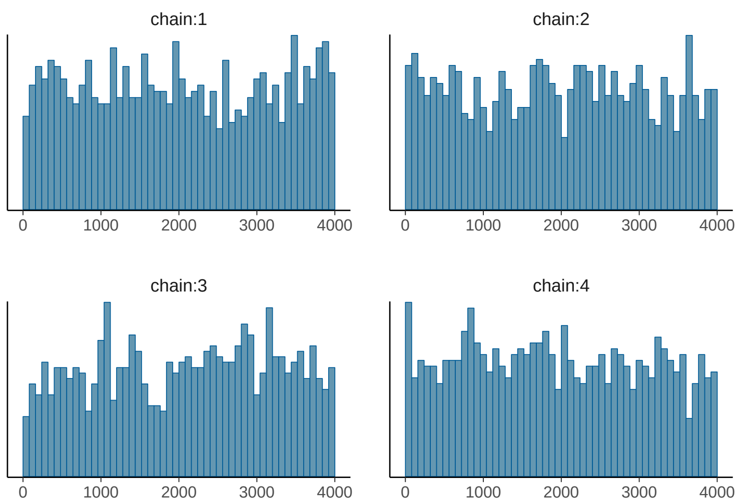
Due to the `<lower=0>` constraint, the sampling was made in the `log(x)` space, and we can also check the performance in that space.

$\log(x)$ is quite close to Gaussian, and thus classic effective sample size is also close to rank normalized ESS which is exactly the same as for the original x as rank normalization is invariant to bijective transformations.

Result: The rank normalized effective sample size is close to the classic effective sample size for transformations which make the distribution close to Gaussian.

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.





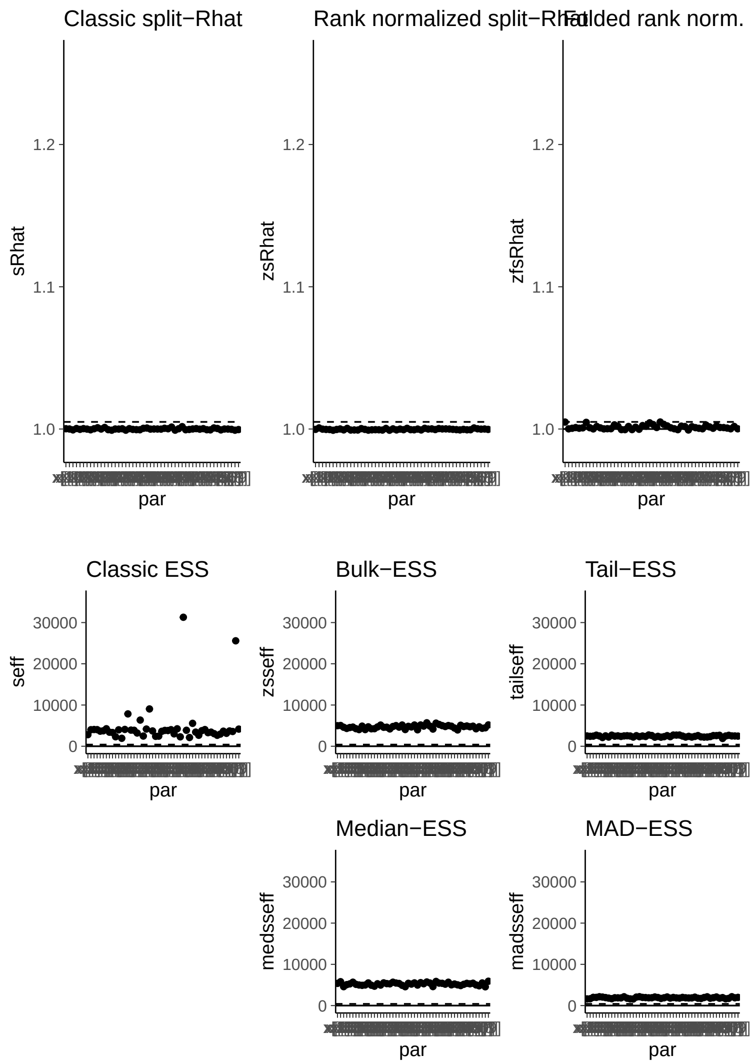
The effective sample size is good overall, with only a small dip in tails. We can also examine the effective sample size of different quantile estimates.

The rank plot visualisation of x[32], which has the smallest tail-ESS of 1742 among x, looks good.

The rank plot visualisation of `lp__` reveals some small differences in the scales, but it's difficult to know whether this small variation from uniform is relevant.

Alternative parameterization of the half-Cauchy distribution

```
parameters {
  vector<lower=0>[50] x_a;
  vector<lower=0>[50] x_b;
}

transformed parameters {
  vector[50] x = x_a .* sqrt(x_b);
}
```



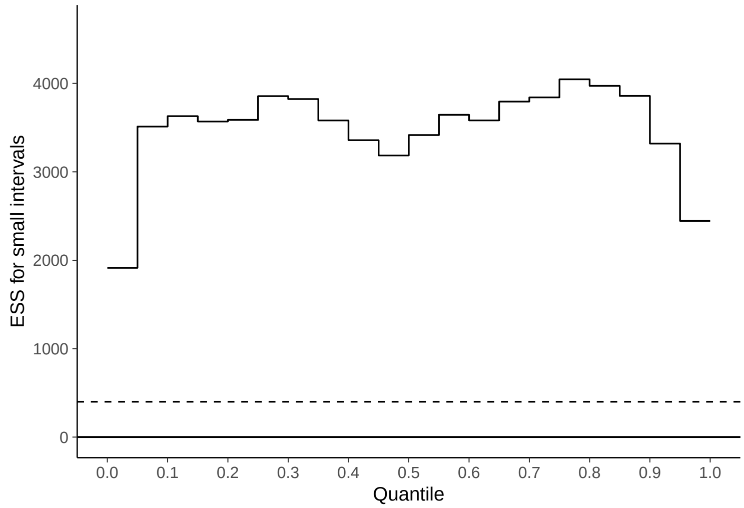

```
model {
  x_a ~ normal(0, 1);
  x_b ~ inv_gamma(0.5, 0.5);
}

generated quantities {
  real I = fabs(x[1]) < 1 ? 1 : 0;
}
```

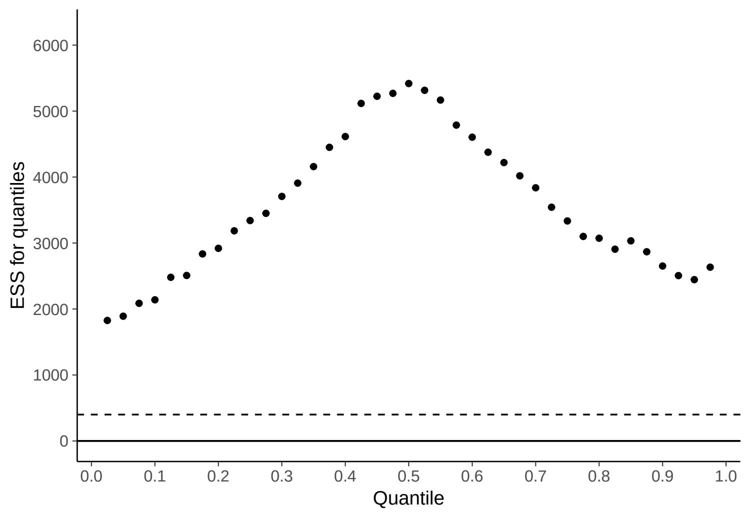
Run half-Cauchy with alternative parameterization

There are no warnings and the sampling is as fast for the half-Cauchy nominal model.

Result: The Rank normalized relative efficiencies have less variation than classic ones which is not well defined for the Cauchy distribution. Based on bulk-ESS and median-ESS, the efficiency for central quantities is much lower, but based on tail-ESS and MAD-ESS, the efficiency in the tails is slightly better than for the half-Cauchy distribution with nominal parameterization. We also see that a parameterization which is good for the full Cauchy distribution is not necessarily good for the half-Cauchy distribution as the `<lower=0>` constraint additionally changes the parameterization.

We also check the `lp__` values:






```
lp__: Bulk-ESS = 977
```

```
lp__: Tail-ESS = 1750
```

We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small interval probability estimates.

We also examine the effective sample size for different quantile estimates.

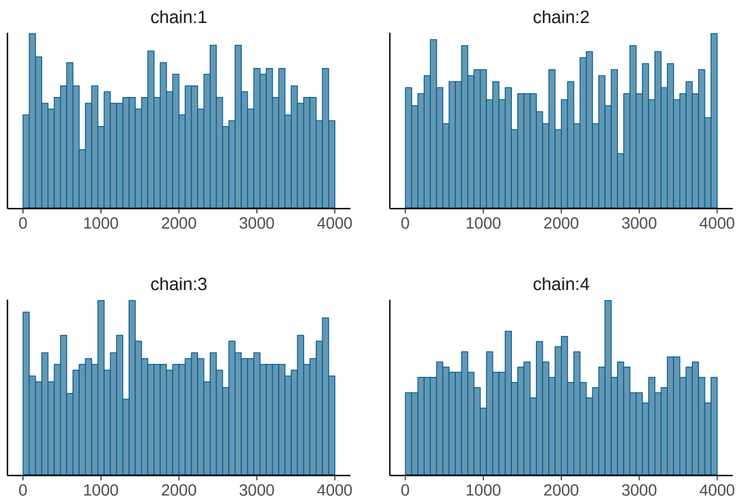
The effective sample size near zero is much worse than for the half-Cauchy distribution with nominal parameterization.

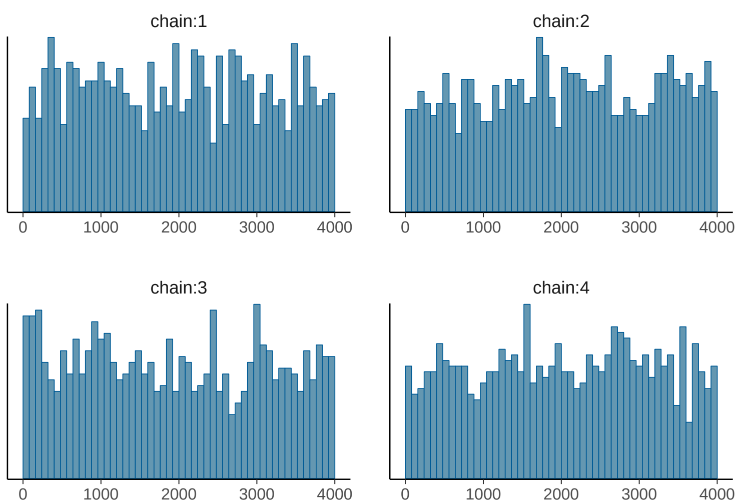
The Rank plot visualisation of x[20], which has the smallest tail-ESS of NaN among the x, reveals deviations from uniformity, which is expected with lower effective sample size.

A similar result is obtained when looking at the rank plots of `lp__`.

The Cauchy distribution with Jags

So far, we have run all models in Stan, but we want to also investigate whether similar problems arise with probabilistic programming languages that use other samplers than variants of Hamiltonian Monte-Carlo.





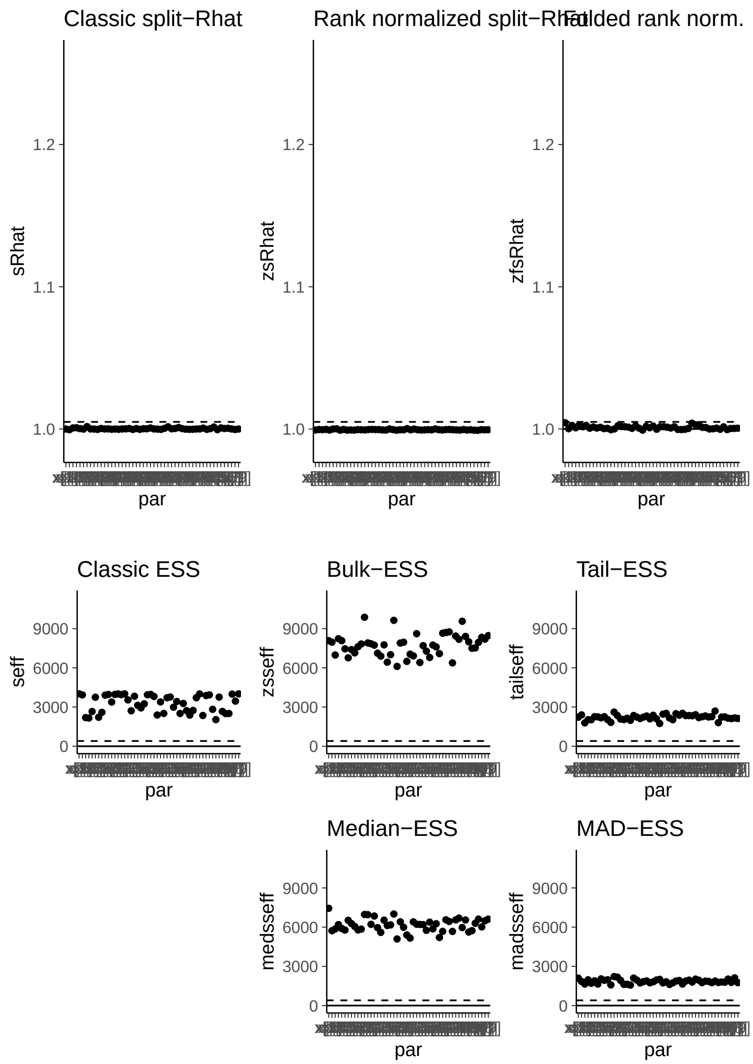
Thus, we will fit the eight schools models also with Jags, which uses a dialect of the BUGS language to specify models. Jags uses a clever mix of Gibbs and Metropolis-Hastings sampling. This kind of sampling does not scale well to high dimensional posteriors of strongly interdependent parameters, but for the relatively simple models discussed in this case study it should work just fine.

The Jags code for the nominal parameteriztion of the cauchy distribution looks as follows:

```
model {
  for (i in 1:50) {
    x[i] ~ dt(0, 1, 1)
  }
}
```

First, we initialize the Jags model for reusage later.

```
Compiling model graph
   Resolving undeclared variables
   Allocating nodes
Graph information:
   Observed stochastic nodes: 0
   Unobserved stochastic nodes: 50
```



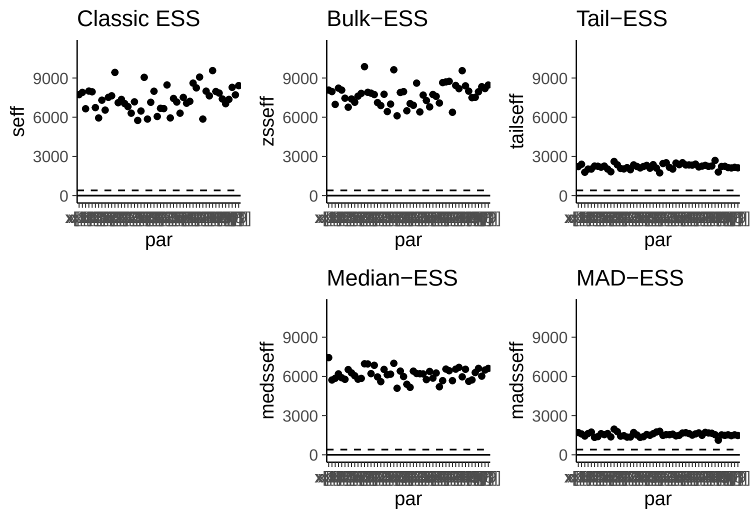

```
Total graph size: 52
```

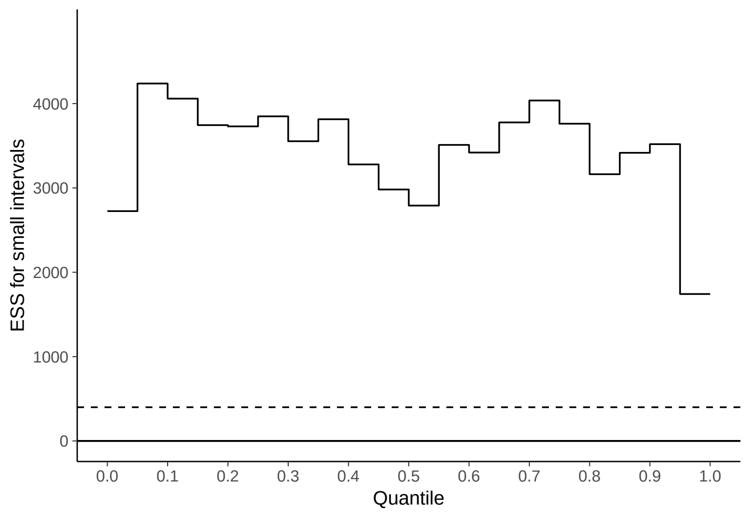
```
Initializing model
```

Next, we sample 1000 iterations for each of the 4 chains for easy comparison with the corresponding Stan results.

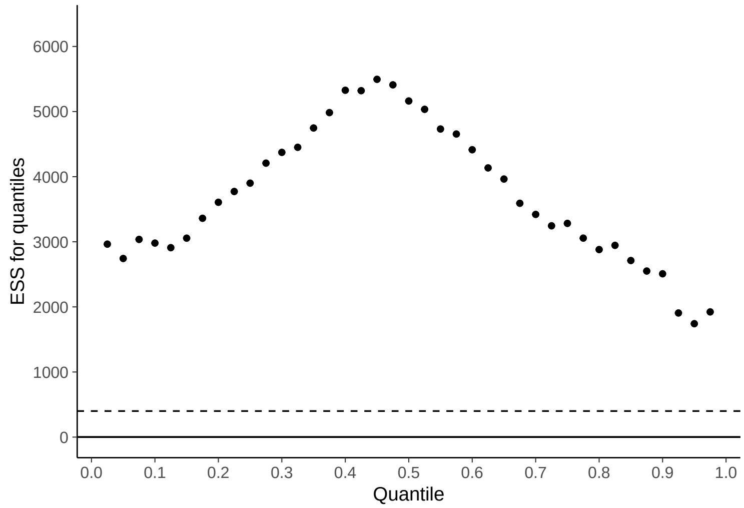
We summarize the model as follows:

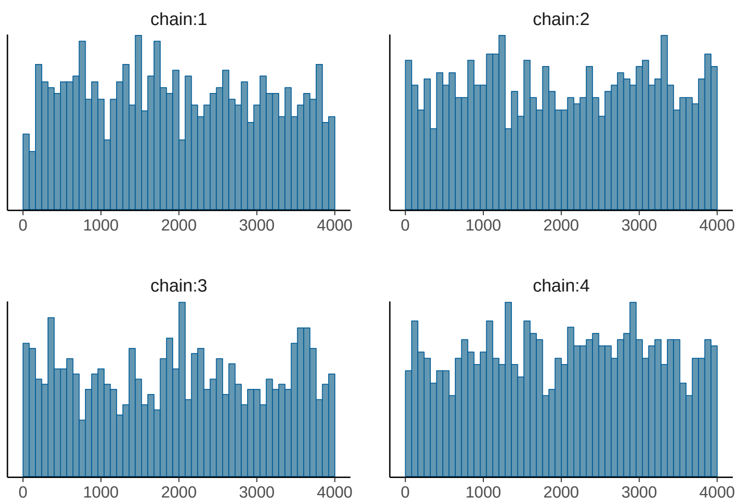
```
Inference for the input samples (4 chains: each with iter = 1000; warmup = 0):

        Q5   Q50  Q95  Mean    SD  Rhat Bulk_ESS Tail_ESS
x[1]  -6.16 -0.02 5.78  -3.03 297.0     1     3933     4085
x[2]  -6.73  0.00 6.07  -1.13  57.9     1     4091     3930
x[3]  -6.66  0.01 6.70  -1.23  57.4     1     4026     3826
x[4]  -5.73  0.02 6.51  -0.18  26.2     1     3971     3930
x[5]  -5.72 -0.02 6.20   1.60 119.0     1     4023     3766
x[6]  -6.80 -0.01 5.86   4.80 258.0     1     4037     3925
x[7]  -5.73  0.02 5.85  -0.88  43.8     1     3871     3905
x[8]  -6.19  0.00 6.62   0.21 144.0     1     4103     3753
```



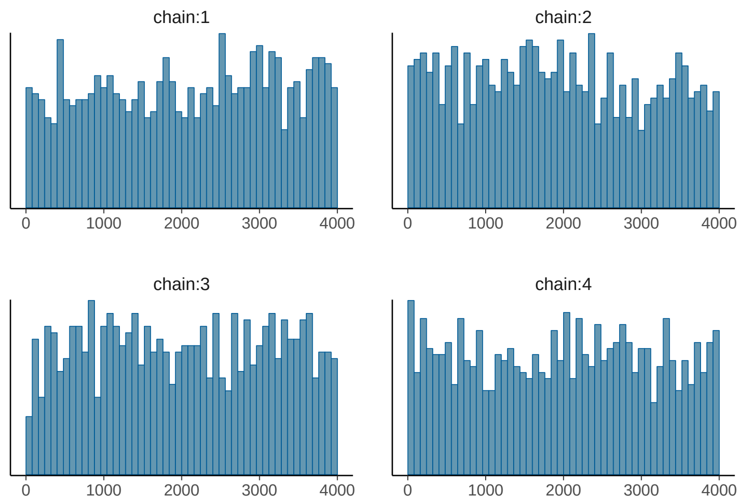


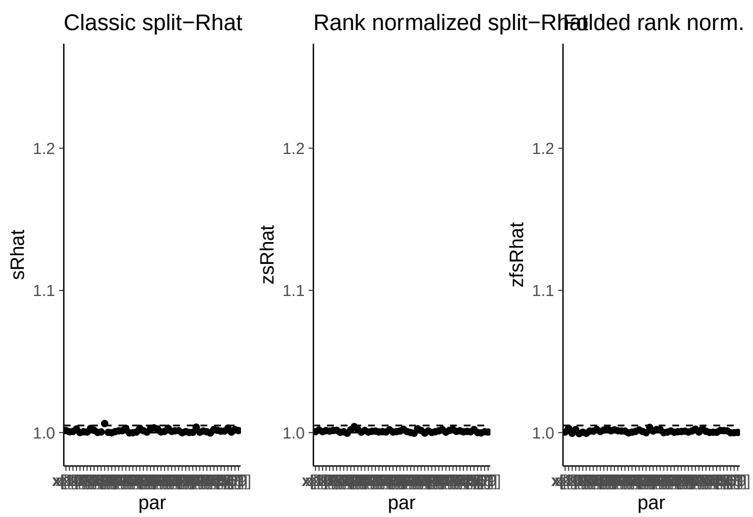

```
x[9]  -6.36  0.00 6.63   0.01  28.0     1     4001     4012
x[10] -5.94  0.01 6.99  -0.34  98.4     1     4237     3914
x[11] -6.94 -0.01 6.32  -0.56  25.0     1     3917     3894
x[12] -5.47 -0.01 6.16   0.62  27.7     1     3780     3846
x[13] -6.88 -0.07 6.05  -1.24  91.1     1     3424     3719
x[14] -6.53 -0.03 6.39   2.22 163.0     1     4011     3801
x[15] -6.61 -0.01 6.78   0.11  35.4     1     3628     3685
x[16] -6.46  0.00 5.72 -12.40 521.0     1     4050     3996
x[17] -5.81  0.00 6.42   0.13  37.5     1     4081     3917
x[18] -6.16  0.01 6.35  -8.24 342.0     1     4142     3958
x[19] -6.16  0.00 6.38  -0.24  70.4     1     3879     3785
x[20] -6.59  0.02 6.33   5.38 278.0     1     3864     3888
x[21] -6.46  0.00 5.95   0.91  37.9     1     3820     3598
x[22] -6.33  0.01 6.28  -7.71 518.0     1     3906     3773
x[23] -6.27  0.00 6.82  -3.28 217.0     1     4128     4015
x[24] -7.49 -0.04 5.80   2.30 191.0     1     3993     4103
x[25] -6.19  0.00 5.48   0.36  61.3     1     4163     3852
x[26] -6.12 -0.07 6.31  -2.66 281.0     1     3132     3734
x[27] -6.47  0.02 6.32   1.17  65.6     1     3985     3867
```





x[28]	-6.28	0.02	6.77	3.67	109.0	1	3961	3973
x[29]	-5.88	-0.01	6.08	-2.32	68.4	1	3983	3908
x[30]	-6.44	0.01	7.10	1.35	55.3	1	4075	3941
x[31]	-6.08	0.02	6.21	-0.63	34.1	1	4078	3687
x[32]	-5.36	-0.02	6.46	-2.29	73.4	1	3815	3891
x[33]	-5.90	0.00	5.84	-0.24	17.7	1	4001	3412
x[34]	-6.24	-0.03	6.42	-1.51	132.0	1	3968	3865
x[35]	-6.18	0.01	6.41	1.18	49.7	1	3810	3931
x[36]	-7.02	-0.01	5.90	6.74	484.0	1	3953	3770
x[37]	-6.65	-0.02	6.13	0.14	33.9	1	4048	4101
x[38]	-5.83	0.01	6.22	1.97	114.0	1	4172	3840
x[39]	-6.28	0.01	6.19	0.15	82.9	1	3933	3929
x[40]	-6.31	-0.01	6.57	1.04	97.9	1	4218	3891
x[41]	-5.74	0.00	6.57	0.71	54.1	1	3669	3699
x[42]	-5.49	0.02	5.59	-0.66	58.2	1	4068	3852
x[43]	-6.79	-0.04	6.45	-0.02	109.0	1	3777	3949
x[44]	-5.93	0.02	6.17	-0.16	32.9	1	3649	3857
x[45]	-6.64	0.00	6.47	-0.33	49.4	1	3919	3869
x[46]	-5.41	0.02	6.86	3.27	145.0	1	4069	4013





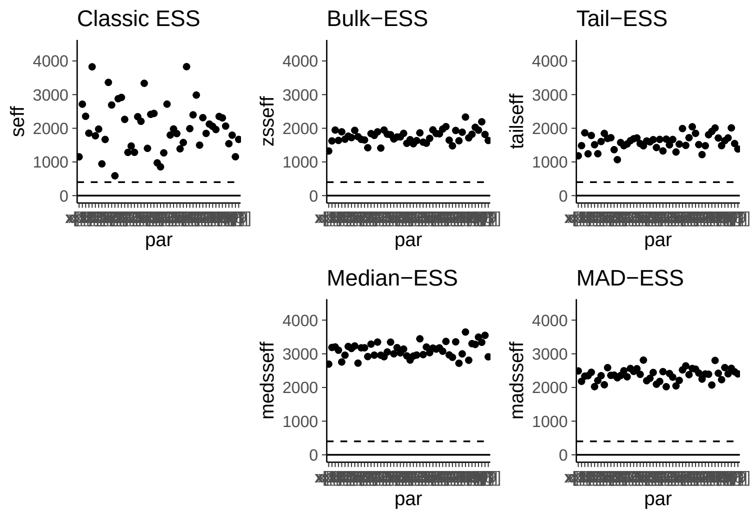

```
x[47] -6.27  0.00 5.96  -0.68  22.6     1     3962     4013
x[48] -6.64 -0.02 5.79  -2.35  71.5     1     4015     4016
x[49] -6.71  0.01 6.10   5.69 562.0     1     3886     3809
x[50] -7.00  0.00 6.21   8.79 614.0     1     3830     3884

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

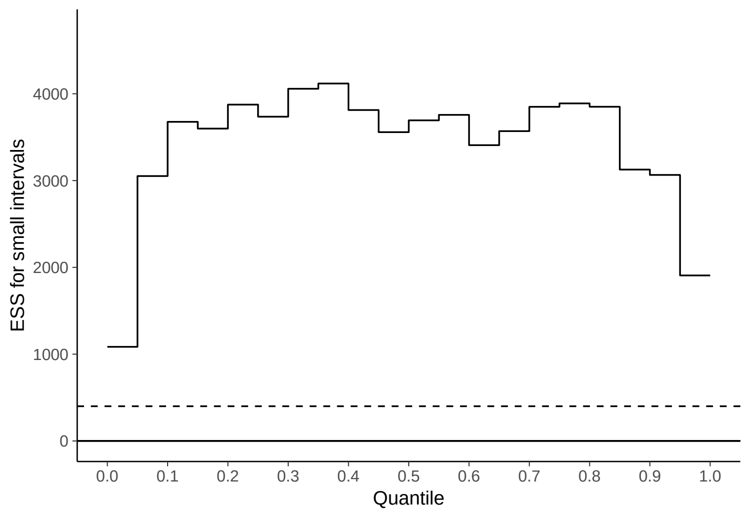
The overall results look very promising with Rhats = 1 and ESS values close to the total number of draws of 4000. We take a detailed look at x[26], which has the smallest bulk-ESS of 3132.

We examine the sampling efficiency in different parts of the posterior by computing the efficiency estimates for small interval probability estimates.

The efficiency estimate is good in all parts of the posterior. Further, we examine the sampling efficiency of different quantile estimates.

Rank plots also look rather similar across chains.





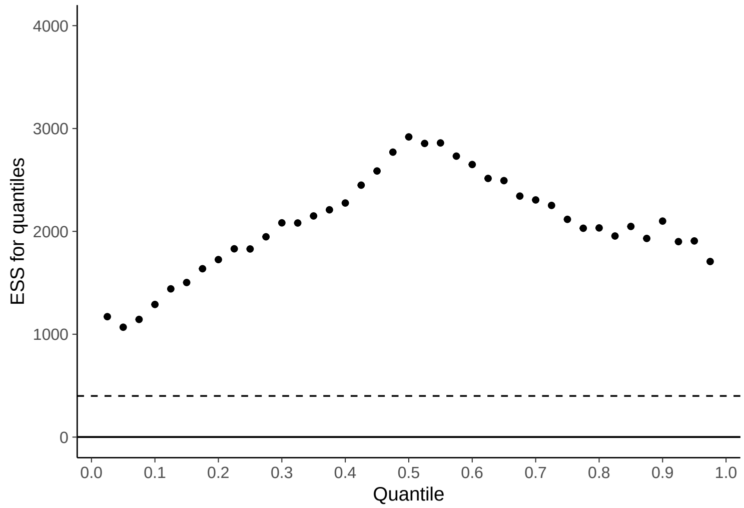
Result: Jags seems to be able to sample from the nominal parameterization of the Cauchy distribution just fine.

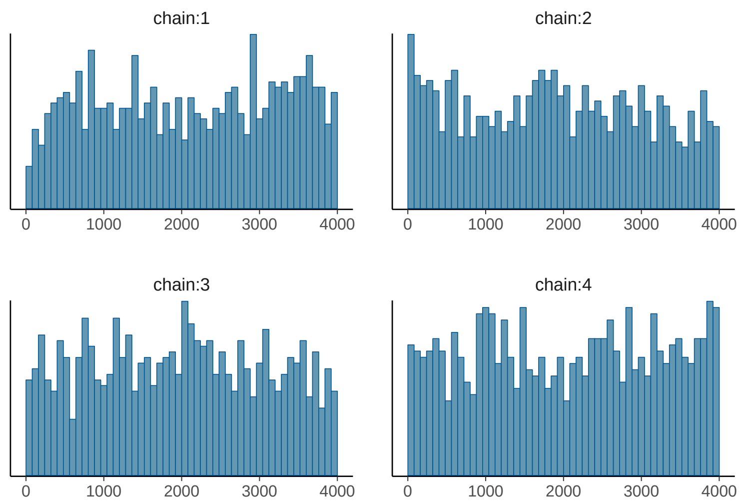
Appendix F: Hierarchical model: Eight Schools

We continue with our discussion about hierarchical models on the Eight Schools data, which we started in Section Eight Schools. We also analyse the performance of different variants of the diagnostics.

A Centered Eight Schools model

```
data {
  int<lower=0> J;
  real y[J];
  real<lower=0> sigma[J];
}

parameters {
```



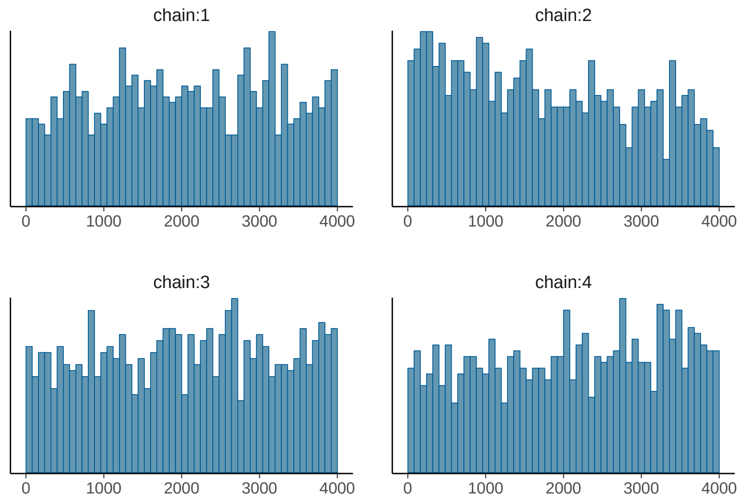


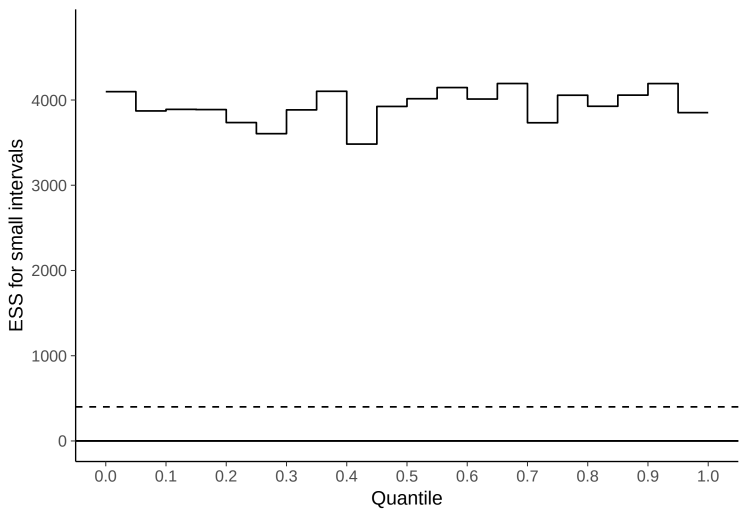

```
  real mu;
  real<lower=0> tau;
  real theta[J];
}

model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 5);
  theta ~ normal(mu, tau);
  y ~ normal(theta, sigma);
}
```

In the main text, we observed that the centered parameterization of this hierarchical model did not work well with the default MCMC options of Stan plus increased `adapt_delta`, and so we directly try to fit the model with longer chains.

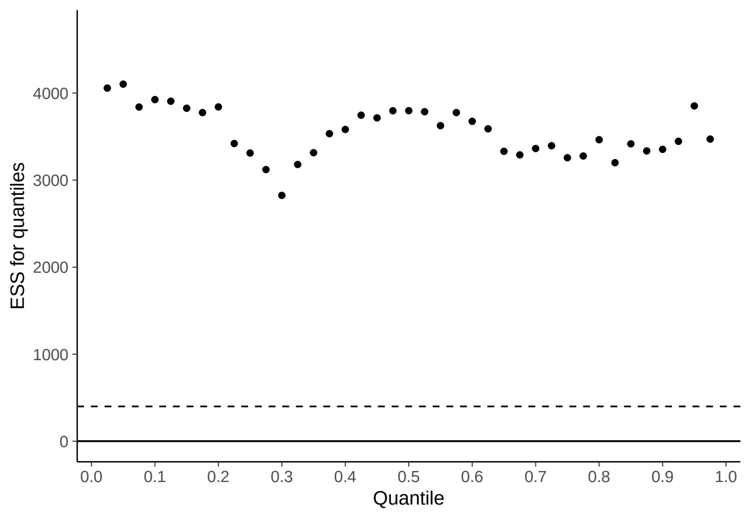
4.2.2.4 Centered parameterization with longer chains

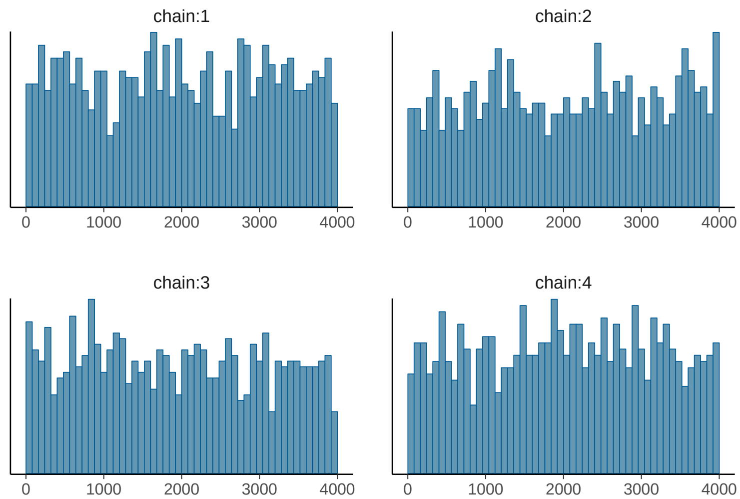
Low efficiency can be sometimes compensated with longer chains. Let's check 10 times longer chain.



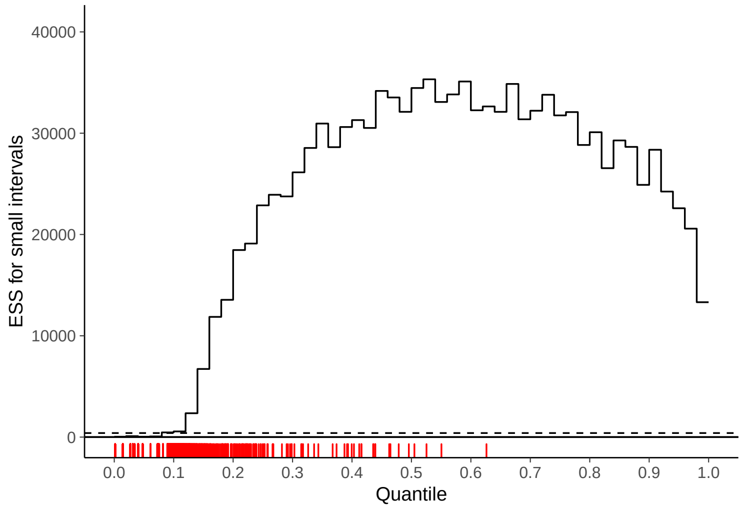



```
Inference for the input samples (4 chains: each with iter = 20000; warmup = 10000):

              Q5    Q50   Q95   Mean   SD  Rhat Bulk_ESS Tail_ESS
mu         -0.99   4.84 10.30   4.88 3.57  1.05       71      189
tau         0.33   2.81 10.00   3.67 3.31  1.08       45       17
theta[1]   -1.36   6.43 16.30   6.76 5.64  1.01      407     9491
theta[2]   -2.48   5.47 12.60   5.42 4.80  1.02      153     9429
theta[3]   -4.92   4.66 11.50   4.41 5.43  1.03      117    10374
theta[4]   -2.89   5.34 12.40   5.23 4.97  1.03      140     9670
theta[5]   -4.48   4.32 10.70   4.09 4.94  1.04       89     4758
theta[6]   -4.15   4.70 11.30   4.49 5.08  1.03      118    11277
theta[7]   -0.88   6.60 15.50   6.83 5.11  1.01      449    11102
theta[8]   -3.46   5.41 13.30   5.34 5.49  1.02      172    10408
lp__      -24.90 -14.80  0.22 -13.80 7.59  1.07       50       86

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```






```
Inference for the input samples (4 chains: each with iter = 20000; warmup = 10000):

           mean se_mean   sd     Q5    Q50   Q95 seff reff sseff zseff
mu         4.88    0.49 3.57  -0.99   4.84 10.30   53 0.00    71    54
tau        3.67    0.30 3.31   0.33   2.81 10.00  123 0.00   173    35
theta[1]   6.76    0.22 5.64  -1.36   6.43 16.30  666 0.02  1060   281
theta[2]   5.42    0.43 4.80  -2.48   5.47 12.60  124 0.00   169   113
theta[3]   4.41    0.53 5.43  -4.92   4.66 11.50  105 0.00   146    86
theta[4]   5.23    0.46 4.97  -2.89   5.34 12.40  118 0.00   163   105
theta[5]   4.09    0.57 4.94  -4.48   4.32 10.70   76 0.00   102    69
theta[6]   4.49    0.51 5.08  -4.15   4.70 11.30  100 0.00   137    87
theta[7]   6.83    0.23 5.11  -0.88   6.60 15.50  512 0.01   745   309
theta[8]   5.34    0.43 5.49  -3.46   5.41 13.30  162 0.00   231   125
lp__     -13.80    1.32 7.59 -24.90 -14.80  0.22   33 0.00    44    37
         zsseff zsreff Rhat sRhat zRhat zsRhat zfsRhat zfsseff zfsreff
mu           71   0.00 1.05  1.05  1.05   1.05    1.02     152    0.00
tau          45   0.00 1.02  1.02  1.08   1.08    1.01    1040    0.03
theta[1]    407   0.01 1.01  1.01  1.01   1.01    1.00    3300    0.08
theta[2]    153   0.00 1.02  1.02  1.02   1.02    1.00    1820    0.05
```




```
theta[3]     117   0.00  1.03  1.02  1.03   1.03    1.01     736    0.02
theta[4]     140   0.00  1.02  1.02  1.03   1.03    1.01    1470    0.04
theta[5]      89   0.00  1.03  1.03  1.04   1.04    1.01     375    0.01
theta[6]     118   0.00  1.03  1.03  1.03   1.03    1.01     644    0.02
theta[7]     449   0.01  1.01  1.01  1.01   1.01    1.00    2760    0.07
theta[8]     172   0.00  1.02  1.02  1.02   1.02    1.00    2820    0.07
lp__          50   0.00  1.08  1.08  1.07   1.07    1.06      55    0.00
         tailseff tailreff medsseff medsreff madsseff madsreff
mu            189     0.00      174        0      174     0.00
tau            17     0.00      175        0      167     0.00
theta[1]     9490     0.24      177        0      268     0.01
theta[2]     9430     0.24      173        0      177     0.00
theta[3]    10400     0.26      168        0      172     0.00
theta[4]     9670     0.24      167        0      167     0.00
theta[5]     4760     0.12      170        0      178     0.00
theta[6]    11300     0.28      176        0      176     0.00
theta[7]    11100     0.28      179        0      852     0.02
theta[8]    10400     0.26      166        0      191     0.00
lp__           86     0.00      170        0      157     0.00
```

We still get a whole bunch of divergent transitions so it's clear that the results can't be trusted even if all other diagnostics were good. Still, it may be worth looking at additional diagnostics to better understand what's happening.

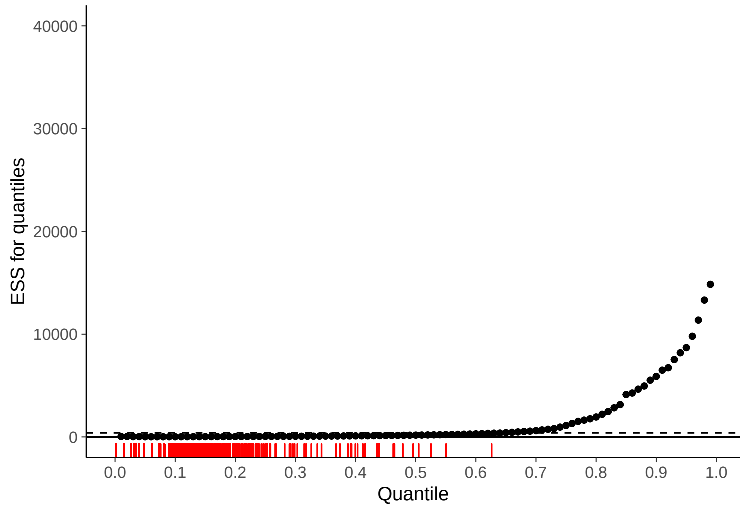
Some rank-normalized split-Rhats are still larger than 1.01. Bulk-ESS for `tau` and `lp__` are around 800 which corresponds to low relative efficiency of 1%, but is above our recommendation of ESS>400. In this kind of cases, it is useful to look at the local efficiency estimates, too (and the larger number of divergences is clear indication of problems, too).

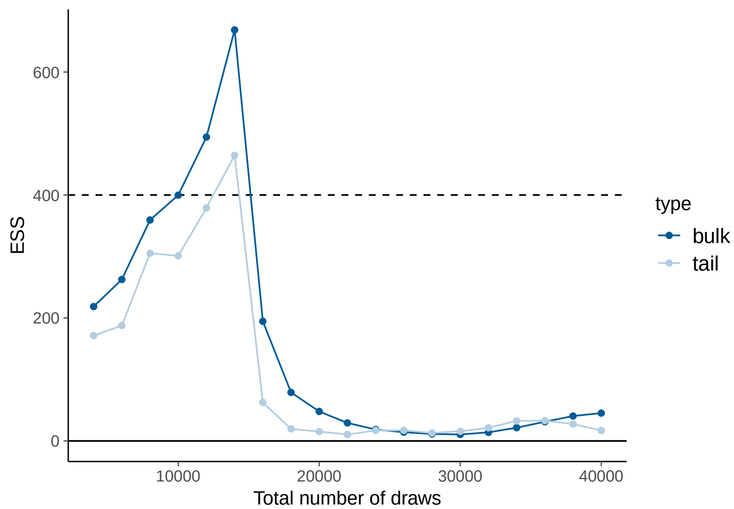
We examine the sampling efficiency in different parts of the posterior by computing the effective sample size for small intervals for `tau`.

We see that the sampling has difficulties in exploring small `tau` values. As ESS<400 for small probability intervals in case of small `tau` values, we may suspect that we may miss substantial amount of posterior mass and get biased estimates.

We also examine the effective sample size of different quantile estimates.

Several quantile estimates have ESS<400, which raises a doubt that there are convergence problems and we





may have significant bias.

Let's see how the Bulk-ESS and Tail-ESS changes when we use more and more draws.

We see that given recommendation that Bulk-ESS>400 and Tail-ESS>400, they are not sufficient to detect convergence problems in this case, even the tail quantile estimates are able to detect these problems.

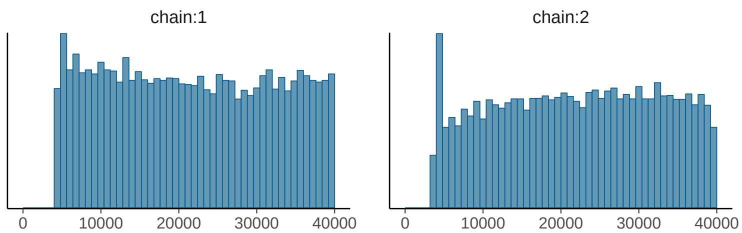
The rank plot visualisation of `tau` also shows clear sticking and mixing problems.

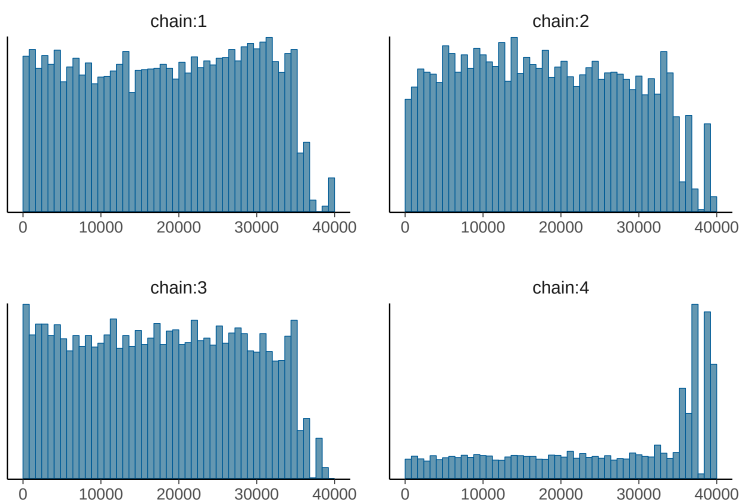
Similar results are obtained for `lp__`, which is closely connected to `tau` for this model.

We may also examine small interval efficiencies for `mu`.

There are gaps of poor efficiency which again indicates problems in the mixing of the chains. However, these problems do not occur for any specific range of values of `mu` as was the case for `tau`. This tells us that it's probably not `mu` with which the sampler has problems, but more likely `tau` or a related quantity.

As we observed divergences, we shouldn't trust any Monte Carlo standard error (MCSE) estimates as they are likely biased, as well. However, for illustration purposes, we compute the MCSE, tail quantiles and corresponding effective sample sizes for the median of `mu` and `tau`. Comparing to the shorter MCMC run, using 10 times more draws has not reduced the MCSE to one third as would be expected without problems in the mixing of the chains.





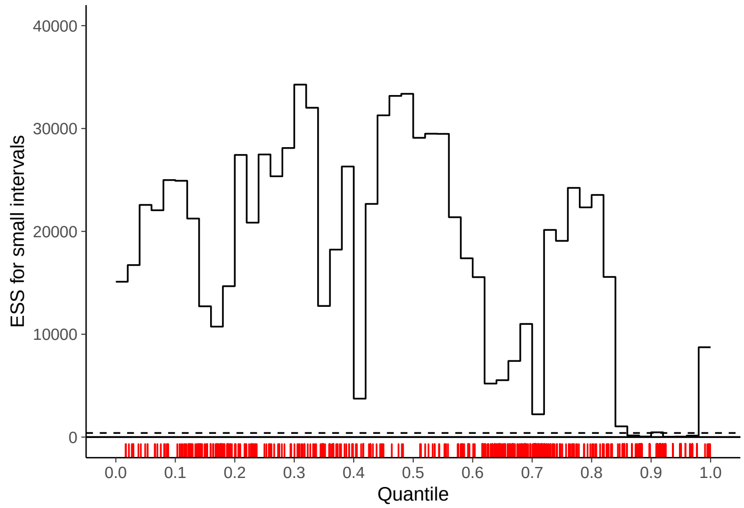

```
  mcse  Q05  Q95   Seff
1 0.37 4.22 5.43 173.52
```

```
  mcse  Q05  Q95   Seff
1 0.27 2.38 3.27 174.86
```

4.2.2.5 Centered parameterization with very long chains

For further evidence, let's check 100 times longer chains than the default. This is not something we would recommend doing in practice, as it is not able to solve any problems with divergences as illustrated below.

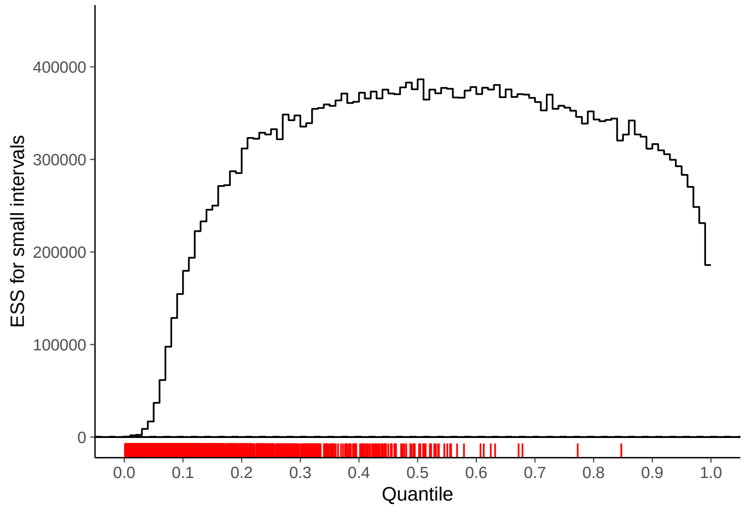
```
Inference for the input samples (4 chains: each with iter = 200000; warmup = 100000):

              Q5   Q50   Q95  Mean   SD  Rhat Bulk_ESS Tail_ESS
mu         -1.10  4.37  9.83  4.37 3.33     1    18335    30265
tau         0.47  2.94 10.00  3.80 3.21     1     2200      769
theta[1]   -1.59  5.73 16.40  6.29 5.69     1    23832   110854
theta[2]   -2.53  4.85 12.80  4.94 4.76     1    27789   136002
theta[3]   -5.06  4.09 11.90  3.87 5.36     1    39355   122761
theta[4]   -2.95  4.68 12.60  4.75 4.86     1    32607   138545
```

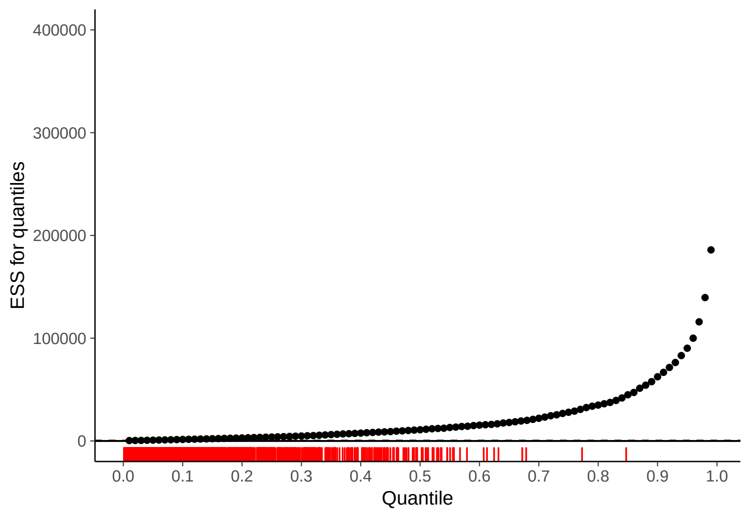



```
theta[5]  -4.55   3.79 10.80   3.55 4.72     1     34479     44492
theta[6]  -4.16   4.16 11.60   4.01 4.91     1     37000     92227
theta[7]  -1.03   5.92 15.60   6.38 5.16     1     20685     58049
theta[8]  -3.49   4.74 13.50   4.85 5.39     1     36212    125498
lp__     -25.00 -15.20 -2.08 -14.60 6.87     1      2541      1074
```

```
For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

```
Inference for the input samples (4 chains: each with iter = 200000; warmup = 100000):

           mean se_mean   sd     Q5    Q50   Q95  seff reff sseff zseff
mu         4.37    0.02 3.33  -1.10   4.37  9.83 18400 0.05 18400 18400
tau        3.80    0.03 3.21   0.47   2.94 10.00  9360 0.02  9390  2210
theta[1]   6.29    0.03 5.69  -1.59   5.73 16.40 31000 0.08 31100 23800
theta[2]   4.94    0.03 4.76  -2.53   4.85 12.80 32900 0.08 33000 27700
theta[3]   3.87    0.02 5.36  -5.06   4.09 11.90 53600 0.13 53600 39200
theta[4]   4.75    0.02 4.86  -2.95   4.68 12.60 39500 0.10 39700 32500
theta[5]   3.55    0.02 4.72  -4.55   3.79 10.80 41400 0.10 41800 34300
theta[6]   4.01    0.02 4.91  -4.16   4.16 11.60 45900 0.11 46100 36800
theta[7]   6.38    0.03 5.16  -1.03   5.92 15.60 24700 0.06 24700 20700
theta[8]   4.85    0.02 5.39  -3.49   4.74 13.50 50200 0.13 50200 36400
lp__     -14.60    0.14 6.87 -25.00 -15.20 -2.08  2410 0.01  2410  2540
         zsseff zsreff  Rhat sRhat zRhat zsRhat zfsRhat zfsseff zfsreff
mu        18300   0.05     1     1     1      1       1   28800    0.07
tau        2200   0.01     1     1     1      1       1   32900    0.08
theta[1]  23800   0.06     1     1     1      1       1   40600    0.10
theta[2]  27800   0.07     1     1     1      1       1   41800    0.10
theta[3]  39400   0.10     1     1     1      1       1   31400    0.08
theta[4]  32600   0.08     1     1     1      1       1   38700    0.10
theta[5]  34500   0.09     1     1     1      1       1   37200    0.09
theta[6]  37000   0.09     1     1     1      1       1   36600    0.09
theta[7]  20700   0.05     1     1     1      1       1   35100    0.09
theta[8]  36200   0.09     1     1     1      1       1   38900    0.10
```



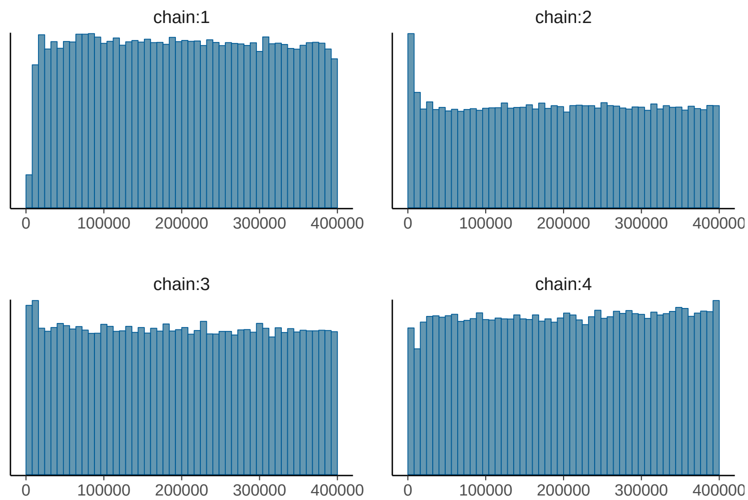



```
lp__        2540   0.01      1       1       1       1        1     2940     0.01
         tailseff tailreff medsseff medsreff madsseff madsreff
mu          30300     0.08    16300     0.04    18300     0.05
tau           769     0.00    10900     0.03    15400     0.04
theta[1]   111000     0.28    15300     0.04    18800     0.05
theta[2]   136000     0.34    15100     0.04    18500     0.05
theta[3]   123000     0.31    16700     0.04    22100     0.06
theta[4]   139000     0.35    16500     0.04    19000     0.05
theta[5]    44500     0.11    16600     0.04    18900     0.05
theta[6]    92200     0.23    16400     0.04    18200     0.05
theta[7]    58000     0.15    14800     0.04    17400     0.04
theta[8]   125000     0.31    15400     0.04    16100     0.04
lp__         1070     0.00    10100     0.03    13800     0.03
```

Rhat, Bulk-ESS and Tail-ESS are not able to detect problems, although Tail-ESS for `tau` is suspiciously low compared to total number of draws.

And the rank plots of `tau` also show sticking and mixing problems for small values of `tau`.

What we do see is an advantage of rank plots over trace plots as even with 100000 draws per chain, rank



plots don't get crowded and the mixing problems of chains is still easy to see.

With centered parameterization the mean estimate tends to get smaller with more draws. With 400000 draws using the centered parameterization the mean estimate is 3.77 (se 0.03). With 40000 draws using the non-centered parameterization the mean estimate is 3.6 (se 0.02). The difference is more than 8 sigmas. We are able to see the convergence problems in the centered parameterization case, if we do look carefully (or use divergence diagnostic), but we do see that Rhat, Bulk-ESS, Tail-ESS and Monte Carlo error estimates for the mean can't be trusted if other diagnostics indicate convergence problems!

4.2.2.6 Centered parameterization with very long chains and thinning

When autocorrelation time is high, it has been common to thin the chains by saving only a small portion of the draws. This will throw away useful information also for convergence diagnostics. With 400000 iterations per chain, thinning of 200 and 4 chains, we again end up with 4000 iterations as with the default settings.

We observe several divergent transitions and the estimated Bayesian fraction of missing information is also low, which indicate convergence problems and potentially biased estimates.

Unfortunately the thinning makes Rhat and ESS estimates to miss the problems. The posterior mean is still biased, being more than 3 sigmas away from the estimate obtained using non-centered parameterization.

```
Inference for the input samples (4 chains: each with iter = 400000; warmup = 200000):

             Q5    Q50   Q95   Mean   SD  Rhat Bulk_ESS Tail_ESS
mu        -0.91   4.46  9.73   4.40 3.24     1     3784     3648
tau        0.46   2.89 10.00   3.75 3.16     1     3625     2447
theta[1]  -1.66   5.63 16.20   6.24 5.74     1     4101     3691
theta[2]  -2.17   4.84 12.60   5.04 4.62     1     3950     3946
theta[3]  -4.54   4.16 11.90   3.98 5.21     1     4121     3819
theta[4]  -3.02   4.73 12.40   4.75 4.83     1     4026     4188
theta[5]  -4.38   3.75 10.60   3.55 4.68     1     3790     3839
theta[6]  -3.76   4.30 11.80   4.18 4.86     1     4057     4059
theta[7]  -0.96   5.91 15.40   6.34 5.00     1     4154     3813
theta[8]  -3.54   4.64 13.50   4.78 5.33     1     4040     3968
lp__     -25.10 -15.00 -1.64 -14.40 6.99     1     3689     2616

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
```

```
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

```
Inference for the input samples (4 chains: each with iter = 400000; warmup = 200000):

           mean se_mean   sd     Q5    Q50   Q95 seff reff sseff zseff
mu         4.40    0.05 3.24  -0.91   4.46  9.73 3740 0.93  3780  3740
tau        3.75    0.05 3.16   0.46   2.89 10.00 4010 1.00  4000  3620
theta[1]   6.24    0.09 5.74  -1.66   5.63 16.20 4060 1.02  4070  4100
theta[2]   5.04    0.07 4.62  -2.17   4.84 12.60 3920 0.98  3940  3940
theta[3]   3.98    0.08 5.21  -4.54   4.16 11.90 4100 1.02  4100  4120
theta[4]   4.75    0.08 4.83  -3.02   4.73 12.40 3960 0.99  4010  3970
theta[5]   3.55    0.08 4.68  -4.38   3.75 10.60 3720 0.93  3810  3740
theta[6]   4.18    0.08 4.86  -3.76   4.30 11.80 3940 0.99  4030  4010
theta[7]   6.34    0.08 5.00  -0.96   5.91 15.40 4120 1.03  4130  4140
theta[8]   4.78    0.08 5.33  -3.54   4.64 13.50 3970 0.99  3990  4010
lp__     -14.40    0.12 6.99 -25.10 -15.00 -1.64 3500 0.88  3560  3690
         zsseff zsreff  Rhat sRhat zRhat zsRhat zfsRhat zfsseff zfsreff
mu         3780   0.95     1     1     1      1       1    3660    0.91
tau        3620   0.91     1     1     1      1       1    4100    1.02
theta[1]   4100   1.03     1     1     1      1       1    4200    1.05
theta[2]   3950   0.99     1     1     1      1       1    4050    1.01
theta[3]   4120   1.03     1     1     1      1       1    3810    0.95
theta[4]   4030   1.01     1     1     1      1       1    3920    0.98
theta[5]   3790   0.95     1     1     1      1       1    3580    0.90
theta[6]   4060   1.01     1     1     1      1       1    3880    0.97
theta[7]   4150   1.04     1     1     1      1       1    4060    1.02
theta[8]   4040   1.01     1     1     1      1       1    3750    0.94
lp__       3690   0.92     1     1     1      1       1    3190    0.80
         tailseff tailreff medsseff medsreff madsseff madsreff
mu           3650     0.91     4190     1.05     3800     0.95
tau          2450     0.61     3960     0.99     3820     0.95
theta[1]     3690     0.92     4120     1.03     3900     0.98
theta[2]     3950     0.99     3560     0.89     4060     1.01
theta[3]     3820     0.95     4080     1.02     3810     0.95
theta[4]     4190     1.05     3500     0.87     3880     0.97
theta[5]     3840     0.96     3830     0.96     3840     0.96
theta[6]     4060     1.01     4000     1.00     3820     0.96
theta[7]     3810     0.95     4260     1.06     3870     0.97
theta[8]     3970     0.99     4140     1.03     3830     0.96
lp__         2620     0.65     3840     0.96     3910     0.98
```

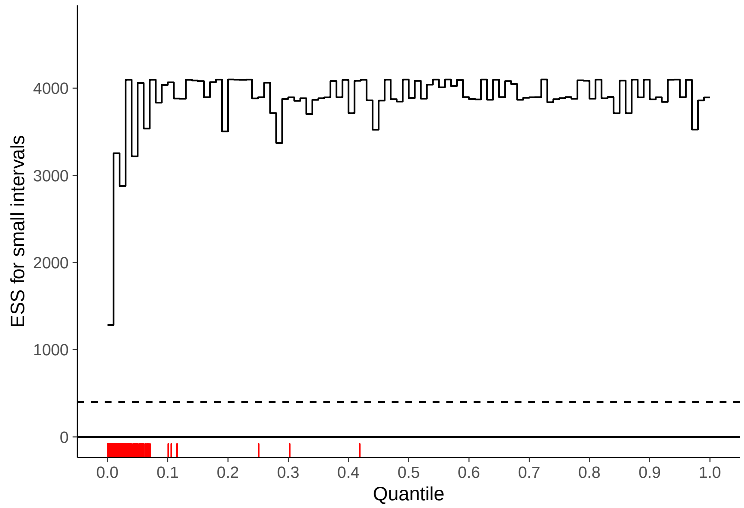
Diagnostic plots for `tau` look reasonable as well.

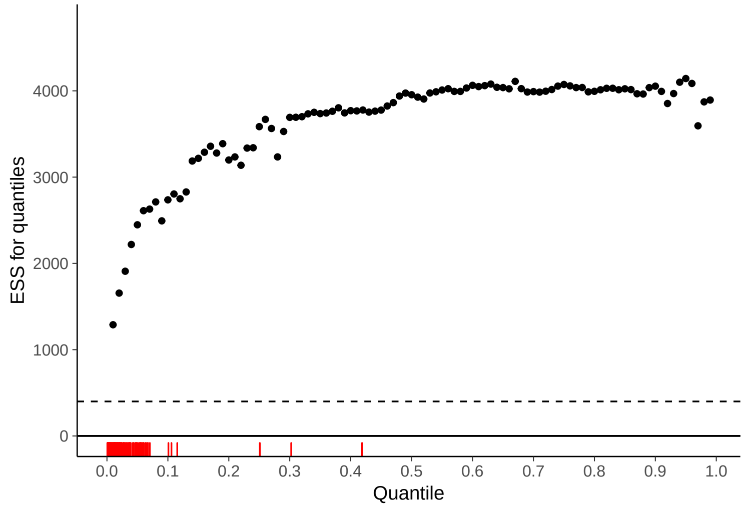
However, the rank plots seem still to show the problem.

Non-centered Eight Schools model

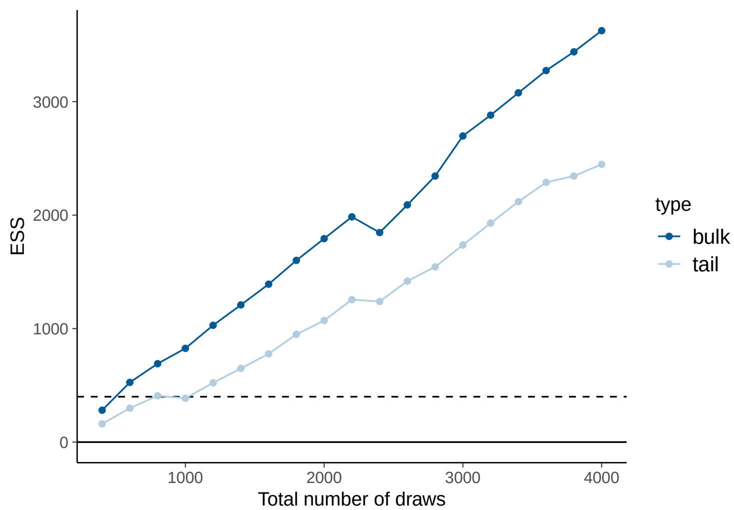
In the following, we want to expand our understanding of the non-centered parameterization of the hierarchical model fit to the eight schools data.

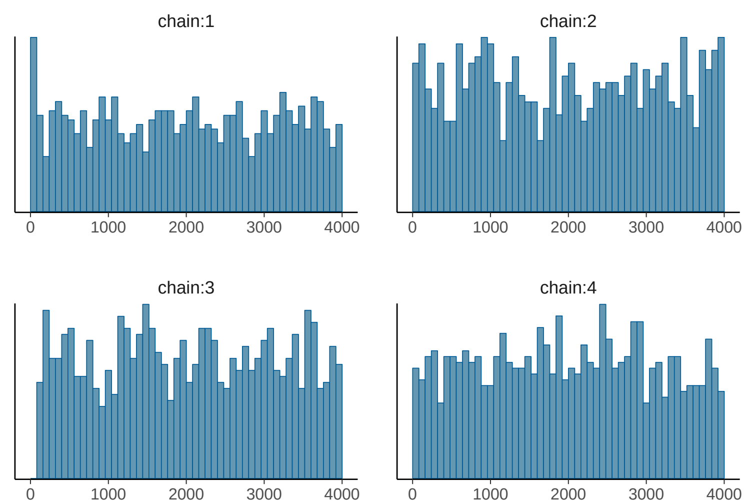
```
data {
  int<lower=0> J;
  real y[J];
  real<lower=0> sigma[J];
```






```
}

parameters {
  real mu;
  real<lower=0> tau;
  real theta_tilde[J];
}

transformed parameters {
  real theta[J];
  for (j in 1:J)
    theta[j] = mu + tau * theta_tilde[j];
}

model {
  mu ~ normal(0, 5);
  tau ~ cauchy(0, 5);
  theta_tilde ~ normal(0, 1);
  y ~ normal(theta, sigma);
```





}

4.2.2.7 Non-centered parameterization with default MCMC options

In the main text, we have already seen that the non-centered parameterization works better than the centered parameterization, at least when we use an increased `adapt_delta` value. Let's see what happens when using the default MCMC option of Stan.

We observe a few divergent transitions with the default of `adapt_delta=0.8`. Let's analyze the sample.

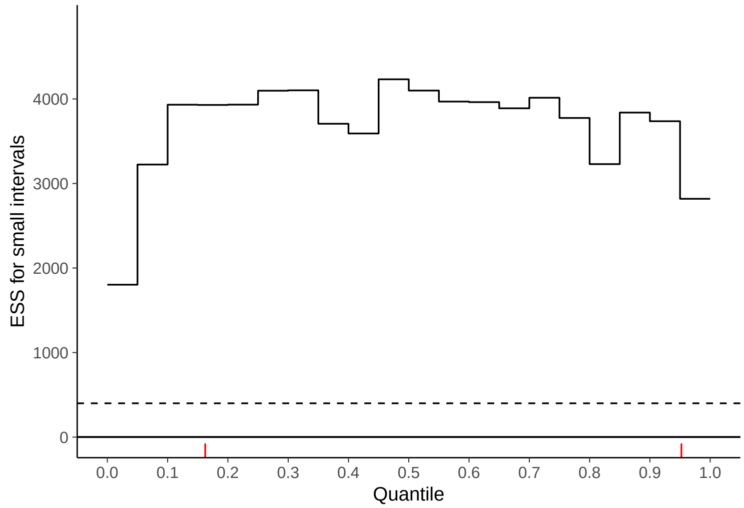
```
Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

                  Q5   Q50   Q95  Mean   SD  Rhat Bulk_ESS Tail_ESS
mu             -0.98  4.41  9.52  4.38 3.24     1     4083     2378
tau             0.25  2.77  9.77  3.61 3.16     1     2303     1795
theta_tilde[1] -1.31  0.35  1.88  0.32 0.97     1     4571     2604
theta_tilde[2] -1.41  0.14  1.64  0.12 0.92     1     5771     3078
theta_tilde[3] -1.62 -0.10  1.49 -0.09 0.96     1     4966     3054
theta_tilde[4] -1.43  0.03  1.51  0.05 0.91     1     5442     2830
theta_tilde[5] -1.67 -0.17  1.35 -0.16 0.91     1     4273     3005
```

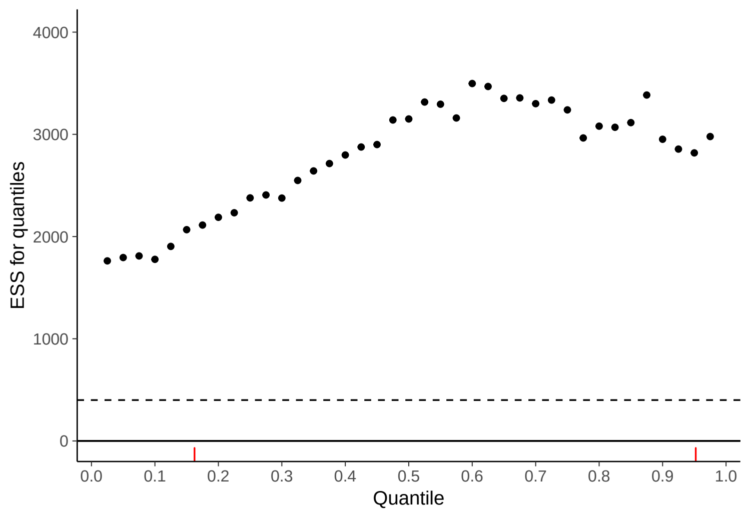
```
theta_tilde[6]  -1.64 -0.08  1.48 -0.07 0.95     1     5192     2981
theta_tilde[7]  -1.25  0.39  1.88  0.36 0.97     1     3898     2800
theta_tilde[8]  -1.51  0.07  1.68  0.08 0.97     1     4848     2863
theta[1]        -1.38  5.68 15.80  6.27 5.60     1     3790     2549
theta[2]        -2.29  4.88 12.80  5.03 4.62     1     5002     2920
theta[3]        -4.28  4.08 11.90  3.95 5.24     1     4001     3036
theta[4]        -2.74  4.66 12.10  4.64 4.63     1     4699     3063
theta[5]        -4.13  3.89 10.40  3.63 4.54     1     4310     3184
theta[6]        -4.11  4.19 11.30  3.95 4.88     1     4965     2806
theta[7]        -0.84  5.86 15.20  6.28 4.94     1     4599     3296
theta[8]        -3.24  4.77 13.50  4.91 5.37     1     4461     3288
lp__           -11.10 -6.47 -3.68 -6.81 2.30     1     1711     2385

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).

Inference for the input samples (4 chains: each with iter = 2000; warmup = 1000):

                mean se_mean   sd     Q5   Q50   Q95 seff reff sseff zseff
mu              4.38    0.05 3.24  -0.98  4.41  9.52 4020 1.01  4040  4070
tau             3.61    0.06 3.16   0.25  2.77  9.77 2680 0.67  2700  2290
theta_tilde[1]  0.32    0.01 0.97  -1.31  0.35  1.88 4530 1.13  4570  4530
theta_tilde[2]  0.12    0.01 0.92  -1.41  0.14  1.64 5740 1.44  5760  5750
theta_tilde[3] -0.09    0.01 0.96  -1.62 -0.10  1.49 4930 1.23  4970  4920
theta_tilde[4]  0.05    0.01 0.91  -1.43  0.03  1.51 5370 1.34  5440  5380
theta_tilde[5] -0.16    0.01 0.91  -1.67 -0.17  1.35 4220 1.06  4270  4230
theta_tilde[6] -0.07    0.01 0.95  -1.64 -0.08  1.48 5180 1.30  5200  5180
theta_tilde[7]  0.36    0.02 0.97  -1.25  0.39  1.88 3880 0.97  3890  3890
theta_tilde[8]  0.08    0.01 0.97  -1.51  0.07  1.68 4840 1.21  4850  4830
theta[1]        6.27    0.09 5.60  -1.38  5.68 15.80 3500 0.88  3530  3770
theta[2]        5.03    0.07 4.62  -2.29  4.88 12.80 4890 1.22  4930  4960
theta[3]        3.95    0.09 5.24  -4.28  4.08 11.90 3800 0.95  3820  3970
theta[4]        4.64    0.07 4.63  -2.74  4.66 12.10 4550 1.14  4580  4680
theta[5]        3.63    0.07 4.54  -4.13  3.89 10.40 4130 1.03  4170  4260
theta[6]        3.95    0.07 4.88  -4.11  4.19 11.30 4730 1.18  4820  4920
theta[7]        6.28    0.07 4.94  -0.84  5.86 15.20 4420 1.10  4420  4520
theta[8]        4.91    0.08 5.37  -3.24  4.77 13.50 4050 1.01  4070  4440
lp__           -6.81    0.06 2.30 -11.10 -6.47 -3.68 1680 0.42  1680  1700
               zsseff zsreff  Rhat sRhat zRhat zsRhat zfsRhat zfsseff
mu               4080   1.02     1     1     1      1       1    1780
tau              2300   0.58     1     1     1      1       1    3130
theta_tilde[1]   4570   1.14     1     1     1      1       1    2140
theta_tilde[2]   5770   1.44     1     1     1      1       1    1980
theta_tilde[3]   4970   1.24     1     1     1      1       1    2140
theta_tilde[4]   5440   1.36     1     1     1      1       1    2010
theta_tilde[5]   4270   1.07     1     1     1      1       1    2260
theta_tilde[6]   5190   1.30     1     1     1      1       1    2080
theta_tilde[7]   3900   0.97     1     1     1      1       1    2260
theta_tilde[8]   4850   1.21     1     1     1      1       1    1900
theta[1]         3790   0.95     1     1     1      1       1    2530
theta[2]         5000   1.25     1     1     1      1       1    2300
theta[3]         4000   1.00     1     1     1      1       1    2550
```

```
theta[4]         4700   1.17     1     1      1      1        1    2650
theta[5]         4310   1.08     1     1      1      1        1    2780
theta[6]         4960   1.24     1     1      1      1        1    2670
theta[7]         4600   1.15     1     1      1      1        1    2490
theta[8]         4460   1.12     1     1      1      1        1    2470
lp__             1710   0.43     1     1      1      1        1    2490
               zfsreff tailseff tailreff medsseff medsreff madsseff
mu                0.44     2380     0.59     4240     1.06     2340
tau               0.78     1800     0.45     3150     0.79     3170
theta_tilde[1]    0.54     2600     0.65     4490     1.12     2490
theta_tilde[2]    0.50     3080     0.77     5350     1.34     2410
theta_tilde[3]    0.53     3050     0.76     5400     1.35     2450
theta_tilde[4]    0.50     2830     0.71     4820     1.21     2420
theta_tilde[5]    0.57     3000     0.75     4280     1.07     2690
theta_tilde[6]    0.52     2980     0.75     4760     1.19     2410
theta_tilde[7]    0.56     2800     0.70     3820     0.96     2780
theta_tilde[8]    0.48     2860     0.72     4350     1.09     2000
theta[1]          0.63     2550     0.64     4360     1.09     2790
theta[2]          0.58     2920     0.73     4230     1.06     2540
theta[3]          0.64     3040     0.76     4000     1.00     2970
theta[4]          0.66     3060     0.77     4550     1.14     2860
theta[5]          0.70     3180     0.80     4520     1.13     2690
theta[6]          0.67     2810     0.70     4760     1.19     3150
theta[7]          0.62     3300     0.82     4320     1.08     2910
theta[8]          0.62     3290     0.82     4400     1.10     2640
lp__              0.62     2380     0.60     1990     0.50     2800
               madsreff
mu                 0.59
tau                0.79
theta_tilde[1]     0.62
theta_tilde[2]     0.60
theta_tilde[3]     0.61
theta_tilde[4]     0.60
theta_tilde[5]     0.67
theta_tilde[6]     0.60
theta_tilde[7]     0.70
theta_tilde[8]     0.50
theta[1]           0.70
theta[2]           0.64
theta[3]           0.74
theta[4]           0.71
theta[5]           0.67
theta[6]           0.79
theta[7]           0.73
theta[8]           0.66
lp__               0.70
```

All Rhats are close to 1, and ESSs are good despite a few divergent transitions. Small interval and quantile plots of `tau` reveal some sampling problems for small `tau` values, but not nearly as strong as for the centered parameterization.

Overall, the non-centered parameterization looks good even for the default settings of `adapt_delta`, and increasing it to 0.95 gets rid of the last remaining problems. This stands in sharp contrast to what we observed for the centered parameterization, where increasing `adapt_delta` didn't help at all. Actually, this is something we observe quite often: A suboptimal parameterization can cause problems that are not simply





solved by tuning the sampler. Instead, we have to adjust our model to achieve trustworthy inference.

Eight Schools with Jags

We will also run the centered and non-centered parameterizations of the eight schools model with Jags.

4.2.2.8 Centered Eight Schools Model

The Jags code for the centered eight schools model looks as follows:

```
model {
  for (j in 1:J) {
    sigma_prec[j] <- pow(sigma[j], -2)
    theta[j] ~ dnorm(mu, tau_prec)
    y[j] ~ dnorm(theta[j], sigma_prec[j])
  }
  mu ~ dnorm(0, pow(5, -2))
  tau ~ dt(0, pow(5, -2), 1)T(0, )
```

```
  tau_prec <- pow(tau, -2)
}
```

First, we initialize the Jags model for reusage later.

```
Compiling model graph
   Resolving undeclared variables
   Allocating nodes
Graph information:
   Observed stochastic nodes: 8
   Unobserved stochastic nodes: 10
   Total graph size: 40

Initializing model
```

Next, we sample 1000 iterations for each of the 4 chains for easy comparison with the corresponding Stan results.

Convergence diagnostics indicate problems in the sampling of `mu` and `tau`, but also to a lesser degree in all other paramters.

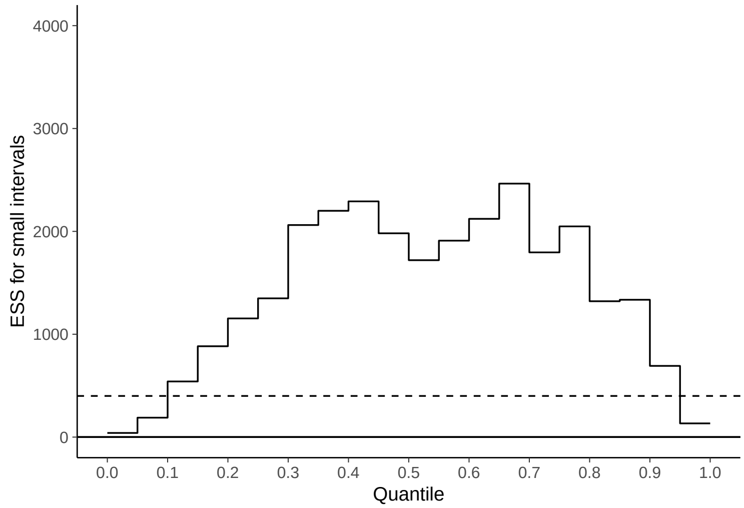
```
Inference for the input samples (4 chains: each with iter = 1000; warmup = 0):

             Q5  Q50   Q95 Mean   SD  Rhat Bulk_ESS Tail_ESS
mu        -1.00 4.41  9.82 4.42 3.26  1.02      189      447
tau        0.29 2.99  9.96 3.73 3.11  1.08       59       53
theta[1] -1.42 5.71 16.70 6.37 5.57  1.02      280      685
theta[2] -2.33 5.03 13.00 5.03 4.66  1.01      364      956
theta[3] -5.08 4.26 11.90 3.97 5.24  1.01      317      995
theta[4] -2.76 4.92 12.60 4.83 4.82  1.01      374     1001
theta[5] -4.67 3.83 10.70 3.58 4.79  1.01      341      889
theta[6] -4.20 4.29 11.70 4.12 4.83  1.01      377     1052
theta[7] -0.68 5.87 15.40 6.37 4.98  1.02      256      736
theta[8] -3.69 4.97 13.60 4.89 5.35  1.01      415      805

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

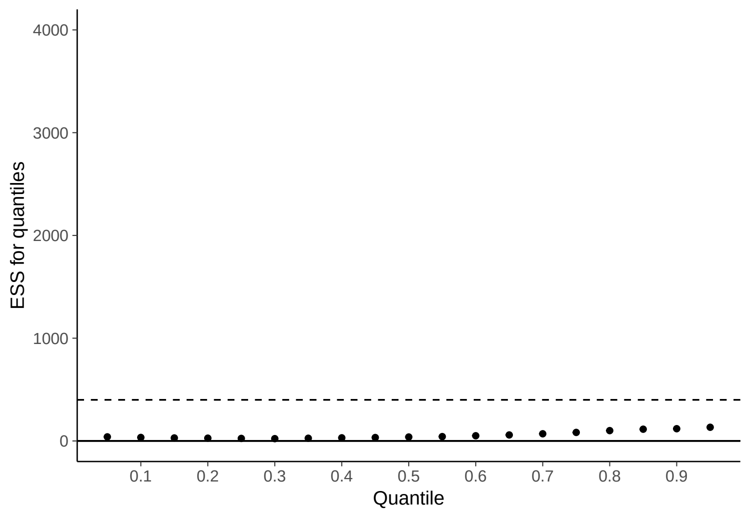
We also see problems in the sampling of `tau` using various diagnostic plots.

Let's see what happens if we run 10 times longer chains.

Convergence looks better now, although `tau` is still estimated not very efficiently.

```
Inference for the input samples (4 chains: each with iter = 1000; warmup = 0):

             Q5  Q50   Q95 Mean   SD  Rhat Bulk_ESS Tail_ESS
mu        -0.89 4.39 10.20 4.40 3.35  1.06       71      251
tau        0.13 2.37  8.37 3.07 2.69  1.09       36       32
theta[1] -1.34 5.35 14.70 5.79 5.07  1.06       88      924
theta[2] -1.70 4.89 12.30 4.83 4.49  1.04      106      959
theta[3] -3.77 4.10 11.60 3.94 4.89  1.03      148      591
theta[4] -2.34 4.73 12.40 4.68 4.61  1.04      126     1054
theta[5] -3.44 4.01 11.10 3.85 4.46  1.03      153      374
theta[6] -3.37 4.23 11.60 4.07 4.70  1.03      154      619
theta[7] -0.93 5.39 14.60 5.94 4.74  1.07       98      450
```






```
theta[8] -2.54 4.68 12.60 4.74 4.82  1.04      130      850

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

The diagnostic plots of quantiles and small intervals tell a similar story.

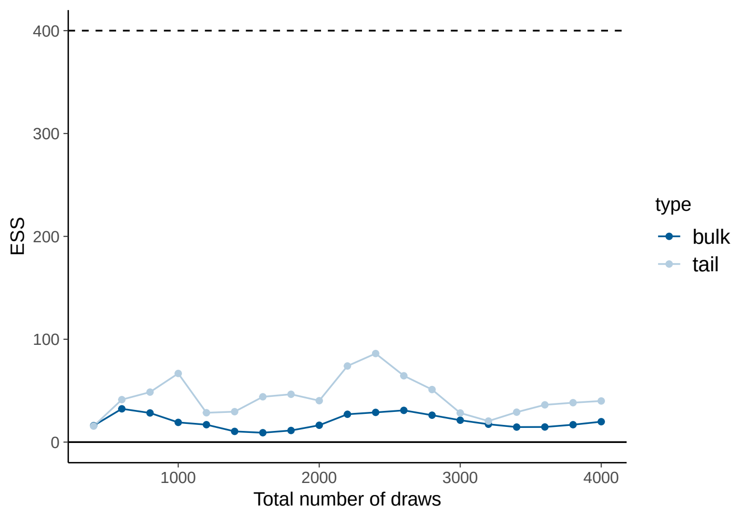
Notably, however, the increase in effective sample size of tau is linear in the total number of draws indicating that convergence for `tau` may be achieved by simply running longer chains.

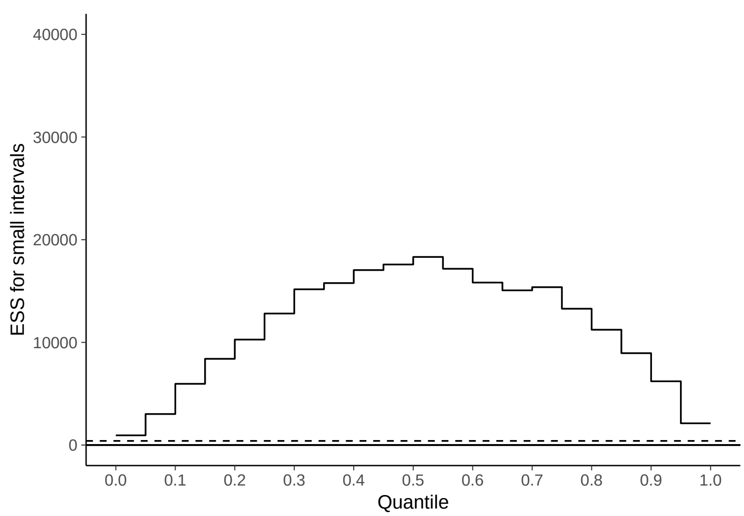
Result: Similar to Stan, Jags also has convergence problems with the centered parameterization of the eight schools model.

4.2.2.9 Non-Centered Eight Schools Model

The Jags code for the non-centered eight schools model looks as follows:

```
model {
  for (j in 1:J) {
```

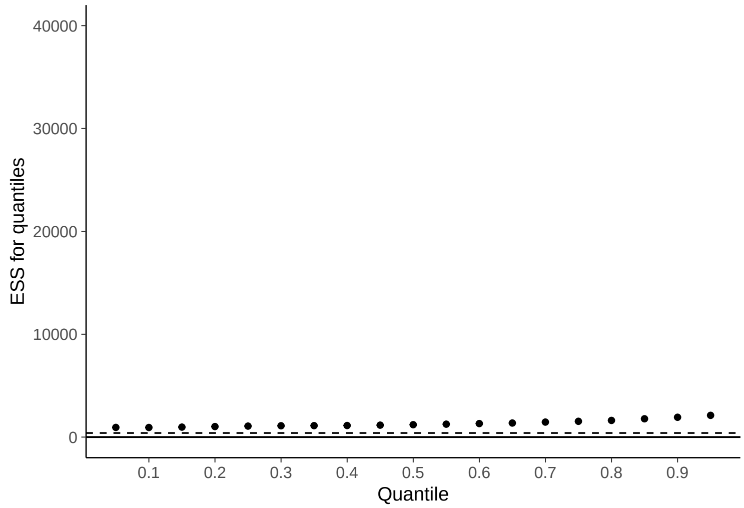


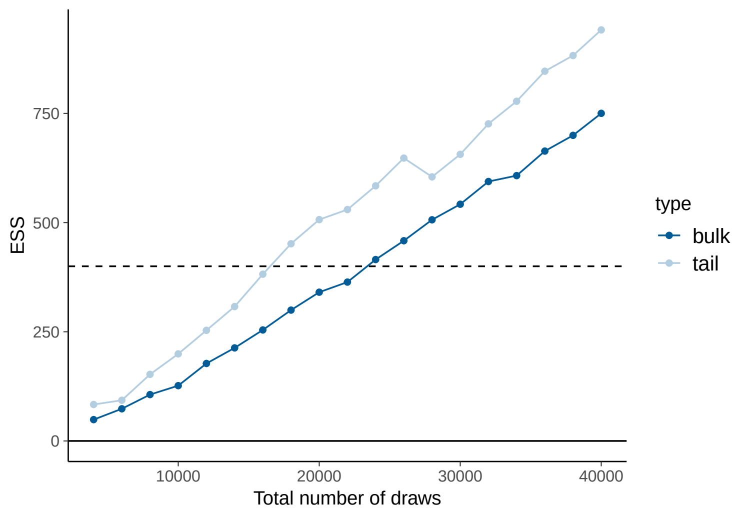



```
    sigma_prec[j] <- pow(sigma[j], -2)
    theta_tilde[j] ~ dnorm(0, 1)
    theta[j] = mu + tau * theta_tilde[j]
    y[j] ~ dnorm(theta[j], sigma_prec[j])
  }
  mu ~ dnorm(0, pow(5, -2))
  tau ~ dt(0, pow(5, -2), 1)T(0, )
}
```

First, we initialize the Jags model for reusage later.

```
Compiling model graph
   Resolving undeclared variables
   Allocating nodes
Graph information:
   Observed stochastic nodes: 8
   Unobserved stochastic nodes: 10
   Total graph size: 55

Initializing model
```

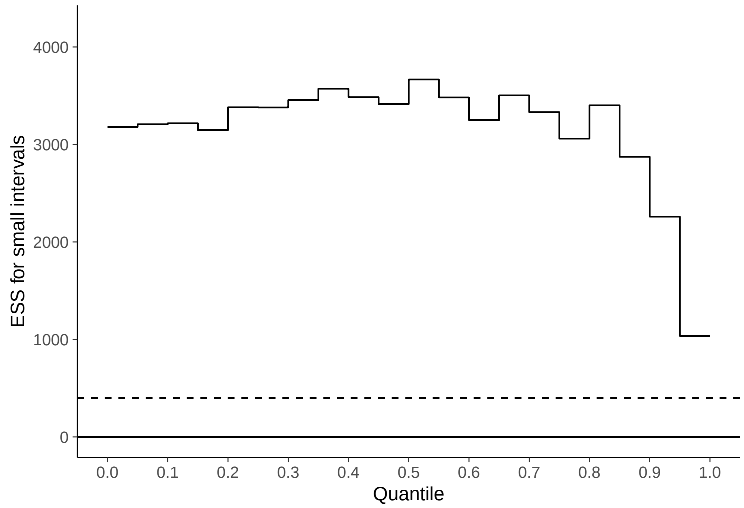


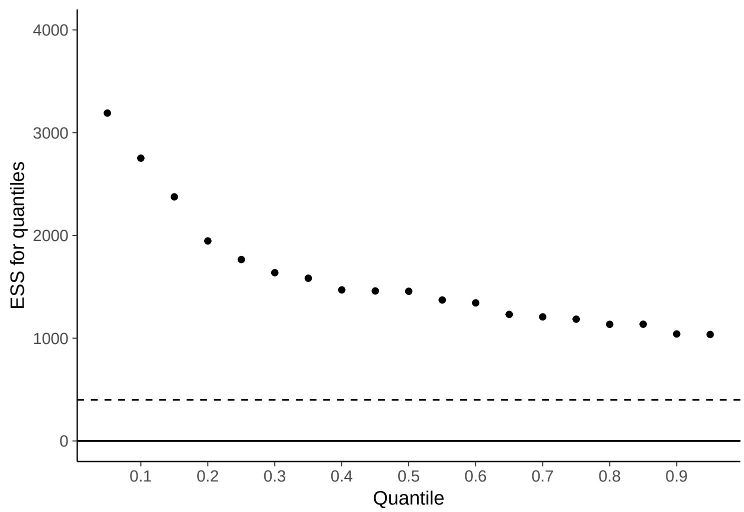


Next, we sample 1000 iterations for each of the 4 chains for easy comparison with the corresponding Stan results.

Convergence diagnostics indicate much better mixing than for the centered eight school model.

```
Inference for the input samples (4 chains: each with iter = 1000; warmup = 0):

            Q5  Q50  Q95 Mean   SD  Rhat Bulk_ESS Tail_ESS
mu       -1.00 4.43 10.1 4.44 3.39     1     2897     3447
tau       0.26 2.74 10.2 3.64 3.28     1     1031      965
theta[1] -1.63 5.63 16.5 6.30 5.76     1     3218     2337
theta[2] -2.60 4.91 12.8 5.00 4.78     1     4015     2912
theta[3] -5.00 4.07 11.9 3.86 5.35     1     3189     2725
theta[4] -2.54 4.78 12.4 4.88 4.79     1     3440     3488
theta[5] -4.44 3.91 10.9 3.64 4.67     1     3480     3560
theta[6] -4.16 4.12 11.4 3.94 4.77     1     3345     2715
theta[7] -1.06 5.95 15.9 6.42 5.16     1     3081     2721
theta[8] -3.43 4.83 13.7 4.92 5.36     1     4112     3115

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
```






```
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

Specifically, the mixing of `tau` looks much better although we still see some problems in the estimation of larger quantiles.

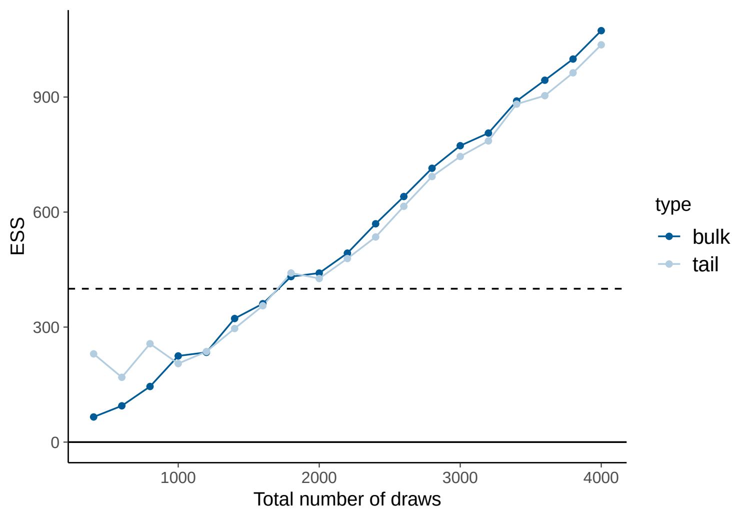
Change in effective sample size is roughly linear indicating that some remaining convergence problems are likely to be solved by running longer chains.

Result: Similar to Stan, Jags can sample from the non-centered parameterization of the eight schools model much better than from the centered parameterization.

Appendix G: Dynamic HMC and effective sample size

We have already seen that the effective sample size of dynamic HMC can be higher than with independent draws. The next example illustrates interesting relative efficiency phenomena due to the properties of dynamic HMC algorithms.

We sample from a simple 16-dimensional standard normal model.

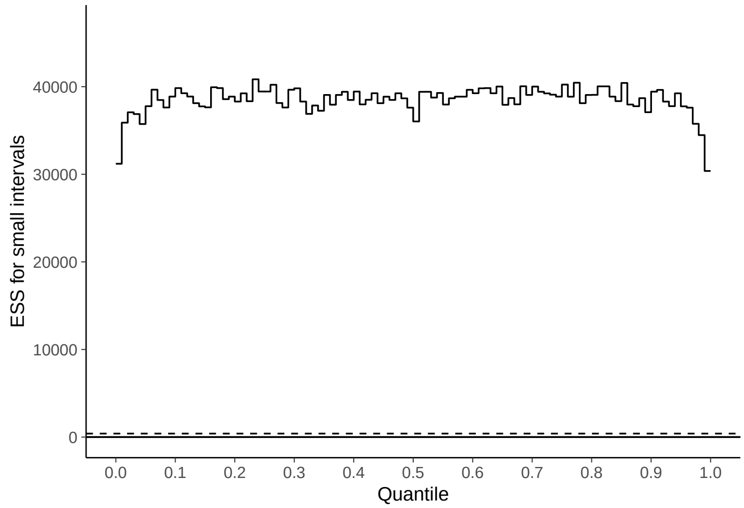


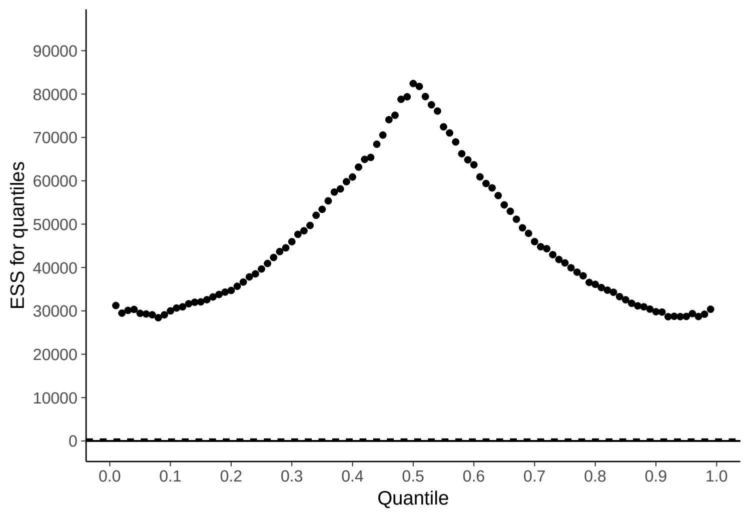

```
data {
  int<lower=1> J;
}
parameters {
  vector[J] x;
}
model {
  x ~ normal(0, 1);
}
```

```
Inference for the input samples (4 chains: each with iter = 10000; warmup = 0):

          Q5   Q50   Q95  Mean   SD  Rhat Bulk_ESS Tail_ESS
x[1]   -1.66  0.00  1.65  0.00 1.00     1    98264    28709
x[2]   -1.64 -0.01  1.64  0.00 1.00     1    95812    29664
x[3]   -1.63  0.00  1.62  0.00 0.99     1    98640    28669
x[4]   -1.65  0.00  1.66  0.01 1.01     1    97302    29166
x[5]   -1.64  0.00  1.63  0.00 1.00     1   101542    29930
x[6]   -1.65  0.00  1.65  0.00 1.00     1    96292    28376
x[7]   -1.63  0.01  1.63  0.00 0.99     1    96016    29238
x[8]   -1.65 -0.01  1.65  0.00 1.00     1   100375    29893
x[9]   -1.64  0.01  1.65  0.00 1.00     1   101141    28621
x[10]  -1.62 -0.01  1.63  0.00 0.99     1   103126    29411
x[11]  -1.65  0.01  1.66  0.00 1.00     1    95886    28488
x[12]  -1.62  0.00  1.63  0.01 0.99     1    98433    29228
x[13]  -1.62  0.01  1.65  0.00 0.99     1    98181    27421
x[14]  -1.63  0.00  1.63  0.00 0.99     1    97313    27507
x[15]  -1.63  0.01  1.64  0.01 0.99     1    95223    29139
x[16]  -1.66  0.00  1.65  0.00 1.01     1    99980    29639
lp__  -13.00 -7.66 -3.92 -7.95 2.79     1    14489    19627

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

```
Inference for the input samples (4 chains: each with iter = 10000; warmup = 0):
```

```
       mean se_mean   sd     Q5   Q50   Q95   seff reff  sseff  zseff
x[1]   0.00    0.00 1.00  -1.66  0.00  1.65  97800 2.45  98400  97700
x[2]   0.00    0.00 1.00  -1.64 -0.01  1.64  95400 2.39  95700  95500
x[3]   0.00    0.00 0.99  -1.63  0.00  1.62  98400 2.46  98700  98300
x[4]   0.01    0.00 1.01  -1.65  0.00  1.66  96600 2.42  97300  96700
x[5]   0.00    0.00 1.00  -1.64  0.00  1.63 101000 2.53 102000 101000
x[6]   0.00    0.00 1.00  -1.65  0.00  1.65  96000 2.40  96300  96000
x[7]   0.00    0.00 0.99  -1.63  0.01  1.63  95600 2.39  96100  95500
x[8]   0.00    0.00 1.00  -1.65 -0.01  1.65  99900 2.50 100000  99900
x[9]   0.00    0.00 1.00  -1.64  0.01  1.65 101000 2.52 101000 101000
x[10]  0.00    0.00 0.99  -1.62 -0.01  1.63 102000 2.55 103000 102000
x[11]  0.00    0.00 1.00  -1.65  0.01  1.66  95200 2.38  95900  95200
x[12]  0.01    0.00 0.99  -1.62  0.00  1.63  97800 2.45  98400  97900
x[13]  0.00    0.00 0.99  -1.62  0.01  1.65  97700 2.44  98200  97700
x[14]  0.00    0.00 0.99  -1.63  0.00  1.63  96800 2.42  97300  96800
x[15]  0.01    0.00 0.99  -1.63  0.01  1.64  94900 2.37  95200  95000
x[16]  0.00    0.00 1.01  -1.66  0.00  1.65  99500 2.49 100000  99400
lp__  -7.95    0.02 2.79 -13.00 -7.66 -3.92  14900 0.37  14900  14500
      zsseff zsreff  Rhat sRhat zRhat zsRhat zfsRhat zfsseff zfsreff
x[1]   98300   2.46     1     1     1      1       1   16400    0.41
x[2]   95800   2.40     1     1     1      1       1   16500    0.41
x[3]   98600   2.47     1     1     1      1       1   16200    0.40
x[4]   97300   2.43     1     1     1      1       1   16100    0.40
x[5]  102000   2.54     1     1     1      1       1   16800    0.42
x[6]   96300   2.41     1     1     1      1       1   16600    0.41
x[7]   96000   2.40     1     1     1      1       1   17100    0.43
x[8]  100000   2.51     1     1     1      1       1   16400    0.41
x[9]  101000   2.53     1     1     1      1       1   15900    0.40
x[10] 103000   2.58     1     1     1      1       1   16500    0.41
x[11]  95900   2.40     1     1     1      1       1   16000    0.40
x[12]  98400   2.46     1     1     1      1       1   15300    0.38
x[13]  98200   2.45     1     1     1      1       1   15400    0.38
x[14]  97300   2.43     1     1     1      1       1   16500    0.41
x[15]  95200   2.38     1     1     1      1       1   16700    0.42
x[16] 100000   2.50     1     1     1      1       1   16400    0.41
lp__   14500   0.36     1     1     1      1       1   21500    0.54
      tailseff tailreff medsseff medsreff madsseff madsreff
x[1]     28700     0.72    82400     2.06    19200     0.48
x[2]     29700     0.74    75500     1.89    19200     0.48
x[3]     28700     0.72    78600     1.97    18700     0.47
x[4]     29200     0.73    81100     2.03    19100     0.48
x[5]     29900     0.75    80000     2.00    20100     0.50
x[6]     28400     0.71    79000     1.98    19600     0.49
x[7]     29200     0.73    81700     2.04    19500     0.49
x[8]     29900     0.75    79300     1.98    18800     0.47
x[9]     28600     0.72    81100     2.03    18700     0.47
x[10]    29400     0.74    76900     1.92    19200     0.48
x[11]    28500     0.71    79200     1.98    18300     0.46
x[12]    29200     0.73    81800     2.05    18700     0.47
x[13]    27400     0.69    80600     2.02    18200     0.46
x[14]    27500     0.69    77600     1.94    19000     0.48
x[15]    29100     0.73    80400     2.01    19600     0.49
x[16]    29600     0.74    82300     2.06    18800     0.47
```






```
lp__      19600     0.49    17100     0.43    23600     0.59
```

The Bulk-ESS for all x is larger than 95223. However tail-ESS for all x is less than 29930. Further, bulk-ESS for `lp__` is only 14489.

If we take a look at all the Stan examples in this notebook, we see that the bulk-ESS for `lp__` is always below 0.5. This is because `lp__` correlates strongly with the total energy in HMC, which is sampled using a random walk proposal once per iteration. Thus, it's likely that `lp__` has some random walk behavior, as well, leading to autocorrelation and a small relative efficiency. At the same time, adaptive HMC can create antithetic Markov chains which have negative auto-correlations at odd lags. This results in a bulk-ESS greater than S for some parameters.

Let's check the effective sample size in different parts of the posterior by computing the effective sample size for small interval estimates for `x[1]`.

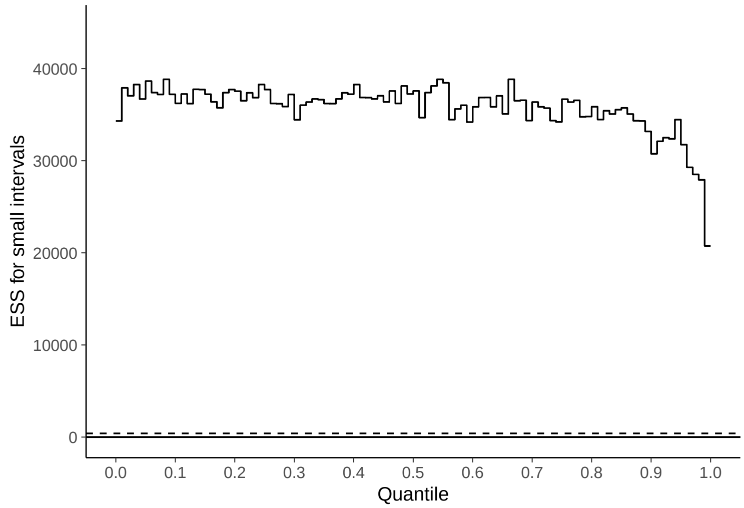
The effective sample size for probability estimate for a small interval is close to 1 with a slight drop in the tails. This is a good result, but far from the effective sample size for the bulk, mean, and median estimates. Let's check the effective sample size for quantiles.

Central quantile estimates have higher effective sample size than tail quantile estimates.

The total energy of HMC should affect how far in the tails a chain in one iteration can go. Fat tails of the target have high energy, and thus only chains with high total energy can reach there. This will suggest that the random walk in total energy would cause random walk in the variance of x. Let's check the second moment of x.

```
Inference for the input samples (4 chains: each with iter = 10000; warmup = 0):

      Q5  Q50  Q95 Mean   SD  Rhat Bulk_ESS Tail_ESS
x[1]   0 0.46 3.85 1.01 1.44     1    16443    18225
x[2]   0 0.44 3.80 0.99 1.42     1    16492    19392
x[3]   0 0.45 3.80 0.98 1.39     1    16148    18342
x[4]   0 0.45 3.95 1.01 1.46     1    16070    18288
x[5]   0 0.45 3.86 1.00 1.42     1    16785    18672
x[6]   0 0.45 3.91 1.00 1.42     1    16572    17525
x[7]   0 0.45 3.74 0.99 1.39     1    17097    19120
x[8]   0 0.46 3.80 1.00 1.42     1    16397    18152
x[9]   0 0.45 3.81 1.00 1.41     1    15922    18049
x[10]  0 0.44 3.73 0.98 1.39     1    16461    18098
x[11]  0 0.46 3.85 1.00 1.41     1    16008    19463
x[12]  0 0.45 3.75 0.99 1.41     1    15368    17674
x[13]  0 0.44 3.83 0.98 1.38     1    15371    16755
x[14]  0 0.45 3.75 0.98 1.37     1    16461    17715
x[15]  0 0.45 3.77 0.98 1.38     1    16655    19241
x[16]  0 0.47 3.86 1.01 1.41     1    16400    19741

For each parameter, Bulk_ESS and Tail_ESS are crude measures of
effective sample size for bulk and tail quantities respectively (good values is
ESS > 400), and Rhat is the potential scale reduction factor on rank normalized
split chains (at convergence, Rhat = 1).
```

```
Inference for the input samples (4 chains: each with iter = 10000; warmup = 0):

      mean se_mean   sd Q5  Q50  Q95  seff reff sseff zseff zsseff zsreff
x[1]  1.01    0.01 1.44  0 0.46 3.85 14700 0.37 14700 16400  16400   0.41
x[2]  0.99    0.01 1.42  0 0.44 3.80 15500 0.39 15500 16500  16500   0.41
x[3]  0.98    0.01 1.39  0 0.45 3.80 14700 0.37 14700 16100  16100   0.40
x[4]  1.01    0.01 1.46  0 0.45 3.95 14500 0.36 14500 16000  16100   0.40
x[5]  1.00    0.01 1.42  0 0.45 3.86 15000 0.38 15000 16800  16800   0.42
x[6]  1.00    0.01 1.42  0 0.45 3.91 14400 0.36 14400 16500  16600   0.41
x[7]  0.99    0.01 1.39  0 0.45 3.74 15500 0.39 15500 17100  17100   0.43
x[8]  1.00    0.01 1.42  0 0.46 3.80 14800 0.37 14800 16400  16400   0.41
x[9]  1.00    0.01 1.41  0 0.45 3.81 13400 0.34 13500 15900  15900   0.40
x[10] 0.98    0.01 1.39  0 0.44 3.73 14700 0.37 14700 16400  16500   0.41
x[11] 1.00    0.01 1.41  0 0.46 3.85 15100 0.38 15100 16000  16000   0.40
x[12] 0.99    0.01 1.41  0 0.45 3.75 14200 0.36 14200 15300  15400   0.38
x[13] 0.98    0.01 1.38  0 0.44 3.83 13500 0.34 13500 15400  15400   0.38
x[14] 0.98    0.01 1.37  0 0.45 3.75 14500 0.36 14600 16400  16500   0.41
x[15] 0.98    0.01 1.38  0 0.45 3.77 15400 0.39 15400 16700  16700   0.42
x[16] 1.01    0.01 1.41  0 0.47 3.86 15600 0.39 15600 16400  16400   0.41
       Rhat sRhat zRhat zsRhat zfsRhat zfsseff zfsreff tailseff tailreff
x[1]      1     1     1      1       1   18400    0.46    18200     0.46
x[2]      1     1     1      1       1   19700    0.49    19400     0.48
x[3]      1     1     1      1       1   18500    0.46    18300     0.46
x[4]      1     1     1      1       1   19000    0.47    18300     0.46
x[5]      1     1     1      1       1   19500    0.49    18700     0.47
x[6]      1     1     1      1       1   17500    0.44    17500     0.44
```

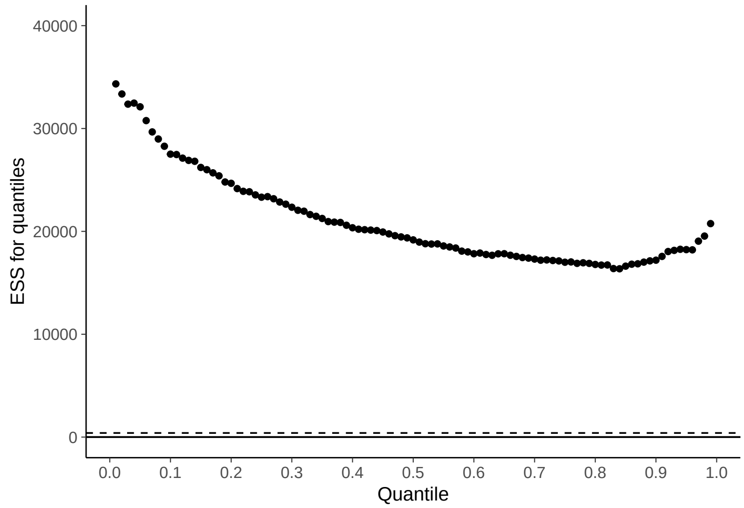


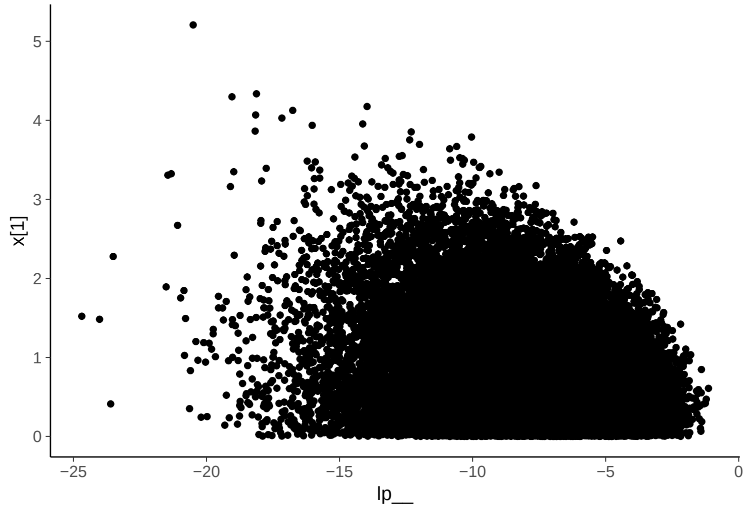

```
x[7]        1     1     1      1       1   19000    0.48    19100      0.48
x[8]        1     1     1      1       1   18900    0.47    18200      0.45
x[9]        1     1     1      1       1   18400    0.46    18000      0.45
x[10]       1     1     1      1       1   18600    0.46    18100      0.45
x[11]       1     1     1      1       1   19500    0.49    19500      0.49
x[12]       1     1     1      1       1   18700    0.47    17700      0.44
x[13]       1     1     1      1       1   18500    0.46    16800      0.42
x[14]       1     1     1      1       1   18800    0.47    17700      0.44
x[15]       1     1     1      1       1   19600    0.49    19200      0.48
x[16]       1     1     1      1       1   20100    0.50    19700      0.49
      medsseff medsreff madsseff madsreff
x[1]     19200     0.48    23300     0.58
x[2]     19300     0.48    24900     0.62
x[3]     18700     0.47    23900     0.60
x[4]     19200     0.48    23900     0.60
x[5]     20100     0.50    25000     0.63
x[6]     19600     0.49    22600     0.57
x[7]     19600     0.49    23300     0.58
x[8]     18800     0.47    24200     0.60
x[9]     18700     0.47    22200     0.55
x[10]    19100     0.48    23900     0.60
x[11]    18400     0.46    24700     0.62
x[12]    18600     0.46    24000     0.60
x[13]    18300     0.46    24100     0.60
x[14]    19100     0.48    23400     0.59
x[15]    19600     0.49    24500     0.61
x[16]    18800     0.47    24400     0.61
```

The mean of the bulk-ESS for x_j^2 is 16290.62, which is quite close to the bulk-ESS for `lp__`. This is not that surprising as the potential energy in normal model is proportional to $\sum_{j=1}^{J} x_j^2$.

Let's check the effective sample size in different parts of the posterior by computing the effective sample size for small interval probability estimates for `x[1]^2`.

The effective sample size is mostly a bit below 1, but for the right tail of x_1^2 the effective sample size drops. This is likely due to only some iterations having high enough total energy to obtain draws from the high energy part of the tail. Let's check the effective sample size for quantiles.

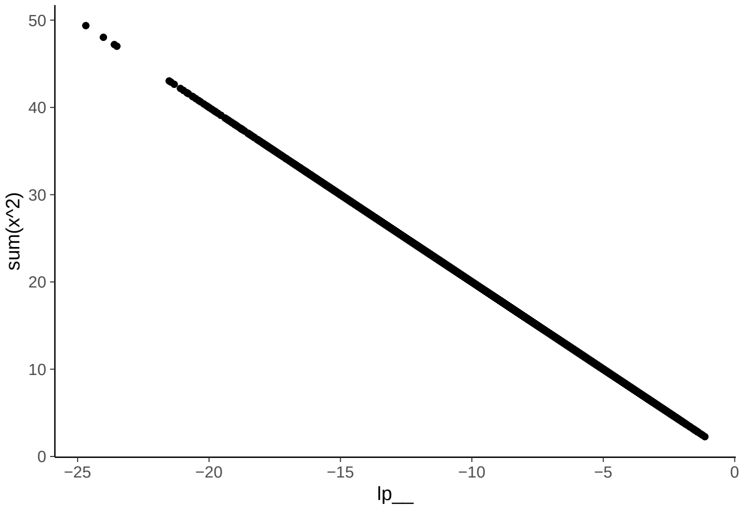




We can see the correlation between `lp__` and magnitude of `x[1]` in the following plot.

Low `lp__` values corresponds to high energy and more variation in `x[1]`, and high `lp__` corresponds to low energy and small variation in `x[1]`. Finally $\sum_{j=1}^{J} x_j^2$ is perfectly correlated with `lp__`.

This shows that even if we get high effective sample size estimates for central quantities (like mean or median), it is important to look at the relative efficiency of scale and tail quantities, as well. The effective sample size of `lp__` can also indicate problems of sampling in the tails.



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