

Probabilistic Machine Learning

Bayesian (Generalised) Linear Models

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Abstract

This should be an abstract

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1 Introduction

1. Motivation (warum reden wir über bayesianische (G)LMs, warum ist das wichtig?)
2. Schwäche bisheriger Methoden, was fehlt bei nicht-bayesianischen GLMs (zitieren)
3. Wie lösen wir das hier?
 - Limits of frequentist methods (as a motivation for Bayesian GLMs - Motivation of bayesian GLMs: - uncertainty quantification, - regularization, (especially where data information is limited (Fahrmeir 2021)) - incorporation of domain knowledge, - small data sets - Current research and related work - Structure of the paper

2 Linear Bayesian Model

The (frequentist) Linear Regression Model is probably the most widely used model in statistics and machine learning. Both the frequentist and the Bayesian Linear Models are described in many introductory texts on statistical modelling, such as Fahrmeir et al. (2021) or Gelman, Carlin, Stern, Dunson, Vehtari and Rubin (2013).

2.1 Model definition

We observe an i.i.d. sample $\mathbf{D} = ((y_1, \mathbf{x}_1), \dots, (y_n, \mathbf{x}_n)) = (\mathbf{y}, \mathbf{X})$ and assume a linear relationship between \mathbf{X} and \mathbf{y} . The frequentist linear regression model then assumes

$$\mathbf{y} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I}), \quad (1)$$

where the weight parameter $\boldsymbol{\theta}$ and the variance σ^2 are estimated to obtain the fitted model. A condition on \mathbf{X} is always implicit.

To view Linear Regression from a Bayesian perspective, we simply reinterpret the parameters as random variables. Conditioning on $\boldsymbol{\theta}$ and σ^2 , the likelihood takes the same form as in Equation 1:

$$\mathbf{y} \mid \boldsymbol{\theta}, \sigma^2 \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I}), \quad (2)$$

Note that to predict multiple outputs, an extension to Multivariate Linear Regression is possible.

2.2 Prior choice

Normal (Inverse Gamma) Prior

To complete the Bayesian linear model specification, we place conjugate priors on both $\boldsymbol{\theta}$ and σ^2 .

$$\begin{aligned} \boldsymbol{\theta} \mid \sigma^2 &\sim \mathcal{N}(\check{\boldsymbol{\mu}}, \sigma^2 \check{\boldsymbol{\Sigma}}) \\ \sigma^2 &\sim \text{IG}(\check{a}, \check{b}), \end{aligned} \quad (3)$$

where $\check{\boldsymbol{\mu}}, \check{\boldsymbol{\Sigma}}, \check{a}$ and \check{b} are the prior parameters. We choose a Gaussian prior on $\boldsymbol{\theta}$ because it is conjugate to the Gaussian likelihood of \mathbf{y} . Since the Inverse-Gamma distribution of σ^2 is conjugate to the Gaussian conditional distribution of $\boldsymbol{\theta}$, the joint prior of $\boldsymbol{\theta}$ and σ^2

$$p(\boldsymbol{\theta}, \sigma^2) \stackrel{\text{Bayes' rule}}{=} p(\boldsymbol{\theta} \mid \sigma^2) p(\sigma^2)$$

follows a Normal Inverse Gamma (NIG) distribution. We can then use Bayes' rule once again to derive the unconditional prior distribution of $\boldsymbol{\theta}$ as a multivariate Student t-distribution.

$$\boldsymbol{\theta} \sim \mathcal{T}(2\check{a}, \check{\boldsymbol{\mu}}, \frac{\check{a}}{\check{b}} \check{\boldsymbol{\Sigma}})$$

Uninformative Prior

The idea of an uninformative (or flat) prior is to maximize the influence of the data on the posterior in the absence of prior knowledge. Especially when little to no prior information is available, we can flatten the NIG prior by setting

$$\check{\boldsymbol{\mu}} = \mathbf{0}, \quad \check{\Sigma}^{-1} = \mathbf{0} \text{ i.e. } \check{\Sigma} \rightarrow \infty$$

and choosing $\check{a} = -\frac{p}{2}$ and $\check{b} = 0$, where p is the number of features in the model.

We can easily see that with this assumption, the prior for $\boldsymbol{\theta}$ becomes very flat while still retaining the useful qualities from the setup described in Equation 3.

The prior distributional assumptions would then be:

$$\begin{aligned} \boldsymbol{\theta} \mid \sigma^2 &\stackrel{a}{\sim} \mathcal{N}(\check{\boldsymbol{\mu}}, \sigma^2 \infty)^1, & p(\boldsymbol{\theta} \mid \sigma^2) &\propto 1 \\ \sigma^2 &\sim \text{IG}(-\frac{p}{2}, 0), & p(\sigma^2) &\propto \frac{1}{\sigma^2} \end{aligned} \quad (4)$$

Note that we generally have to be careful with completely flat priors; it is necessary to check if the resulting posterior is proper (which is the case here).

Another good solution for use-cases with little prior knowledge that still require a proper posterior is Zellner's g-prior (Zellner, 1986).

Regularization Priors

Regularization (or penalization) regulates the trade off between model complexity and out-of-sample performance, or equivalently bias vs. variance. In frequentist statistics, we minimize the Penalized Least Squares criterion (PLS)

$$\text{PLS}(\boldsymbol{\theta}) = (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta}) + \lambda \text{pen}(\boldsymbol{\theta}).$$

where $\lambda > 0$ controls the balance of the tradeoff and therefore the strength of regularization.

In the Bayesian view, we introduce a regularization prior on $\boldsymbol{\theta}$. Concretely:

$$\begin{aligned} \mathbf{y} \mid \boldsymbol{\theta}, \sigma^2 &\sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I}),^2 \\ \boldsymbol{\theta} &\sim \text{regularization prior} \\ \sigma^2 &\sim \text{IG}(\check{a}, \check{b}), \end{aligned}$$

although there are many options for regularization priors, we are going to focus on regularization priors that align directly with familiar frequentist penalties.

¹Informally stated for demonstrational purposes.

²Usually, it does not make sense to regularize the intercept. To be completely accurate, we would need to separate the intercept from $\boldsymbol{\theta}$, i.e. split $\boldsymbol{\theta}$ into $(\theta_0, \boldsymbol{\theta}'^\top)$ and consequently set \mathbf{X}' as the design matrix without a column for the intercept. We would then specify the model as $\mathbf{y} \mid \boldsymbol{\theta}, \sigma^2 \sim \mathcal{N}(\theta_0 \mathbf{I} + \mathbf{X}'\boldsymbol{\theta}', \sigma^2 \mathbf{I})$. We chose to simplify this and stick to the previously established definitions because we aim for an understandable explanation of the basic concept of Bayesian regularization.

Ridge regularization (Hoerl and Kennard, 1970a,b) uses $\text{pen}(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_2^2$ and the Bayesian analogue (e.g. Hsiang, 1975, MacKay, 1992) specifies

$$\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}), \quad (5)$$

with τ^2 controlling the degree of regularization akin to the role of λ . In contrast to λ , τ^2 does not need to be set in advance or optimized as a hyperparameter. We can simply embed it in a hierarchical model by specifying a prior for τ^2 , e.g. $\tau^2 \sim \text{IG}(\check{a}_\tau, \check{b}_\tau)$, and estimate it alongside $\boldsymbol{\theta}$ and σ^2 .

Lasso regularization (Tibshirani, 1996) uses $\text{pen}(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_1$ to perform variable selection by setting elements θ_j of $\boldsymbol{\theta}$ to 0 during estimation. This means that Lasso regularization promotes a *sparse* solution. The Bayesian Lasso specifies a Laplace prior on $\boldsymbol{\theta}$ via the scale-mixture representation (Park and Casella, 2008)

$$\begin{aligned} \boldsymbol{\theta} \mid \tau^2 &\sim \mathcal{N}(\mathbf{0}, \tau^2 \mathbf{I}) \\ \tau_j^2 &\stackrel{\text{i.i.d.}}{\sim} \text{Exp}(0.5\lambda^2), \quad j = 1, \dots, p, \end{aligned} \quad (6)$$

where the regularization parameter λ^2 is often given a (hyper-) prior, e.g. $\lambda^2 \sim \text{G}(\check{a}_\lambda, \check{b}_\lambda)$.

Because Bayesian Lasso does not promote a sparse solution, discrete-mixture Spike-and-Slab priors (Mitchell and Beauchamp, 1988) (which are necessary for categorical covariates) or the heavy-tailed horseshoe prior (Carvalho et al., 2010) are preferred for variable selection.

2.3 Bayesian inference with closed form priors

Parameter posterior distribution

In a frequentist linear model, we use least-squares (LS) estimation to obtain the estimate

$$\hat{\boldsymbol{\theta}}_{LS} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \quad (7)$$

for $\boldsymbol{\theta}$. Under Gaussian errors, this satisfies

$$\hat{\boldsymbol{\theta}}_{LS} \sim \mathcal{N}(\boldsymbol{\theta}, \sigma^2 (\mathbf{X}^\top \mathbf{X})^{-1}).$$

To quantify the uncertainty in the estimation, we can compute confidence intervals for $\boldsymbol{\theta}$, but these reflect only the variability in the estimator, not uncertainty about the true parameter itself.

In contrast, the Bayesian approach yields a full posterior distribution on $\boldsymbol{\theta}$ by updating the prior distribution with observed data using Bayes' rule. With the NIG prior introduced in Equation 3, conjugacy implies for the joint posterior $p(\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y})$ that

$$\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y} \sim \text{NIG}(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\Sigma}}, \hat{a}, \hat{b})$$

with posterior mean and variance ³

$$\hat{\boldsymbol{\mu}} = \hat{\Sigma}(\check{\Sigma}^{-1}\check{\boldsymbol{\mu}} + \mathbf{X}^\top \mathbf{y}), \quad \hat{\Sigma} = (\mathbf{X}^\top \mathbf{X} + \check{\Sigma}^{-1})^{-1}. \quad (8)$$

Integrating out σ^2 yields $\boldsymbol{\theta} \mid \mathbf{y} \sim \mathcal{T}(2\hat{a}, \hat{\boldsymbol{\mu}}, \hat{b}/\hat{a}\hat{\Sigma})$ and Bayesian credibility intervals can be derived directly from this distribution (see e.g. Held and Sabanés Bové, 2020).

Since we defined the non-information prior Equation 4 as a special case of the NIG-distributed prior, we can use Equation 8 to directly calculate the posterior mean and variance as

$$\hat{\boldsymbol{\mu}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}, \quad \hat{\Sigma} = \mathbf{X}^\top \mathbf{X}.$$

The posterior mean $\hat{\boldsymbol{\mu}}$ coincides with $\hat{\boldsymbol{\beta}}_{LS}$ (Equation 7), so a Bayesian linear model with a non-informative prior converges to the frequentist solution. More generally, as the prior variance $\check{\Sigma}$ grows, $\hat{\boldsymbol{\mu}}$ approaches $\hat{\boldsymbol{\beta}}_{LS}$, since the likelihood (and thus the data) dominates the posterior.

Bayesian Ridge regression is simply the NIG case in Equation 3 with finite $\check{\Sigma}$, resulting in the same posterior update in Equation 8. By contrast, the Bayesian Lasso's Laplace prior has no closed-form posterior, but we can easily sample from it using Gibbs sampling (Park and Casella, 2008). We will go more into depth on approximate inference for Bayesian regression models in subsection 3.3.

Posterior predictive distribution

In many applications, we care more about predictions $\tilde{\mathbf{y}}$ for new, unseen inputs $\tilde{\mathbf{X}}$ (or test data $(\tilde{\mathbf{y}}, \tilde{\mathbf{X}})$), independent of the training data \mathbf{D} , than about $\boldsymbol{\theta}$ itself. The Bayesian answer to this is the *posterior predictive distribution* (PPD) (Box, 1980, Barbieri, 2015, see e.g.)

$$p(\tilde{\mathbf{y}} \mid \mathbf{y}) = \int p(\tilde{\mathbf{y}}, \boldsymbol{\theta} \mid \mathbf{y}) d\boldsymbol{\theta} = \int p(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \mathbf{y}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} \stackrel{\tilde{\mathbf{y}} \perp \mathbf{y} \mid \boldsymbol{\theta}}{=} \int p(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta},$$

which is an average of conditional probabilities over the posterior distribution of $\boldsymbol{\theta}$.⁴ For the NIG prior in Equation 3, one can show⁵ that

$$\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \sigma^2, \mathbf{y} \sim \mathcal{T}(2\hat{a}, \tilde{\mathbf{X}}\boldsymbol{\theta}, \frac{\hat{b}}{\hat{a}}(\mathbf{I} + \tilde{\mathbf{X}}\hat{\Sigma}\tilde{\mathbf{X}}^\top)).$$

Interestingly, the posterior predictive mean $\hat{\boldsymbol{\mu}} = \tilde{\mathbf{X}}\boldsymbol{\theta}$ of the t-distribution coincides with the least squares prediction and its scale matrix reflects both observational noise and posterior uncertainty. Bayesian inference with the Gaussian conjugate is more thoroughly described by Murphy (n.d.).

If no closed form exists, the PPD can also be simulated (see subsection 3.3)

³For the full calculation see Appendix A

⁴A note on intuition: In essence, the PPD is the marginal distribution of $\tilde{\mathbf{y}}$, conditioned on the data \mathbf{y} . We recognize the marginal distribution of \mathbf{y} from Bayes' rule as the normalization constant, i.e. $p(\mathbf{y}) = \int p(\mathbf{y}, \boldsymbol{\theta}) d\boldsymbol{\theta} = \int p(\mathbf{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$.

⁵see Appendix A

3 Logistic Bayesian Model

3.1 Bayesian Generalized Linear Regression Model

Bayesian generalized linear models extend the familiar Bayesian linear regression framework by replacing the Gaussian distributional assumption on \mathbf{y} with an arbitrary exponential-family distribution (Nelder and Wedderburn, 1972, West et al., 1985). In their most general form, we assume

$$\mathbf{y} \mid \boldsymbol{\theta} \sim F(g^{-1}(\mathbf{X}\boldsymbol{\theta})),$$

where F is any exponential-family distribution (e.g. Binomial, Poisson, Gamma) and g^{-1} is the inverse link function. Priors for the parameter $\boldsymbol{\theta}$ can be set in the same way as for the Bayesian linear model. However, in practice, the prior choice also depends on the link function (West et al., 1985).

3.2 Bayesian Logistic Regression Model

We are going to illustrate Bayesian GLMs with the example of Logistic regression models, which have a wide variety of applications in statistics, from text classification to medicine and genetic modelling. (SOURCE)

Model definition

The Bayesian logistic regression model is defined as

$$\begin{aligned} \mathbf{y}_i \mid \boldsymbol{\theta} &\sim \text{Bin}(1, g^{-1}(\mathbf{x}_i\boldsymbol{\theta})), \quad i = 1, \dots, n \\ g^{-1}(\mathbf{x}_i\boldsymbol{\theta}) &= \sigma(\mathbf{x}_i\boldsymbol{\theta}). \end{aligned} \tag{9}$$

where $\sigma(\mathbf{x}_i\boldsymbol{\theta}) = \frac{\exp(\mathbf{x}_i\boldsymbol{\theta})}{1+\exp(\mathbf{x}_i\boldsymbol{\theta})}$ is the logistic (sigmoid) function. Other choices like the probit link can also be used.

Prior choice

Unlike the Gaussian linear model, the logistic likelihood breaks conjugacy. Nevertheless, we can use a Gaussian prior (Equation 3) or an (improper) flat prior (Equation 4) for $\boldsymbol{\theta}$, but both require approximate inference (see subsection 3.3).

To address separation (i.e. perfect prediction) and to induce shrinkage, heavier-tailed priors are commonly employed. Gelman et al. (2008) introduced the t-distribution as a prior for low-information settings and mentions the Cauchy distribution as another possibility, which is elaborated on by Ghosh et al. (2017).

Regularization can also be achieved with the same prior distributions as introduced for Bayesian linear regression in section 2.2 (see e.g. Van Erp et al., 2019, Fahrmeir et al., 2010, O’Hara and Sillanpää, 2009).

3.3 Approximate Bayesian inference

Unlike for the linear model, Bayesian inference with closed-form posteriors is not possible in most cases. To sample from the posterior and PPD, we need to use approximate Bayesian inference methods.

Sampling from the posterior with MCMC methods

Markov Chain Monte Carlo (MCMC) generates samples from the posterior $p(\boldsymbol{\theta} \mid \mathbf{y})$ without making any (explicit) assumptions about the form of the posterior, although MCMC performs best if the parameter posterior is known up to a constant. The Metropolis–Hastings algorithm (Hastings, 1970) for K samples⁶ proceeds as follows:

1. Initialize $\boldsymbol{\theta}^{(1)}$
2. For $k = 1, \dots, K$
 - (a) Draw $\boldsymbol{\theta}^{(*)}$ from the *proposal distribution* $q(\boldsymbol{\theta}^{(*)} \mid \boldsymbol{\theta}^{(k)})$
 - (b) calculate the *acceptance probability*

$$\alpha = \min\left(1, \frac{p(\boldsymbol{\theta}^{(*)} \mid \mathbf{y}) p(\boldsymbol{\theta}^{(*)}) q(\boldsymbol{\theta}^{(k)} \mid \boldsymbol{\theta}^{(*)})}{p(\boldsymbol{\theta}^{(k)} \mid \mathbf{y}) p(\boldsymbol{\theta}^{(k)}) q(\boldsymbol{\theta}^{(*)} \mid \boldsymbol{\theta}^{(k)})}\right)$$

- (c) Accept or discard the proposal $\boldsymbol{\theta}^{(*)}$ (for $u \sim \text{Uni}[0, 1]$)

$$\begin{cases} u \leq \alpha & \boldsymbol{\theta}^{(k+1)} = \boldsymbol{\theta}^{(*)} \\ u > \alpha & \boldsymbol{\theta}^{(k+1)} = \boldsymbol{\theta}^{(k)} \end{cases}$$

The efficiency of Metropolis–Hastings depends critically on the proposal distribution q . A common choice is a Gaussian centered at the current state with covariance given by the (estimated) negative inverse Hessian of the log-posterior, often obtained via IWLS (Gamerman, 1998, Lenk and DeSarbo, 2000, Scott, 2011):⁷

$$q(\boldsymbol{\theta}^{(*)} \mid \boldsymbol{\theta}^{(k)}) \sim \mathcal{N}(\boldsymbol{\theta}^{(k)} \mid -H^{-1}(\boldsymbol{\theta}^{(k)})), \quad H(\boldsymbol{\theta}) = \nabla_{\boldsymbol{\theta}}^2 \log(p(\boldsymbol{\theta}^{(k)} \mid \mathbf{y}) p(\boldsymbol{\theta}^{(k)}))$$

(Scott, 2011) argues that using heavier-tailed proposals (e.g. Student- t) can improve mixing by allowing larger moves.

Beyond Metropolis–Hastings, several advanced samplers are popular:

- Gibbs sampling for models with conditional conjugacy or augmentation (Dellaportas and Smith, 1993).

⁶Note that by construction, the samples are (sometimes heavily) correlated and that the number of repetitions necessary until convergence depends on $\boldsymbol{\theta}^{(0)}$.

⁷The symmetry of the Gaussian distribution simplifies the algorithm to the Metropolis algorithm, where the acceptance probability can be calculated only using $p(\boldsymbol{\theta} \mid \mathbf{y}) p\boldsymbol{\theta}$.

- Hamiltonian Monte Carlo, which exploits gradient information to explore high-dimensional posteriors efficiently (Neal, 1993).
- Data augmentation (Albert and Chib, 1993), using Gaussian scale mixtures and introducing auxiliary latent variables to restore conjugacy in logistic models (Holmes, n.d., Frühwirth-Schnatter and Frühwirth, 2007, Scott, 2011).

Full Bayes with Laplace Approximation

In contrast to MCMC methods, Laplace Approximation (LA) approximates the full posterior distribution by assuming a Gaussian distribution (Tierney et al., 1986):

$$p(\boldsymbol{\theta} \mid \mathbf{y}) \approx \mathcal{N}(\hat{\boldsymbol{\theta}}_{MAP}, H^{-1}(\hat{\boldsymbol{\theta}}_{MAP})),$$

where $\hat{\boldsymbol{\theta}}_{MAP}$ is the maximum posterior estimate, obtained by maximizing the (real) posterior with standard optimization methods.

In the case of the Bayesian logistic model with a simple parameter prior $\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$, this results in

$$\begin{aligned} \hat{\boldsymbol{\theta}}_{MAP} &= \arg \max_{\boldsymbol{\theta}} p(\boldsymbol{\theta} \mid \mathbf{y}) \stackrel{\text{Bayes' rule}}{=} \arg \max_{\boldsymbol{\theta}} p(\mathbf{y} \mid \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} \\ &= \arg \max_{\boldsymbol{\theta}} \sum_{i=1}^n \log \left(\sigma(y_i \mathbf{x}_i \boldsymbol{\theta}) \right) - \frac{1}{2\sigma^2} \boldsymbol{\theta}^\top \boldsymbol{\theta} \\ H(\boldsymbol{\theta}) &= -\nabla_{\boldsymbol{\theta}}^2 \log p(\boldsymbol{\theta} \mid \mathbf{y}) = \frac{1}{\sigma^2} \mathbf{I} + \sum_{i=1}^n \sigma(y_i \mathbf{x}_i \boldsymbol{\theta}) (1 - \sigma(y_i \mathbf{x}_i \boldsymbol{\theta})) \mathbf{x}_i \mathbf{x}_i^\top. \end{aligned}$$

For hierarchical models, Rue et al. (2009) proposed an extended algorithm based on Integrated Nested Laplace Approximation.

Posterior predictive distribution

In a binary classification setting, we obtain the PPD by calculating the distribution of the positive class⁸ $p(\tilde{\mathbf{y}} = 1 \mid \boldsymbol{\theta}, \mathbf{y})$ and inferring the negative class.

As MCMC results in samples from the posterior, we can use the samples $\boldsymbol{\theta}_k$ to approximate the PPD with

$$p(\tilde{\mathbf{y}} = 1 \mid \boldsymbol{\theta}, \mathbf{y}) \approx \frac{1}{K} \sum_{k=1}^K \sigma(\tilde{\mathbf{X}} \boldsymbol{\theta}_k). \quad (10)$$

Under Laplace Approximation, we may either

- draw samples $\boldsymbol{\theta}_s \sim \mathcal{N}(\hat{\boldsymbol{\theta}}_{MAP}, H^{-1}(\hat{\boldsymbol{\theta}}_{MAP}))$ with $s = 1, \dots, S$ and compute Equation 10 or
- use the LA-approximated PPD and compute

$$p(\tilde{\mathbf{y}} = 1 \mid \boldsymbol{\theta}, \mathbf{y}) = \int \sigma(\tilde{\mathbf{X}} \boldsymbol{\theta}) \mathcal{N}_{\boldsymbol{\theta}}(\hat{\boldsymbol{\theta}}_{MAP}, H^{-1}(\hat{\boldsymbol{\theta}}_{MAP})) d\boldsymbol{\theta}.$$

⁸Encoded here with $y_i \in \{0 \text{ (negative)}, 1 \text{ (positive)}\}$

4 Illustrative Examples

4.1 Regularization and variable selection

We now apply three of the previously discussed priors to linear and logistic regression models using synthetic data (consisting of training and test data) under two settings:

- **Scenario A:** a well-behaved setting without collinearity to examine shrinkage:

$$n = 150, n_{train} = 100, n_{test} = 50$$

$$\boldsymbol{\theta} = (2, 1.5, 0, 0, 0)$$

$$\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$

$$\text{linear: } \mathbf{y} \mid \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \mathbf{I}) \quad \text{logistic: } \mathbf{y} \sim \text{Ber}(\sigma(\mathbf{X}\boldsymbol{\theta}))$$

- **Scenario B:** a low-information setting where $n \approx p$ with collinearity between informative and non-informative covariates:

$$n = 150, n_{train} = 30, n_{test} = 120$$

$$\boldsymbol{\theta} = (2, 1.5, 0, \overset{26 \text{ times}}{\dots}, 0)$$

$$\mathbf{X} \sim \mathcal{N}(\mathbf{0}, \Sigma), \quad \Sigma = \begin{pmatrix} 1 & & \\ & S_3 & 0 \\ & 0 & I_{26} \end{pmatrix}, \quad S_3 = \begin{pmatrix} 1 & 0.8 & 0.8 \\ 0.8 & 1 & 0.8 \\ 0.8 & 0.8 & 1 \end{pmatrix}$$

$$\text{linear: } \mathbf{y} \mid \boldsymbol{\theta} \sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \mathbf{I}) \quad \text{logistic: } \mathbf{y} \sim \text{Ber}(\sigma(\mathbf{X}\boldsymbol{\theta}))$$

For each scenario, we fit three linear and three logistic regression models using the following priors: A flat prior as a benchmark, using the conjugate setting described in Equation 4 with the R-package `brms`⁹. A Ridge prior (see Equation 5) and a Lasso prior (see Equation 6) via the `bayesreg` package and automatic optimization of the regularization parameters τ^2 and λ^2 . For all models, we ran MCMC with 20,000 iterations, 1,000 burn-in, and a thinning interval of 10.

Although ridge and lasso shrink coefficients, they do not perform variable selection by themselves. Thus, we used Bayesian credibility intervals as described in van Erp et al. (2019) as a criterion to decide whether a parameter is credibly nonzero.

Our evaluation focuses on:

1. Variable selection accuracy: Number of correctly identified influential covariates (Hits) and falsely as influential declared covariates (FP).
2. Predictive accuracy: Measured on test data by the mean log posterior predictive density (MLPPD) proposed by Gelman, Hwang and Vehtari (2013). Since the log-likelihood is a proper scoring rule, it is well-suited to evaluate Bayesian regression models.

Table 1 shows numerical results, while Figure 1 visualizes parameter estimates and uncertainty.

⁹The Gaussian prior variance was set to 10^6 and for the Gamma prior we set $a = 0.001, b = 0.001$ which results in an uninformative prior.

Model	Prior	Scenario A			Scenario B		
		Hits (of 2)	FP (of 3)	MLPPD	Hits (of 2)	FP (of 28)	MLPPD
Linear	flat	2	0	-1.425	2	1	-1.605
Linear	lasso	2	0	-1.424	2	0	-1.464
Linear	ridge	2	0	-1.427	2	0	-1.575
Logit	flat	2	1	-0.390	0	21	$-\infty$
Logit	lasso	1	0	-0.463	1	0	-0.485
Logit	ridge	1	0	-0.455	1	0	-0.493

Table 1: Evaluation metrics under scenarios A and B. For linear regression, all priors correctly identified the influential variables and produced few or no false positives. The effect of regularization is more pronounced in logistic regression: in both scenarios, regularized models (lasso and ridge) declared fewer coefficients as influential and reduced false positives. In the low-information Scenario B, regularization priors improved both variable selection and predictive accuracy (MLPPD). Except under the flat prior, Bayesian logistic regression achieved slightly better predictive performance than linear regression, though differences in MLPPD between priors were small.

4.2 Performance of approximate inference algorithms in Bayesian regression

In this second experiment, we compared Laplace Approximation (LA) and Metropolis-Hastings MCMC in Bayesian linear and logistic regression.

We generate 1,000 synthetic data sets with $n = 100$:

$$\begin{aligned} \mathbf{X} &\sim \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \boldsymbol{\theta} = (-0.5, 2, 1) \\ \text{linear: } \mathbf{y} \mid \boldsymbol{\theta} &\sim \mathcal{N}(\mathbf{X}\boldsymbol{\theta}, \mathbf{I}), \quad \text{logistic: } \mathbf{y} \mid \boldsymbol{\theta} \sim \text{Ber}(\sigma(\mathbf{X}\boldsymbol{\theta})) \end{aligned}$$

Each dataset was used to fit one linear and one logistic model, using both inference approaches. We assumed $\boldsymbol{\theta} \sim \mathcal{N}(\mathbf{0}, 10\mathbf{I})$ and fixed residual variance $\sigma^2 = 10$. For LA, we used `r-INLA` with settings to default from INLA to simple LA. For MCMC, we used the `MCMCglmm` package with settings specifically to use Metropolis Hastings, a relatively small sample size of 5,000, a burnin period of 500 and a thinning interval of 10. For each method, we recorded CPU runtime, posterior means, and posterior standard deviations of the estimated parameters.

Results for the linear and logistic model can be seen in Figure 2 and Figure 3 respectively. In our experiment, LA was generally slower than MCMC methods. In the case of the Bayesian linear model (Figure 2), there was not much difference in the posterior parameter estimates, although LA leads to much higher standard deviation of parameters. In contrast, LA showed clear advantages in logistic regression (Figure 3): it yielded more accurate parameter estimates and lower posterior uncertainty than MCMC. These results highlight that the performance of approximate inference methods can differ significantly depending on the model and likelihood.

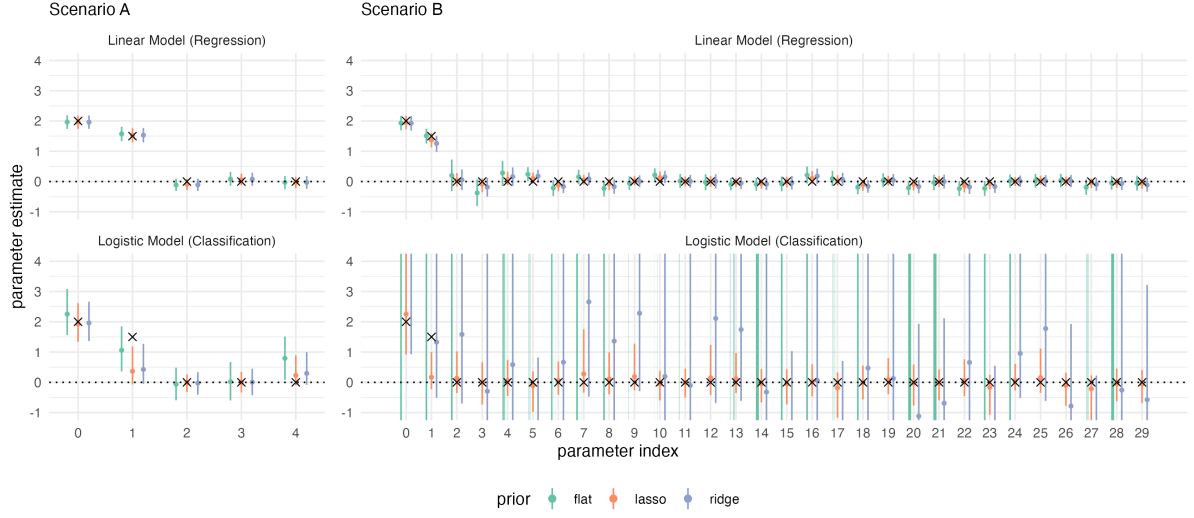


Figure 1: Estimated model parameters with 95% credibility intervals (CI). True parameter values are shown as black crosses. Linear models yielded more accurate estimates with narrower CIs than logistic models. In Scenario B, the uncertainty of the unregularized logistic model becomes especially pronounced, illustrating the need for regularization in high-dimensional, low-information settings.

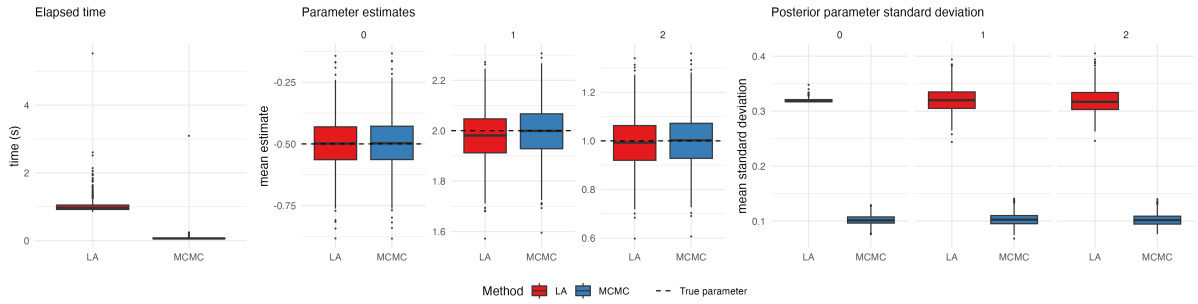


Figure 2: Bayesian linear regression: Comparison of LA (red) and MCMC (blue) across 1,000 simulations. MCMC is faster in this setting. Both methods estimate parameters accurately, though LA yields higher posterior uncertainty.

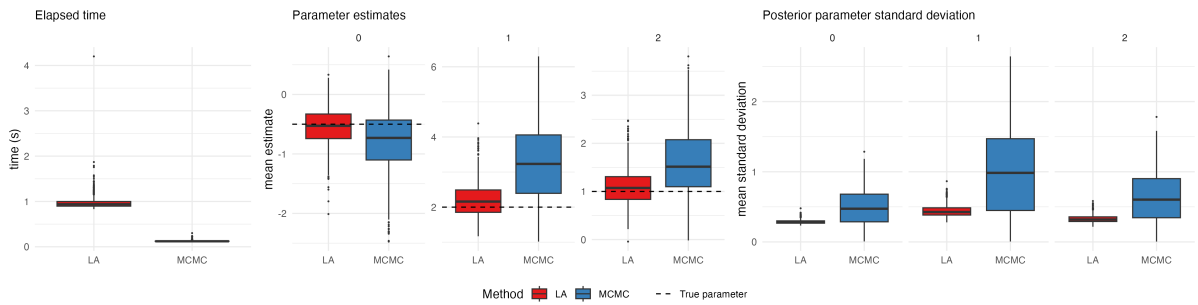


Figure 3: Bayesian logistic regression: Comparison of LA (red) and MCMC (blue) across 1,000 simulations. LA outperforms MCMC in both accuracy and precision of parameter estimates. While LA is slower to compute, it provides more stable estimates.

5 Conclusion and Outlook

We have reviewed the formulation, prior specification and approximate inference methods for Bayesian generalized linear models, with a particular focus on methods for regularization and approximation. We showed that the lack of conjugacy in the logistic likelihood necessitates numerical techniques such as Metropolis–Hastings MCMC and Laplace approximation. We detailed how the prior choice can stabilize estimation in difficult settings and how we can implement familiar regularization schemes in a Bayesian setting.

In an applied example, we examined regularized Bayesian models in difficult data settings. Especially in logistic models, regularization improved predictive performance and reduced falsely as informative declared covariates. In our comparison of MCMC and LA, we saw that although MCMC can be faster in simple linear models, Laplace approximation often provides more accurate and precise estimates in logistic regression despite higher computational cost, which could also be mitigated by the specific implementation used in the experiment. Since these examples were meant to be illustrative, the results should not be overinterpreted. In many cases, more efficient methods for regularization and approximate inference can be used and are readily available.

Some limitations of the described methods have already been mentioned above, such as the need for more complex prior distributions for real variable selection in section 2.2. Additionally, we have only examined how Bayesian GLMs work compared to frequentist GLMs for linear relationships. For more complex scenarios, the Bayesian framework can be extended to hierarchical GLMs to model random effects or to Generalized Additive Models through the inclusion of splines.

A Appendix

Notation

We denote prior parameters with \checkmark and posterior parameters with $\hat{\cdot}$. Vectors are written in bold-face like so \mathbf{x} and matrices are bold capital letters \mathbf{X} . In general, we assume n observations and $p - 1$ covariates (which means that the intercept θ_0 is always included in $\boldsymbol{\theta}$ and that $\mathbf{X} = (\mathbf{1} \ \mathbf{x}_1 \ \cdots \ \mathbf{x}_{p-1})$)

Proofs and Derivations

Posterior of the Normal-Inverse-Gamma prior

For the model described in (3), the posterior distribution is calculated according to Fahrmeir et al. (2021) as

$$\begin{aligned} p(\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y}) &\stackrel{\text{Bayes' rule}}{\propto} \mathcal{L}(\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y}) p(\boldsymbol{\theta}, \sigma^2) \\ &= \mathcal{L}(\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y}) p(\boldsymbol{\theta} \mid \sigma^2) p(\sigma^2) \\ &= \frac{1}{(\sigma^2)^{n/2}} \exp\left(-\frac{1}{2\sigma^2} (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})^\top (\mathbf{y} - \mathbf{X}\boldsymbol{\theta})\right) \\ &= \frac{1}{(\sigma^2)^{p/2}} \exp\left(-\frac{1}{2\sigma^2} (\boldsymbol{\theta} - \check{\boldsymbol{\mu}})^\top \check{\Sigma}^{-1} (\boldsymbol{\theta} - \check{\boldsymbol{\mu}})\right) \\ &= \frac{1}{(\sigma^2)^{\check{a}+1}} \exp\left(-\frac{\check{b}}{\sigma^2}\right), \end{aligned}$$

which is NIG-distributed

$$\boldsymbol{\theta}, \sigma^2 \mid \mathbf{y} \sim \text{NIG}(\hat{\boldsymbol{\mu}}, \hat{\Sigma}, \hat{a}, \hat{b})$$

with parameters

$$\begin{aligned} \hat{\boldsymbol{\mu}} &= \hat{\Sigma}(\check{\Sigma}^{-1}\check{\boldsymbol{\mu}} + \mathbf{X}^\top \mathbf{y}) \\ \hat{\Sigma} &= (\mathbf{X}^\top \mathbf{X} + \check{\Sigma}^{-1})^{-1} \\ \hat{a} &= \check{a} + \frac{n}{2} \\ \hat{b} &= \check{b} + \frac{1}{2}(\mathbf{y}^\top \mathbf{y} + \check{\boldsymbol{\mu}}^\top \check{\Sigma}^{-1} \check{\boldsymbol{\mu}} - \hat{\boldsymbol{\mu}}^\top \hat{\Sigma}^{-1} \hat{\boldsymbol{\mu}}). \end{aligned}$$

For the conditional posteriors it holds that

$$\begin{aligned} \boldsymbol{\theta} \mid \sigma^2, \mathbf{y} &\sim \mathcal{N}(\hat{\boldsymbol{\mu}}, \sigma^2 \hat{\Sigma}) \\ \boldsymbol{\theta} \mid \mathbf{y} &\sim \mathcal{T}(2\hat{a}, \hat{\boldsymbol{\mu}}, \hat{b}/\hat{a}\hat{\Sigma}). \end{aligned}$$

Posterior predictive distribution of the Normal-Inverse-Gamma prior

In the case of (3), the posterior predictive distribution is calculated as

$$\begin{aligned}
 p(\tilde{\mathbf{y}} \mid \mathbf{y}) &= \int \int p(\tilde{\mathbf{y}}, \boldsymbol{\theta}, \sigma^2) d\boldsymbol{\theta} d\sigma^2 \\
 &= \int \int p(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \sigma^2) p(\boldsymbol{\theta}, \sigma^2) d\boldsymbol{\theta} d\sigma^2 \\
 &= \int \int \mathcal{N}(\tilde{\mathbf{y}} \mid \mathbf{X}\boldsymbol{\theta}, \sigma^2 \mathbf{I}) \text{NIG}(\boldsymbol{\theta}, \sigma^2 \mid \boldsymbol{\mu}, \hat{\Sigma}, \hat{a}, \hat{b}).
 \end{aligned}$$

According to e.g. Murphy (n.d.), the result is

$$\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \sigma^2, \mathbf{y} \sim \mathcal{T}(2\hat{a}, \tilde{\mathbf{X}}\boldsymbol{\theta}, \frac{\hat{b}}{\hat{a}}(\mathbf{I} + \tilde{\mathbf{X}}\hat{\Sigma}\tilde{\mathbf{X}}^\top))$$

with posterior predictive mean

$$\mathbb{E}_{\boldsymbol{\theta}}(\mathbb{E}_{\tilde{\mathbf{y}}}(\tilde{\mathbf{y}} \mid \boldsymbol{\theta}, \sigma^2, \mathbf{y}) \mid \sigma^2, \mathbf{y}) = \mathbb{E}(\tilde{\mathbf{X}}\boldsymbol{\theta} \mid \sigma^2, \mathbf{y}) = \tilde{\mathbf{X}}\boldsymbol{\theta},$$

as stated by Gelman, Carlin, Stern, Dunson, Vehtari and Rubin (2013). The posterior predictive variance $\frac{\hat{b}}{\hat{a}}\mathbf{I} + \frac{\hat{b}}{\hat{a}}\tilde{\mathbf{X}}\hat{\Sigma}\tilde{\mathbf{X}}^\top$ consists of measurement noise in the prior from $\frac{\hat{b}}{\hat{a}}$ and uncertainty in the parameter $\boldsymbol{\theta}$ from $\frac{\hat{b}}{\hat{a}}\tilde{\mathbf{X}}\hat{\Sigma}\tilde{\mathbf{X}}^\top$.

B Electronic appendix

Data, code and figures are provided in electronic form. All figures and scripts are available from https://github.com/lona-k/probML_seminar

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