Probabilistic Machine Learning

Bayesian (Generalised) Linear Models

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Abstract

This should be an abstract

Contents

1 Introduction

Bishop (2006) introduced this and that. Another statement that needs a reference, but the authors are not named directly (Bishop, 2006). Another statement where the reference is just one possible source (see, e.g., Bishop, 2006).

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. (n.d.) or Gelman et al. (n.d.).

2.1 Model definition

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

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

where the weight parameter $\boldsymbol{\theta}$ and the variance σ^2 are estimated to obtain the fitted model. A condition on $\boldsymbol{X}$ 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 (1):

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

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.

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

where $\breve{\boldsymbol{\mu}}, \breve{\Sigma}, \breve{a}$ and $\breve{b}$ are the prior parameters. We choose a Gaussian prior on $\boldsymbol{\theta}$ because it is conjugate to the Gaussian likelihood of $\boldsymbol{y}$. 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

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

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.

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

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

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

and choosing $\breve{a} = -\frac{p}{2}$ and $\breve{b} = 0$, 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 (3).
The prior distributional assumptions would then be:

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

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, n.d.).

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)

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

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:

$$\begin{aligned} \boldsymbol{y} \mid \boldsymbol{\theta}, \sigma^2 &\sim \mathcal{N}(\boldsymbol{X}\boldsymbol{\theta}, \sigma^2 \boldsymbol{I}), ^2 \\ \boldsymbol{\theta} &\sim \text{regularization prior} \\ \sigma^2 &\sim \text{IG}(\breve{a}, \breve{b}), \end{aligned} \tag{5}$$

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

[1] Informally stated for demonstational purposes.

[2] Usually, 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 $\boldsymbol{X}'$ as the design matrix without a column for the intercept. We would then specify the model as $\boldsymbol{y} \mid \boldsymbol{\theta}, \sigma^2 \sim \mathcal{N}(\theta_0 \boldsymbol{I} + \boldsymbol{X}'\boldsymbol{\theta}', \sigma^2 \boldsymbol{I})$. 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, n.d.a,n) uses $\text{pen}(\boldsymbol{\theta}) = \|\boldsymbol{\theta}\|_2^2$ and the Bayesian analogue (MacKay, n.d., e.g.) specifies

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

with τ^2 controlling the degree of regularization akin to the role of λ. In constrast 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. $\tau^2 \sim \text{IG}(\breve{a}_\tau, \breve{b}_\tau)$, and estimate it alongside $\boldsymbol{\theta}$ and σ^2.

Lasso regularization (Tibshirani, n.d.) 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, n.d.)

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

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

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

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

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

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

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 (3), conjugacy implies for the joint posterior $p(\boldsymbol{\theta}, \sigma^2 \mid \boldsymbol{y})$ that

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

with posterior mean and variance [3]

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

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

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

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

The posterior mean $\hat{\boldsymbol{\mu}}$ coincides with $\hat{\boldsymbol{\beta}}_{LS}$ (7), so a Bayesian linear model with a non-informative prior converges to the frequentist solution. More generally, as the prior variance $\breve{\Sigma}$ 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 (3) with finite $\hat{\Sigma}$, resulting in the same posterior update in (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, n.d.). We will go more into depth on approximate inference for Bayesian regression models in Section 3.3.

Posterior predictive distribution

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

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

which is an average of conditional probabilities over the posterior distribution of $\boldsymbol{\theta}$.[4]
For the NIG prior in (3), one can show[5] that

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

Interestingly, the posterior predictive mean $\hat{\boldsymbol{\mu}} = \tilde{\boldsymbol{X}}\boldsymbol{\theta}$ 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 (2007).

If no closed form exists, the posterior predictive distribution can also be simulated (see Section 3.3)

[3] For the full calculation see Appendix A

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

[5] see Appendix A

3 Logistic Bayesian Model

3.1 Bayesian Generalized Regression

very short model statement

3.2 Bayesian Logistic Regression

Model definition

motivate logistic regression as very important for medcine and so on, probably the most-used GLM (source??) just define the model

Prior choice

- NIG scale mixture + flat prior - student t prior (Gelman 2008) - more regularization (analogue to sec 2??) - explain that it's basically the same - note similarities with naive bayesian classification!
Regularization priors

3.3 Approximate Bayesian inference

- For e.g these conjugate priors, inference can be done in closed form as explained in section, - but for most priors in GLMs this is not possible - we will introduce 2 algorithms for numerical inference

Sampling from the posterior with MCMC and HM

motivate MCMC methods
state metropolis hastings (with IWLS proposal (Fahrmeir, Gamerman, Link)) explain importance of proposal density (and simple idea for it in the case of logistic regression)
modification with metropolis **gibbs** sampler (to reduce)
note auxilariy variable augmentation (Alber 1993, Holmes) because it's cool and we mentioned scale mixture models

Full Bayes with Laplace Approximation

- Idea of LA (i.e. approximate posterior with Gaussian) - Reference to Herleitung of LA? - state formulas for mean and variance - show in logit case with simple prior
Note INLA for hierarchical models (Rue 2008)

Posterior predictive distribution

state formula (or reference sec 2) explain in general what we do for classes
- MCMC: very simple approximation - LA: - show integral - state approximation with MC integration - note probit approximation (Spiegelhalter 1990)
basically plug-in into the same formula, because we explain it with Monte-Carlo integration

4 Simulation Study

4.1 Regularization and variable selection

Experiment Setup

- Linear Regression - Logistic Regression

Results and Evaluation

4.2 Performance of approximate inference algorithms in Bayesian regression

setup with LA vs. MCMC (MH, HM, Gibbs, etc.?) in a regression environment Evaluation

5 Conclusion

A concise summary of contents and results

A Appendix

Notation

We denote prior parameters with $\breve{}$ and posterior parameters with $\hat{}$. Vectors are written in bold-face like so $\boldsymbol{x}$ and matrices are bold capital letters $\boldsymbol{X}$.

n observations

p covariates

$\boldsymbol{\theta}$ regression weights

Distributions

When deriving equations, we assume the following probability density functions and parameter placements:

$\mathcal{N}(\mu, \sigma^2)$ Gaussian distribution with mean μ and variance σ^2

Gamma distribution

$IG(a, b)$ Inverse Gamma distribution with scale parameter a and location parameter b

(multivariate) Student t-distribution

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. (n.d.) as

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

which is NIG-distributed

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

with parameters

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

For the conditional posteriors it holds that

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

Posterior predictive distribution of the Normal-Inverse-Gamma prior

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

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

According to e.g. Murphy (2007), the result is

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

with posterior predictive mean

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

as stated by Gelman et al. (n.d.). The posterior predictive variance $\frac{\hat{b}}{\hat{a}}\boldsymbol{I} + \frac{\hat{b}}{\hat{a}}\tilde{\boldsymbol{X}}\hat{\Sigma}\tilde{\boldsymbol{X}}^\top$ consists of measurement noise in the prior from $\frac{\hat{b}}{\hat{a}}$ and uncertainty in the parameter $\boldsymbol{\theta}$ from $\frac{\hat{b}}{\hat{a}}\tilde{\boldsymbol{X}}\hat{\Sigma}\tilde{\boldsymbol{X}}^\top$.

B Electronic appendix

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

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