

ON THE HYPERPRIOR CHOICE FOR THE GLOBAL SHRINKAGE PARAMETER IN THE HORSESHOE PRIOR

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Introduction

- ▶ *Sparse estimation*: large number of parameters $\theta = (\theta_1, \dots, \theta_D)$, assume only a few are nonzero
 - ▶ Regression/classification with many candidate predictors
 - ▶ Example dataset: Leukemia classification $D = 7129$, $n = 72$
- ▶ Non-Bayesian approaches: LASSO, elastic net etc.
- ▶ Bayesian approach: sparsifying prior + integrate over uncertainty

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 - ▶ Continuous shrinkage prior
 - ▶ Computationally convenient alternative to the spike-and-slab, with similar or better performance

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- ▶ Horseshoe prior
 - ▶ Continuous shrinkage prior
 - ▶ Computationally convenient alternative to the spike-and-slab, with similar or better performance
- ▶ However:
 - ▶ Previously not clear how to encode prior assumptions about the sparsity to the model (trivial in spike-and-slab)
 - ⇒ This talk

Horseshoe prior

- ▶ Linear regression model with many inputs $\mathbf{x} = (x_1, \dots, x_D)$

$$y_i = \beta^T \mathbf{x}_i + \varepsilon_i, \quad \varepsilon_i \sim \mathbf{N}(0, \sigma^2), \quad i = 1, \dots, n,$$

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- ▶ The horseshoe prior:

$$\begin{aligned} \beta_j | \lambda_j, \tau &\sim \mathbf{N}(0, \lambda_j^2 \tau^2), \\ \lambda_j &\sim \mathbf{C}^+(0, 1), \quad j = 1, \dots, D. \end{aligned}$$

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- ▶ *The global parameter* τ shrinks all β_j towards zero
- ▶ *The local parameters* λ_j allow some β_j to escape the shrinkage

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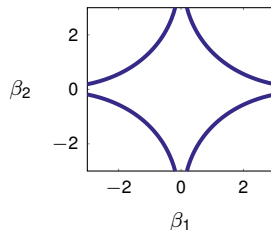
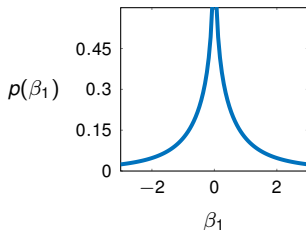
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- ▶ *The global parameter τ shrinks all β_j towards zero*
- ▶ *The local parameters λ_j allow some β_j to escape the shrinkage*



Horseshoe prior

- ▶ Given the hyperparameters, the posterior mean satisfies approximately

$$\bar{\beta}_j = (1 - \kappa_j)\beta_j^{\text{ML}}, \quad \kappa_j = \frac{1}{1 + n\sigma^{-2}\tau^2\lambda_j^2},$$

where κ_j is the *shrinkage factor*

Horseshoe prior

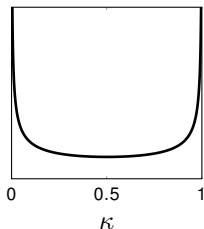
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 1.0$$



We expect both

- ▶ relevant ($\bar{\beta}_j \approx \beta_j^{\text{ML}}$) features
- ▶ irrelevant ($\bar{\beta}_j \approx 0$) features

Horseshoe prior

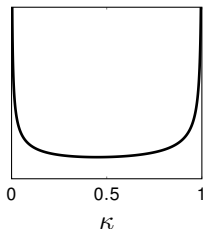
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.9$$



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Horseshoe prior

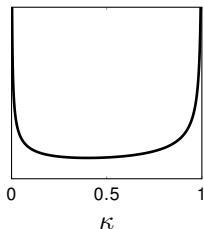
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.8$$



We expect both

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Horseshoe prior

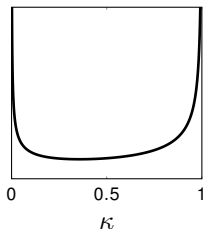
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.7$$



We expect both

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Horseshoe prior

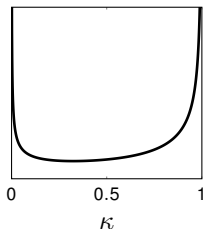
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.6$$



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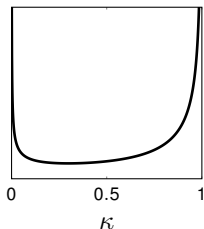
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.5$$



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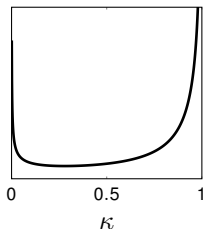
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- ▶ With $\lambda_j \sim C^+(0, 1)$, the prior for κ_j looks like:

$$n\sigma^{-2}\tau^2 = 0.4$$



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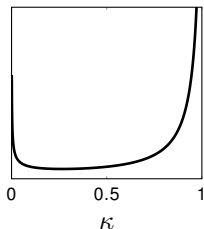
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$$n\sigma^{-2}\tau^2 = 0.3$$



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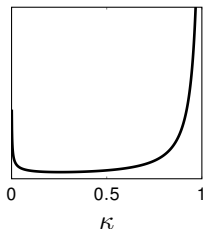
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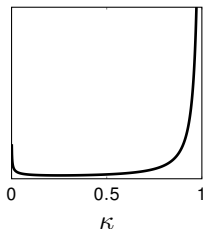
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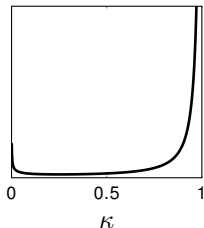
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Small $\tau \Rightarrow$ more coefficients ≈ 0

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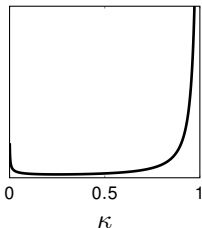
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How to specify prior for τ ?

The global shrinkage parameter τ

- ▶ *Effective number of nonzero coefficients*

$$m_{\text{eff}} = \sum_{j=1}^D (1 - \kappa_j)$$

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$$\mathbf{E}[m_{\text{eff}} \mid \tau, \sigma] = \frac{\tau \sigma^{-1} \sqrt{n}}{1 + \tau \sigma^{-1} \sqrt{n}} D$$

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$$\mathbf{E}[m_{\text{eff}} | \tau, \sigma] = \frac{\tau \sigma^{-1} \sqrt{n}}{1 + \tau \sigma^{-1} \sqrt{n}} D$$

- ▶ Setting $\mathbf{E}[m_{\text{eff}} | \tau, \sigma] = \rho_0$ (prior guess for the number of nonzero coefficients) yields for τ

$$\tau_0 = \frac{\rho_0}{D - \rho_0} \frac{\sigma}{\sqrt{n}}$$

⇒ Prior guess for τ based on our beliefs about the sparsity

Illustration $p(\tau)$ vs. $p(m_{\text{eff}})$

Let $n = 100$, $\sigma = 1$, $\rho_0 = 5$, $\tau_0 = \frac{\rho_0}{D - \rho_0} \frac{\sigma}{\sqrt{n}}$, $D = \text{dimensionality}$

Illustration $p(\tau)$ vs. $p(m_{\text{eff}})$

Let $n = 100$, $\sigma = 1$, $\rho_0 = 5$, $\tau_0 = \frac{\rho_0}{D - \rho_0} \frac{\sigma}{\sqrt{n}}$, $D = \text{dimensionality}$

$p(m_{\text{eff}})$ with different choices of $p(\tau)$:

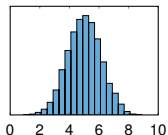
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$$\tau = \tau_0$$

$D = 10$



$D = 1000$

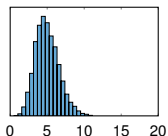


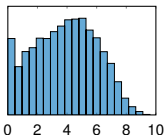
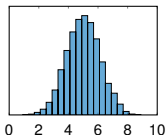
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$\tau = \tau_0$ $\tau \sim \mathbf{N}^+(0, \tau_0^2)$

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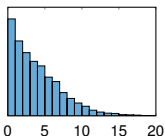
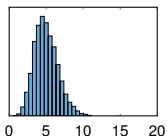


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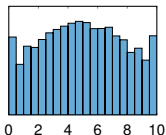
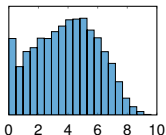
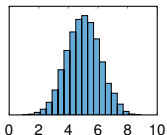
$p(m_{\text{eff}})$ with different choices of $p(\tau)$:

$$\tau = \tau_0$$

$$\tau \sim \mathbf{N}^+(0, \tau_0^2)$$

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$D = 10$



$D = 1000$

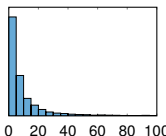
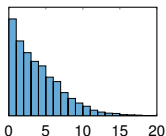
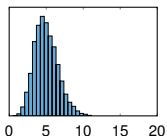
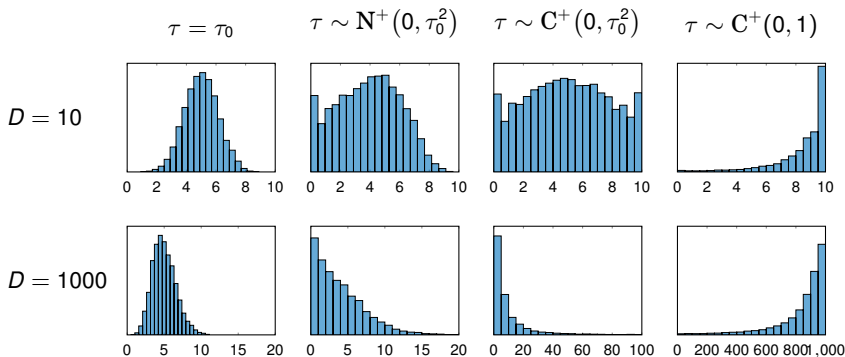


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$p(m_{\text{eff}})$ with different choices of $p(\tau)$:



Non-Gaussian observation models

- ▶ The reference value (reminder):

$$\tau_0 = \frac{\rho_0}{D - \rho_0} \frac{\sigma}{\sqrt{n}}$$

- ▶ The framework can be applied also to non-Gaussian observation models by deriving appropriate plug-in values for σ
 - ▶ Gaussian approximation to the likelihood
 - ▶ E.g. $\sigma = 2$ for logistic regression

Experiments

Table: Summary of the real world datasets, D denotes the number of predictors and n the dataset size.

Dataset	Type	D	n
Ovarian	Classification	1536	54
Colon	Classification	2000	62
Prostate	Classification	5966	102
ALLAML	Classification	7129	72
Corn (4 targets)	Regression	700	80

- ▶ Models implemented and posterior inference using Stan¹.

¹<http://mc-stan.org/>

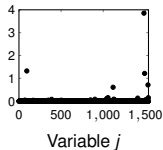
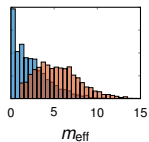
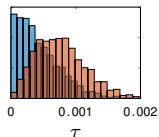
Effect of $p(\tau)$ on parameter estimates

Ovarian cancer data
($n = 54$, $D = 1536$).

Choose τ_0 according to a
prior guess $p_0 = 3$.

Effect of $\rho(\tau)$ on parameter estimates

$$\tau \sim N^+(0, \tau_0^2)$$



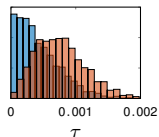
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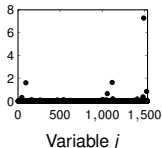
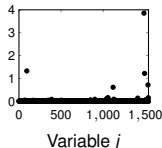
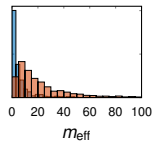
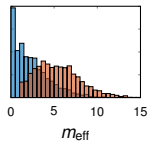
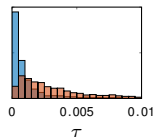
Prior and posterior sam-
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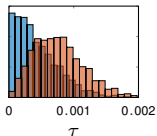
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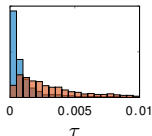
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coefficients $|\bar{\beta}_j|$.

Effect of $\rho(\tau)$ on parameter estimates

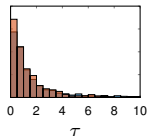
$$\tau \sim N^+(0, \tau_0^2)$$



$$\tau \sim C^+(0, \tau_0^2)$$

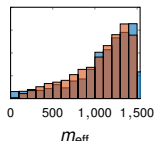
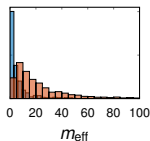
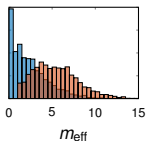


$$\tau \sim C^+(0, 1)$$

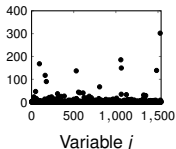
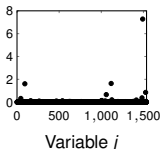
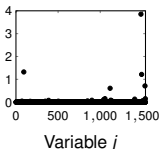


Ovarian cancer data
($n = 54, D = 1536$).

Choose τ_0 according to a
prior guess $\rho_0 = 3$.



Prior and posterior sam-
ples for τ and m_{eff} , and
absolute posterior mean
coefficients $|\bar{\beta}_j|$.

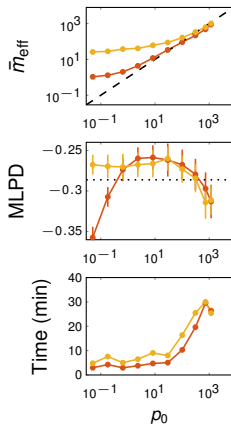


Effect of $p(\tau)$ on prediction accuracy (1/2)

$\tau \sim \mathbf{N}^+(0, \tau_0^2)$ (red) and $\tau \sim \mathbf{C}^+(0, \tau_0^2)$ (yellow),
for various p_0 transformed into τ_0 (largest p_0 corresponds to $\tau_0 = 1$).

Effect of $\rho(\tau)$ on prediction accuracy (1/2)

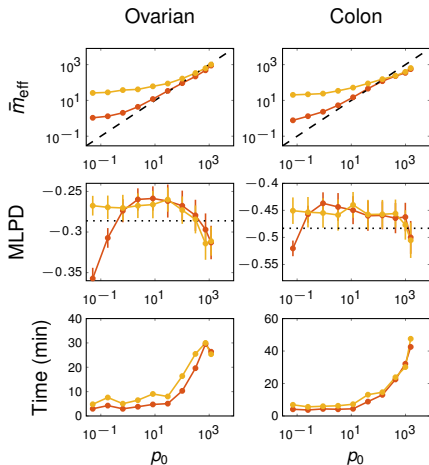
Ovarian



$\tau \sim \mathbf{N}^+(0, \tau_0^2)$ (red) and $\tau \sim \mathbf{C}^+(0, \tau_0^2)$ (yellow),
for various ρ_0 transformed into τ_0 (largest ρ_0 corresponds to $\tau_0 = 1$).

Posterior mean \bar{m}_{eff} , mean log predictive density (MLPD) on test data (dashed line denotes LASSO), and computation time.

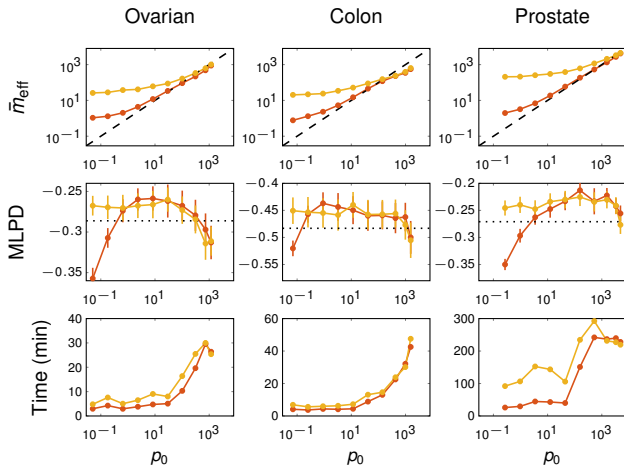
Effect of $\rho(\tau)$ on prediction accuracy (1/2)



$\tau \sim \mathbf{N}^+(0, \tau_0^2)$ (red) and $\tau \sim \mathbf{C}^+(0, \tau_0^2)$ (yellow),
for various ρ_0 transformed into τ_0 (largest ρ_0 corresponds to $\tau_0 = 1$).

Posterior mean \bar{m}_{eff} , mean log predictive density (MLPD) on test data (dashed line denotes LASSO), and computation time.

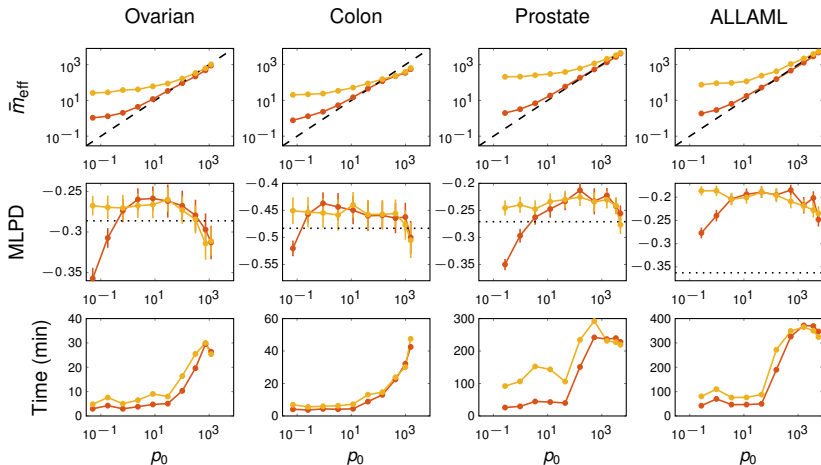
Effect of $\rho(\tau)$ on prediction accuracy (1/2)



$\tau \sim N^+(0, \tau_0^2)$ (red) and $\tau \sim C^+(0, \tau_0^2)$ (yellow),
for various ρ_0 transformed into τ_0 (largest ρ_0 corresponds to $\tau_0 = 1$).

Posterior mean \bar{m}_{eff} , mean log predictive density (MLPD) on test data (dashed line denotes LASSO), and computation time.

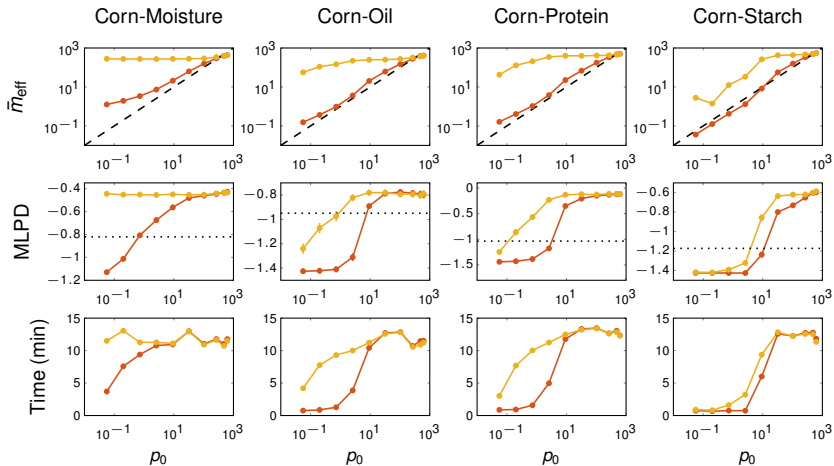
Effect of $\rho(\tau)$ on prediction accuracy (1/2)



$\tau \sim \mathbf{N}^+(0, \tau_0^2)$ (red) and $\tau \sim \mathbf{C}^+(0, \tau_0^2)$ (yellow),
for various ρ_0 transformed into τ_0 (largest ρ_0 corresponds to $\tau_0 = 1$).

Posterior mean \bar{m}_{eff} , mean log predictive density (MLPD) on test data (dashed line denotes LASSO), and computation time.

Effect of $\rho(\tau)$ on prediction accuracy (2/2)



$\tau \sim \mathbf{N}^+(0, \tau_0^2)$ (red) and $\tau \sim \mathbf{C}^+(0, \tau_0^2)$ (yellow),
for various ρ_0 transformed into τ_0 (largest ρ_0 corresponds to $\tau_0 = 1$).

Posterior mean \bar{m}_{eff} , mean log predictive density (MLPD) on test data (dashed line denotes LASSO), and computation time.

Summary

- ▶ The global shrinkage parameter τ effectively determines the level of sparsity
- ▶ The prior for $p(\tau)$ can have a significant effect on the inference results
 - ▶ “Uninformative” $\tau \sim C^+(0, 1)$ often poor choice
- ▶ Our framework allows the user to calibrate the prior for τ based on the prior beliefs about the sparsity
- ▶ The concept of effective number of nonzero regression coefficients m_{eff} could be applied also to other shrinkage priors

Implementation

- ▶ Horseshoe prior is implemented at least in R-packages *rstanarm* and *brms*
 - ▶ Both allow prior specification for the global parameter τ
- ▶ Demo about the model fitting and the subsequent projective variable selection using our R-package *projpred*:

<https://users.aalto.fi/~jtpiiron/projpred/quickstart.html>