

Generalised Decomposition Priors on R2

DAGStat 2025

Javier Aguilar, Paul-Christian Bürkner

25.03.2025

TU Dortmund

javier.aguilar@tu-dortmund.de

Prior specification

The prior is a fundamental part of Bayesian modeling.

Hard question: How to specify the prior?

Prior specification

The prior is a fundamental part of Bayesian modeling.

Hard question: How to specify the prior?

Fundamental question: How to make it easier for the user to specify priors?

Prior specification

The prior is a fundamental part of Bayesian modeling.

Hard question: How to specify the prior?

Fundamental question: How to make it easier for the user to specify priors?

- Build upon **intuition** about the phenomenon.
- Propose **semi automated** and **parsimonious** priors.
- Propose priors on **predictive quantities** that are better understood by the user and move uncertainty.

Priors in Linear Regression

How to select the prior for b ?

1. Scaled Gaussians

$$b \mid \sigma, \Sigma_b \sim N(0, \sigma^2 \Sigma_b), \quad \sigma \sim p(\sigma), \quad \Sigma_b \sim p(\Sigma_b)$$

Priors in Linear Regression

How to select the prior for b ?

1. Scaled Gaussians

$$b \mid \sigma, \Sigma_b \sim N(0, \sigma^2 \Sigma_b), \quad \sigma \sim p(\sigma), \quad \Sigma_b \sim p(\Sigma_b)$$

2. Shrinkage priors

$$b_i \mid \Psi_i \sim N(0, \Psi_i), \quad \Psi_i \sim G(\cdot)$$

$$p(b_i) = \int N(b_i \mid 0, \Psi_i) dG(\Psi_i)$$

- Usual decomposition $\Psi_i = \phi_i \tau^2$
- Includes Spike and Slab, Horseshoe, Dirichlet Laplace, Beta Prime etc.

Prior specification

Question: What is the effect on R^2 ?

$$b_k \sim \mathcal{N}(0,1), \quad \sigma \sim \text{Exp}(1)$$

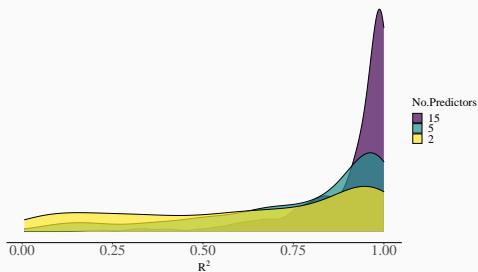


Figure 1: Implied prior distribution on R^2

Basic Idea:

- Set a prior on R^2 to encode domain knowledge.
- Decompose total variance τ^2 among b_k
- Span and jointly regularize all coefficients!

$$R^2 = \frac{\text{var}(x'b)}{\text{var}(x'b) + \sigma^2}$$



The GDR2 prior: Construction

- Assumptions:

- Centered coefficients

$$\mathbb{E}(b_i) = \mathbb{E}(u_{igj}) = 0,$$

- Scaled variances

$$\text{var}(b_i) = \sigma^2 \lambda_i^2$$

The GDR2 prior: Construction

- Assumptions:
 - Centered coefficients
 $\mathbb{E}(b_i) = \mathbb{E}(u_{igj}) = 0,$
 - Scaled variances
 $\text{var}(b_i) = \sigma^2 \lambda_i^2$
- Variance decomposition of the linear predictor $x'b$

$$\text{var}(x'b) = \sum_{i=1}^K \sigma^2 \lambda_i^2$$

The GDR2 prior: Construction

- Assumptions:

- Centered coefficients

$$\mathbb{E}(b_i) = \mathbb{E}(u_{igj}) = 0,$$

- Scaled variances

$$\text{var}(b_i) = \sigma^2 \lambda_i^2$$

- Variance decomposition of the linear predictor $x'b$

$$\text{var}(x'b) = \sum_{i=1}^K \sigma^2 \lambda_i^2$$

- Total explained variance τ^2

$$\tau^2 := \sum_{i=1}^K \lambda_i^2$$

The GDR2 prior: Construction

- Assumptions:

- Centered coefficients

$$\mathbb{E}(b_i) = \mathbb{E}(u_{igj}) = 0,$$

- Scaled variances

$$\text{var}(b_i) = \sigma^2 \lambda_i^2$$

- Variance decomposition of the linear predictor $x'b$

$$\text{var}(x'b) = \sum_{i=1}^K \sigma^2 \lambda_i^2$$

- Total explained variance τ^2

$$\tau^2 := \sum_{i=1}^K \lambda_i^2$$

- Rewrite R^2

$$R^2 = \frac{\sigma^2 \tau^2}{\sigma^2 \tau^2 + \sigma^2} = \frac{\tau^2}{\tau^2 + 1}.$$

The GDR2 prior: R2 prior

1) Set

$$R^2 \sim \text{Beta}(\mu_{R^2}, \varphi_{R^2}) \iff \tau^2 \sim \text{BP}(\mu_{R^2}, \varphi_{R^2})$$

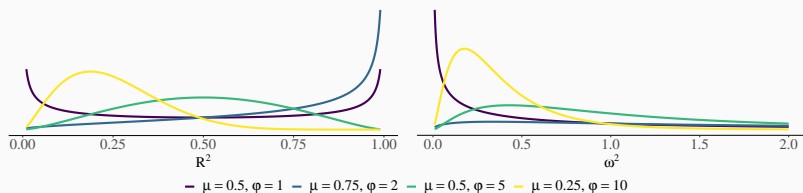
- $\mu_{R^2} \in (0, 1)$ **prior mean**
- $\varphi_{R^2} > 0$ **prior precision**

The GDR2 prior: R² prior

1) Set

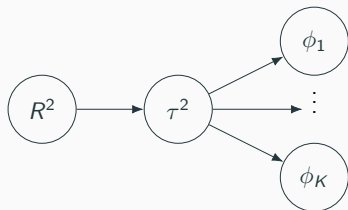
$$R^2 \sim \text{Beta}(\mu_{R^2}, \varphi_{R^2}) \iff \tau^2 \sim \text{BP}(\mu_{R^2}, \varphi_{R^2})$$

- $\mu_{R^2} \in (0, 1)$ **prior mean**
- $\varphi_{R^2} > 0$ **prior precision**



The GDR2 prior: Variance Partitioning

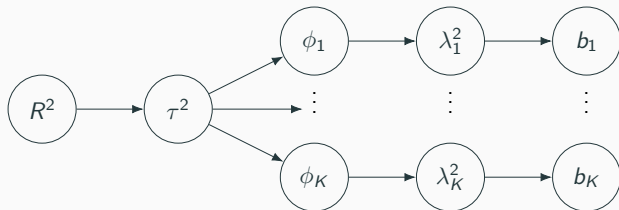
Let ϕ follow a distribution on the simplex \mathcal{S}^{K-1}



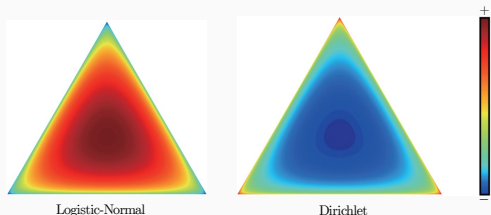
- How should we specify the distribution of ϕ ?
- Which behavior do we want to exhibit in ϕ ?

The GDR2 prior: Coefficients

Set $\lambda_i = \phi_i \tau^2$ and $b \mid \sigma, \lambda \sim N(0, \sigma \lambda_i^2)$



Distributions in the Simplex



Dirichlet $\phi \sim \text{Dir}(\alpha)$

- Tractable analytical properties
- α is easy to understand, but the mean determines covariance.

Logistic Normal

$\eta \sim \mathcal{N}(\mu, \Sigma)$, $\phi = \text{softmax}(\eta)$

- Higher flexibility
- Challenging to select μ, Σ

Hyperparameter specification

Prior for R^2

- User informed
- Since $\text{var}(b) = \mathbb{E}(\tau^2)\text{cov}(\phi)$, set values to imply a heavy tail for b .
Set $(1 - \mu_{R^2})\varphi_{R^2} \leq 1/2$

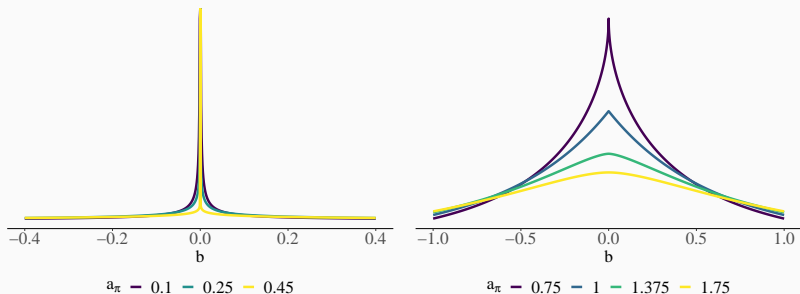
Hyperparameter specification

Prior for R^2

- User informed
- Since $\text{var}(b) = \mathbb{E}(\tau^2)\text{cov}(\phi)$, set values to imply a heavy tail for b .
Set $(1 - \mu_{R^2})\varphi_{R^2} \leq 1/2$

Priors for ϕ : Dirichlet distribution

- Set $\alpha = (a_\pi, \dots, a_\pi)$, $a_\pi > 0$
- If $a_\pi \leq 1/2$ then we get unbounded marginals for b around the origin

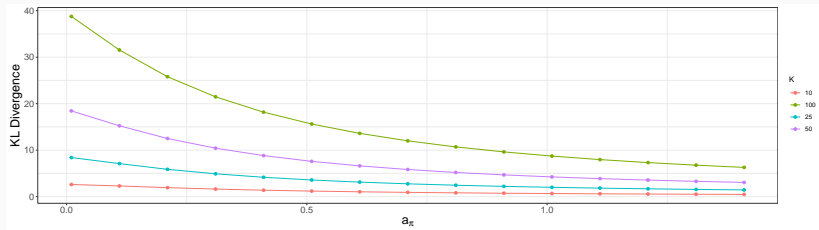


Hyperparameter specification: LN and KL Matching

Priors for ϕ : Logistic Normal distribution

Idea: Minimize KL between $\text{Dir}(\alpha)$ and $\text{LN}(\mu, \Sigma)$.

- Closed form expression.
- Automated and cheap
- Exact matching is neither wished nor achievable as KL doesn't vanish.



Priors for ϕ : Logistic Normal distribution

How to specify μ ?

- $\mu = 0$ means all proportions are equally weighted and $\mathbb{E}[\phi_k] = 1/K$.
- If $\mu_k = c_k, \Sigma = \sigma_\phi^2 I$ then

$$\mathbb{E}[\phi_k] = \mathbb{E} \left(\frac{e^{\eta_k}}{\sum_j e^{\eta_j}} \right) \approx \frac{e^{c_k}}{\sum_j e^{c_j}}$$

- One can also form groups within μ
- Other cases are more involved

Hyperparameter specification: LN and KL Matching

Priors for ϕ : Logistic Normal distribution

Idea: How to specify Σ ? Study the implied prior on the size of the logits η (log ratios)

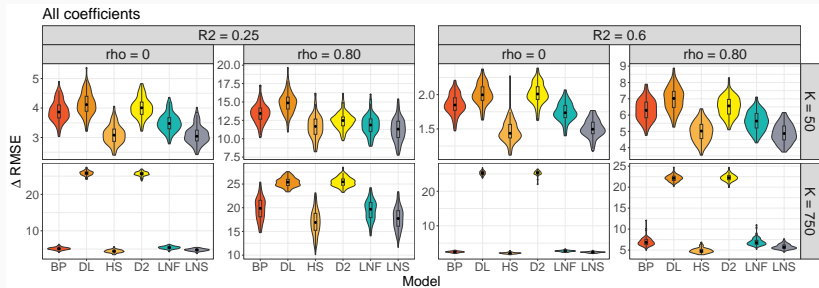
- If $\mu = 0, \Sigma = \sigma_\phi^2 I$ and $\eta \sim N(0, \sigma_\phi^2 I)$ then $\|\eta\|$ concentrates around $\sqrt{K}\sigma_\phi$ since

$$\mathbb{P}\left(\left|\frac{\|\eta\|}{\sqrt{K}\sigma_\phi} - 1\right| \geq t\right) \leq 2 \exp\left(-\frac{K\sigma_\phi^2 t^2}{2C}\right), \quad C > 0$$

- There σ_ϕ specifies a budget.
- $\sigma_\phi \rightarrow 0$, the logits concentrate near zero, resulting in $\phi_k \rightarrow 1/K$
- σ_ϕ increases, the logits spread
- Example: If $\sigma_\phi = \sqrt{\gamma/K}, \gamma > 0$ then $\|\eta\|^2 \approx \gamma$ regardless of K
- Other cases are more involved

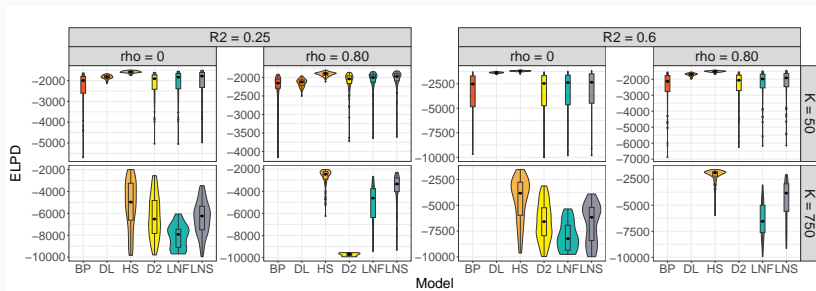
Simulation: Comparison with other priors

Parameter recovery



Simulation: Comparison with other priors

Out of sample predictive performance measured via ELPD



Future directions

1. How can the data inform us about the mean and covariance of ϕ ?
2. Theoretical properties of the prior
3. Even with KL matching we are getting promising results, hence proper hyperparameter selection should improve performance.

Takeaway Message

Key Takeaway:

- Opens the way to think about different relationships among variance components.
- Joint priors based on quantities of interest is a promising avenue for research.

Thank You for Your Attention!

Feel free to reach out for questions or collaborations.

Contact Information:

- ✉ javier.aguilar@tu-dortmund.de
- <https://jear2412.github.io>
- 🐙 [jear2412](#)



References

- [1] Javier Enrique Aguilar and Paul-Christian Bürkner. Intuitive joint priors for Bayesian linear multilevel models: The R2D2M2 prior. *Electronic Journal of Statistics*, 17(1):1711 – 1767, 2023. doi: 10.1214/23-EJS2136. URL <https://doi.org/10.1214/23-EJS2136>.
- [2] Javier Enrique Aguilar and Paul-Christian Bürkner. Generalized decomposition priors on r^2 , 2025. URL <https://arxiv.org/abs/2401.10180>.