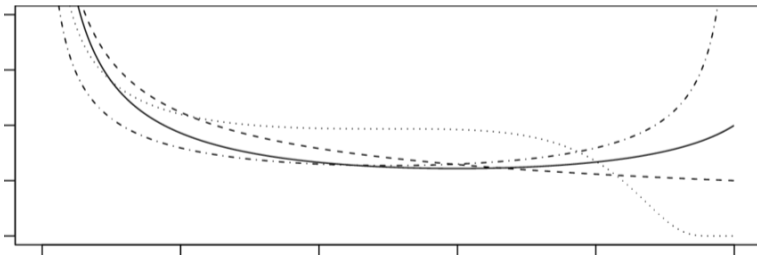


Scalable MCMC for Bayes Shrinkage Priors

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July 2, 2018

Stanford University



Joint work with James Johndrow and Anirban Bhattacharya

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 - Point mass mixture prior, *but*: computation is prohibitive

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- ▶ Global-local priors can achieve this (with some qualifications).
- ▶ But... they are still slow.
 - Lasso: $n \approx 1,000$, $p \approx 1,000,000$;
 - Global-local: $n \approx 1,000$, $p \approx 1,000$.

Model

- ▶ The Horseshoe model*:

$$y_i \mid \beta_j, \lambda_j, \tau, \sigma^2 \stackrel{\text{ind}}{\sim} N(x_i \beta, \sigma^2)$$

$$\beta_j \stackrel{\text{ind}}{\sim} N(0, \tau^2 \lambda_j^2)$$

$$\lambda_j \stackrel{\text{ind}}{\sim} \text{Cauchy}_+(0, 1)$$

$$\tau \sim \text{Cauchy}_+(0, 1)$$

$$\sigma^2 \sim \text{InvGamma}(a_0/2, b_0/2)$$

*[Carvalho et. al, 2010]

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- ▶ It achieves the minimax-adaptive risk for squared error loss up to a constant.
- ▶ Suppose $X = I$, $\|\beta\|_0 = s_n$, then [van der Pas et al., 2014],

$$\sup_{\beta: \|\beta\|_0 \leq s_n} \mathbb{E}_{\beta} \left[\|\hat{\beta}_{HS} - \beta\|_2^2 \right] \leq 4\sigma^2 s_n \log \frac{n}{s_n} \cdot (1 + o(1)),$$

while, for any estimator $\hat{\beta}$, [Donoho et al., 1992] shows

$$\sup_{\beta: \|\beta\|_0 \leq s_n} \mathbb{E}_{\beta} \left[\|\hat{\beta} - \beta\|_2^2 \right] \geq 2\sigma^2 s_n \log \frac{n}{s_n} \cdot (1 + o(1)).$$

Computation

- ▶ State-of-the-art: (i) $\tau \mid \beta, \sigma^2, \lambda$, (ii) $(\beta, \sigma^2) \mid \tau, \lambda$, (iii) slice sampling for λ .

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- ▶ First idea: **block** (β, σ^2, τ) to improve *mixing*;
 1. sample $(\beta, \sigma^2, \tau) \mid \lambda$ by block sampling: $\tau \mid \lambda$, then $\sigma^2 \mid \tau, \lambda$, and finally $\beta \mid \sigma^2, \tau, \lambda$;
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 2. sample $\lambda \mid \beta, \sigma^2$ using slice sampling.
- ▶ Second idea: **truncate** some of the matrices involved to improve the *computational cost per step*.

Gibbs sampling

Let $M = X(\text{diag}(\xi\eta))^{-1}X^T + I$, $\xi = \tau^{-2}$, $\eta_j = \lambda_j^{-2}$, and **block update**:

- ▶ $p(\tau \mid \lambda, y) \propto \frac{1}{\sqrt{\xi(1+\xi)}} |M|^{-1/2} (y^T M^{-1} y + b_0)^{-\frac{n+a_0}{2}}$
- ▶ $p(\sigma^2 \mid \tau, \lambda, y) \sim \text{InvGamma} \left(\frac{n+a_0}{2}, \frac{1}{2} [y^T M^{-1} y + b_0] \right)$
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Then perform slice sampling:

- ▶ $p(\lambda \mid \beta, \sigma^2, \tau, y)$: (i) $U \mid \eta_j \sim \text{Unif} \left[0, \frac{1}{1+\eta_j} \right]$; (ii) $\eta_j \mid u \sim e^{-\frac{\xi\beta_j^2}{2\sigma^2} \eta_j} \mathbb{I}_{\left[\frac{1-u}{u} > \eta_j \right]}$.

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Markov approximation

- ▶ We approximate $M = X \text{diag}((\xi \eta_j)^{-1}) X^T + I$ with

$$M_\delta = X D_\delta X^T + I, \quad D_\delta = \text{diag}((\xi \eta_j)^{-1} \mathbb{I}_{[(\xi_{\max} \eta_j)^{-1} > \delta]})$$

for $\delta \ll 1$, and ξ_{\max} the maximum of the current and proposed ξ .

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Approximating Kernels

Let $\mathcal{P}_\delta(x, \cdot)$ and $\mathcal{P}(x, \cdot)$ denote the Markov operators for the approximate and exact algorithms, with $x = (\beta, \sigma^2, \tau, \lambda)$ the entire state vector. Then

$$\sup_x \|\mathcal{P}_\delta(x, \cdot) - \mathcal{P}(x, \cdot)\|_{\text{TV}} \leq \sqrt{\delta} \|X\| \sqrt{a + \frac{n + a_0}{b_0} + \frac{n}{2} \frac{\|y\|^2}{b_0}} + \mathcal{O}(\delta),$$

for sufficiently small $\delta > 0$.

Simulation

- ▶ We simulate data as follows:

$$x_i \stackrel{\text{iid}}{\sim} N_p(0, \Sigma)$$

$$y_i \sim N(x_i \beta, 4)$$

$$\beta_j = \begin{cases} 2^{-(j/4-9/4)} & \text{if } j < 24, \\ 0 & \text{if } j \geq 24. \end{cases}$$

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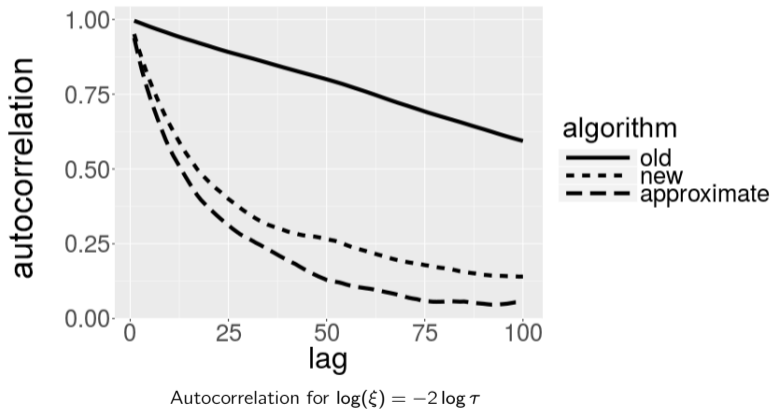
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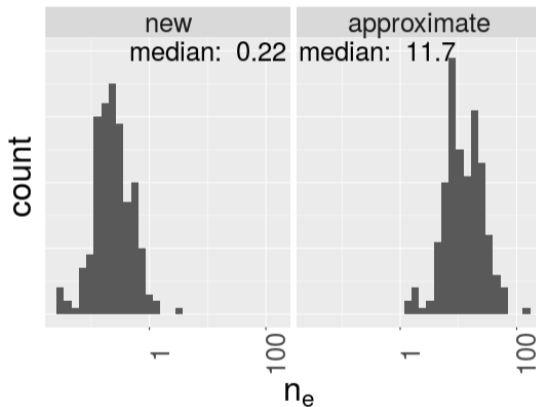
- ▶ There are nulls, clear non-nulls, and some subtle non-nulls.
- ▶ We consider both $\Sigma = I$ (independent design) and $\Sigma_{ij} = 0.9^{|i-j|}$ (correlated design).

Autocorrelation



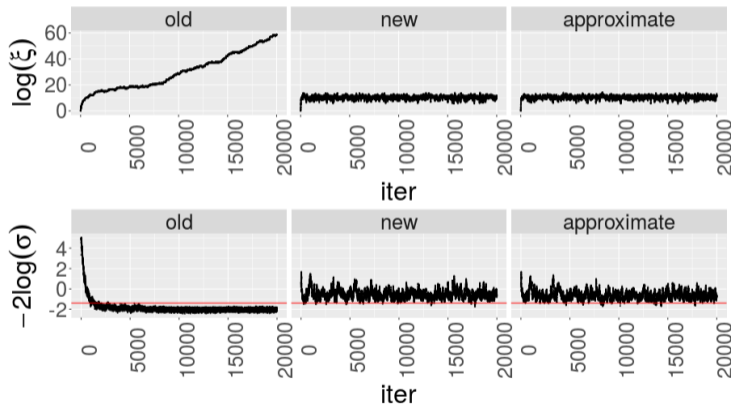
Effective samples per second

- ▶ Approximate algorithm is $50\times$ more efficient with $n = 2,000$ and $p = 20,000$.



Accuracy

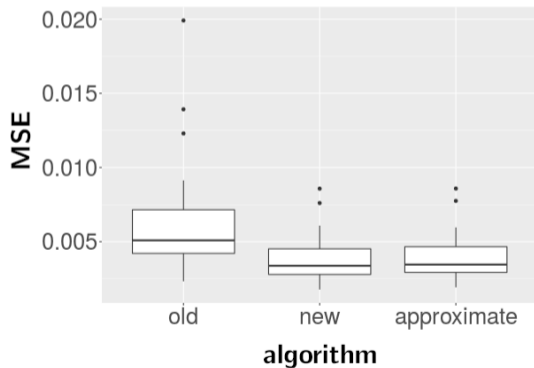
- ▶ Existing algorithms failed to converge, due to numerical underflow.



Trace plots for $-2\log(\sigma)$ and $\log(\xi) = -2\log(\tau)$; truth in red

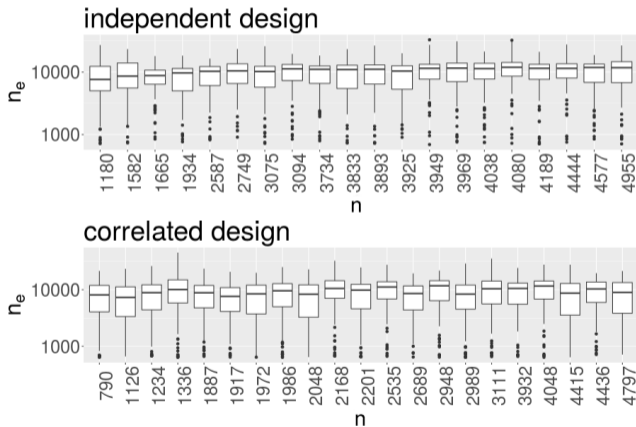
Accuracy

- ▶ In terms of MSE, the approximation costs us little.



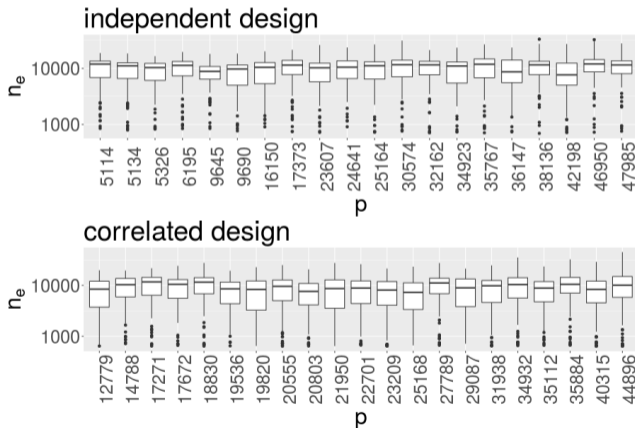
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- Effective sample sizes seem independent of n and p .



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Real application: GWAS

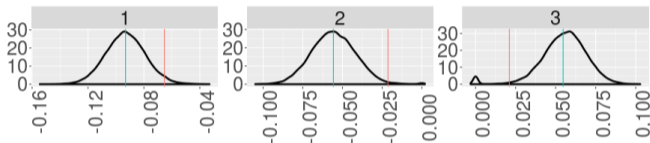
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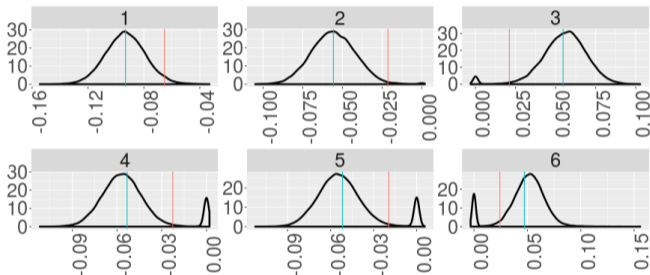
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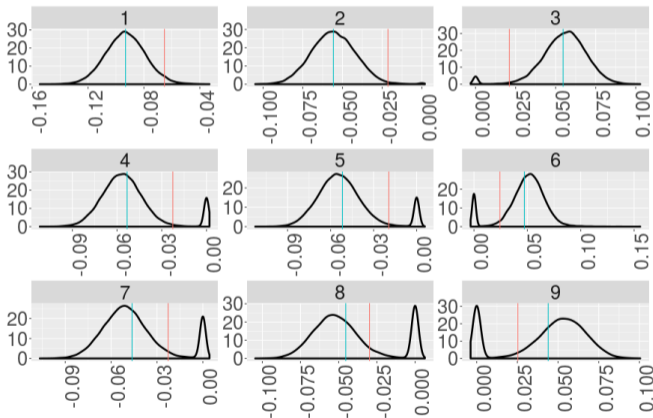
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Bimodal posterior distribution for $\beta_j | y_j$; Lasso (red) shrinks more than Horseshoe (blue)

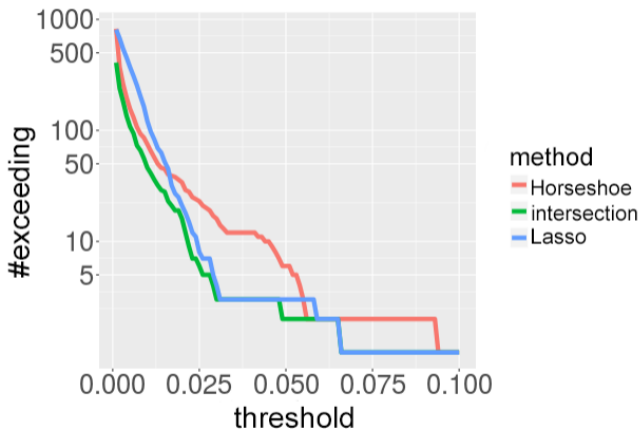
Real application: GWAS

- ▶ $n = 2267$ observations, $p = 98385$ SNPs in the genome of maize.
- ▶ X : maize seeds; y : growing degree days to silking ('growth cycle')



Bimodal posterior distribution for $\beta_j | y$; Lasso (red) shrinks more than Horseshoe (blue)

Variable selection with Horseshoe



Number of variables for which $\hat{\beta}_{\text{HS},j} = \mathbb{E}[\beta_j | y] > t$ or $\hat{\beta}_{\text{Lasso},j} > t$ vs threshold t ;
 both methods largely agree on the identities of the signals

Conclusion

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- ▶ We observed interesting and novel statistical phenomena, e.g., bimodality of β .
- ▶ There is likely more room for improvement.

References

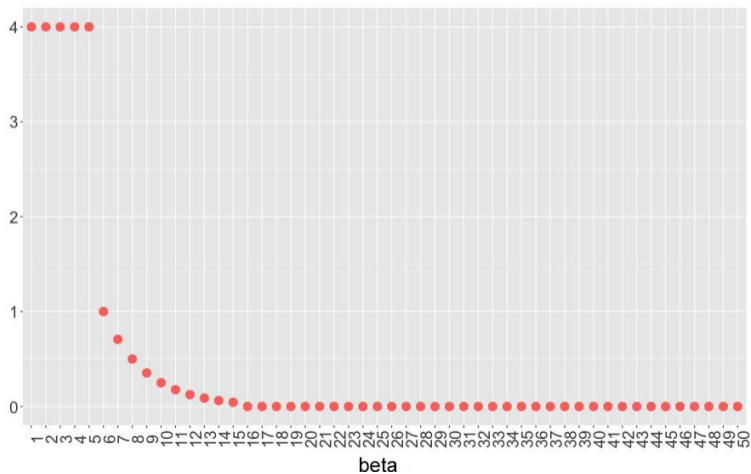
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Extra slides

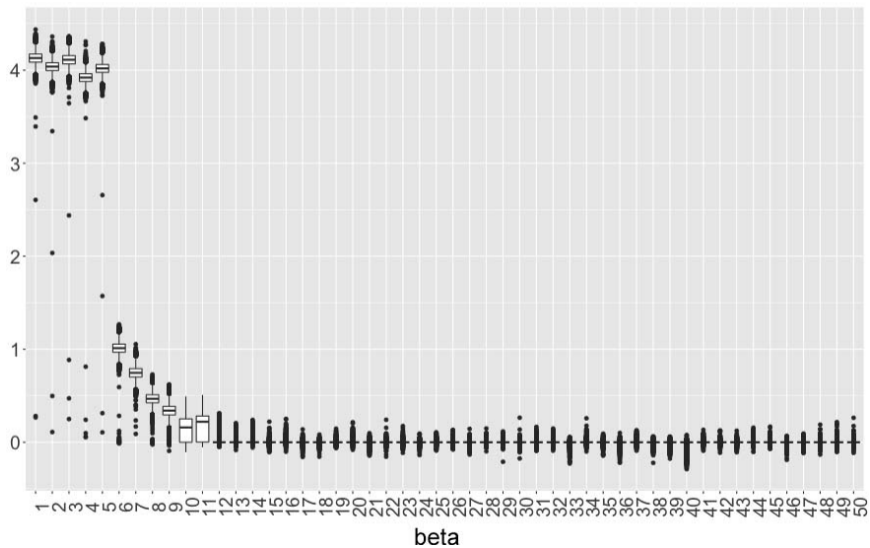
- ▶ More simulation results
- ▶ Why “Horseshoe”?

More simulations

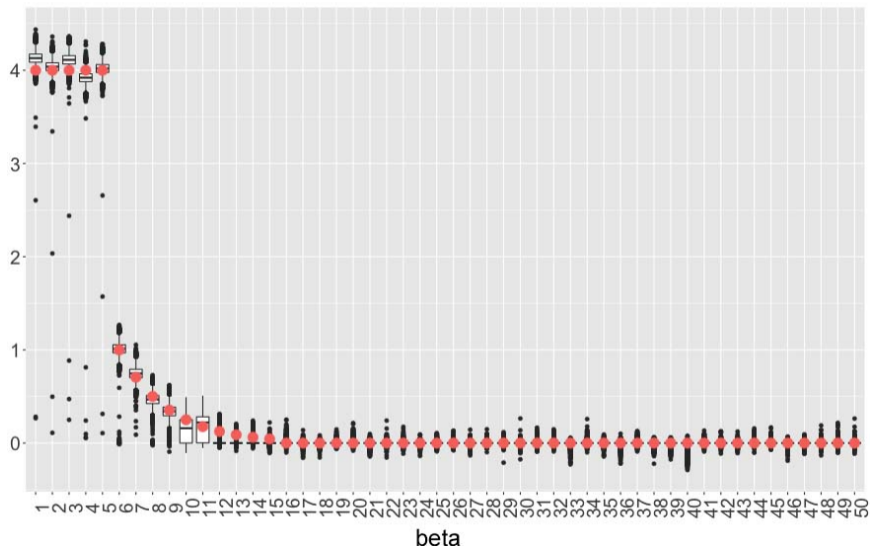
- ▶ We let $n = 1000$ and $p = 20,000$.



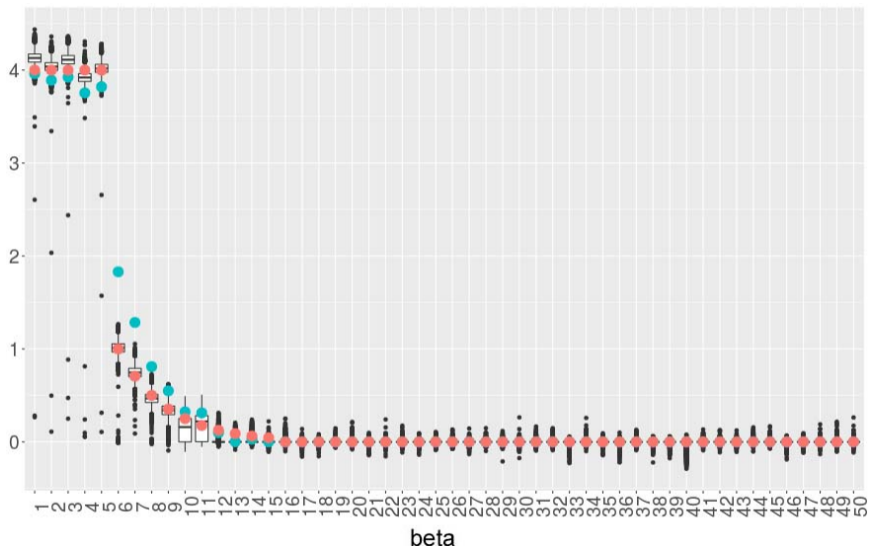
More simulations



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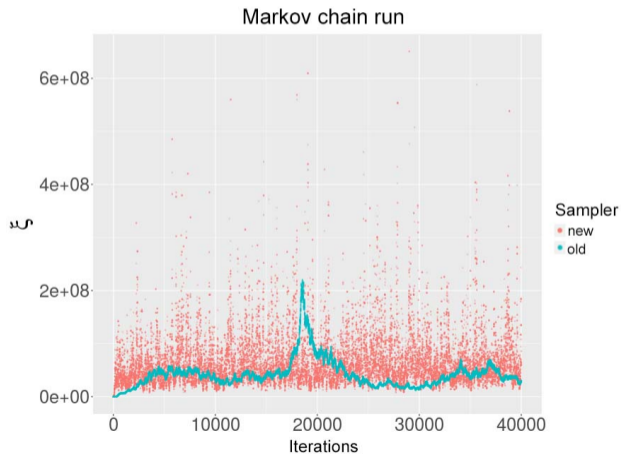


More simulations

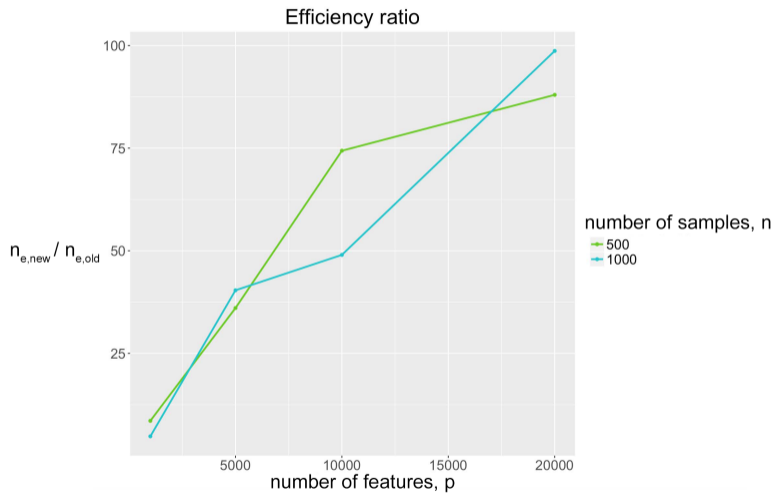


More simulations

- ▶ The new algorithm lead to significant improvement in the autocorrelation:



More simulations



Why "Horseshoe"?

- ▶ In the orthogonal case with $n \geq p$ and $\sigma^2 = \tau = 1$, and defining a shrinkage profile $\kappa_j = 1/(1 + n\lambda_j^2)$, we can write $\mathbb{E}[\beta_j|y] = (1 - \mathbb{E}[\kappa_j|y])\hat{\beta}_j$.

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- ▶ Prior density for κ_j :

