MAST90125: Bayesian Statistical learning

Lecture 17: Empirical Bayes and chains comparison

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What have we done so far?

In the previous three lectures, we have studied regression models in Bayesian context. We did this for both cases where the response variable has

- a normal distribution conditional on the linear predictor $\mathbf{x}'\boldsymbol{\beta}$ (linear models),
- its distribution belonging to an exponential family conditional on the linear predictor $\mathbf{x}'\boldsymbol{\beta}$ (generalised linear models).

In particular, we focused on cases where Gibbs sampling was possible. In so doing, we ended up with cases in which we implicitly considered either

- Empirical Bayes
- Data augmentation.

Meanwhile, you might realize that different choices will lead to different results. So

- How to compare those chains with different initialization?

In this lecture, we will first introduce Empirical Bayes. We will then study how to compare chains (different proposed conditional distributions).

A reminder

Consider Bayes Theorem,

$$p(\boldsymbol{\theta}|y) = \frac{p(\boldsymbol{\theta}, y)}{p(y)} = \frac{p(y|\boldsymbol{\theta})p(\boldsymbol{\theta})}{p(y)} \quad \text{where } y \text{ is the data of size } n \geq 1.$$

- Now assume that $\boldsymbol{\theta}$ is multivariate and partition the vector as $(\boldsymbol{\theta}_1, \ \boldsymbol{\theta}_2)$. With this, we can re-write Bayes theorem as follows:

$$p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2|y) = \frac{p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, y)}{p(y)} = \frac{p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, y)p(\boldsymbol{\theta}_2, y)}{p(y)} = p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, y)p(\boldsymbol{\theta}_2|y)$$

- This may look uninteresting, as it just shows that the joint posterior corresponds to the conditional posterior of $\boldsymbol{\theta}_1$ multiplied by the marginal posterior of $\boldsymbol{\theta}_2$. However, now consider the following:

A reminder

- We know that as n becomes large, $p(\boldsymbol{\theta}|y) \to \mathcal{N}(\hat{\boldsymbol{\theta}}_{MAP}, I(\hat{\boldsymbol{\theta}}_{MAP})^{-1})$, where $I(\hat{\boldsymbol{\theta}}_{MAP})_{ij} = -\frac{\partial^2 \log(p(\boldsymbol{\theta},y))}{\partial \boldsymbol{\theta}_i \partial \boldsymbol{\theta}_j}\big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}_{MAP}}$.
- Furthermore, we know that the posterior variance $\text{Var}(\boldsymbol{\theta}|y)$ will decrease with n. Now assume that $\text{Var}(\boldsymbol{\theta}_2|y) \to 0$ at a faster rate than $\text{Var}(\boldsymbol{\theta}_1|y)$.
- In this scenario, $p(\boldsymbol{\theta}_2|y)$ has a sharper peak than $p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, y)$, and we can write

$$p(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2|y) = p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2, y)p(\boldsymbol{\theta}_2|y) \approx p(\boldsymbol{\theta}_1|\boldsymbol{\theta}_2^*, y)$$

  where $\boldsymbol{\theta}_2^*$ is the mode of $p(\boldsymbol{\theta}_2|y)$.
- Here, rather than undertake a full Bayesian analysis, we replace some parameters by their certain point estimates, and we name this method *Empirical Bayes*.

Where have you used Empirical Bayes before?

- It turns out we have implicitly used Empirical Bayes in this subject before.
  - In our example of Bayesian LASSO in lecture 14, fitted in Lab 7 to the US Judge ratings data, we fixed γ while estimating:

$$\boldsymbol{\beta}, \sigma_e^2, \sigma_j^2; \quad j = 1, \ldots p.$$

  - In the description of the linear mixed model in lecture 14, we assumed $\mathbf{K}$ was known up to proportionality.
  - In Lecture 12, we determined a Gibbs sampler for estimating σ^2, μ_1, μ_2 when $\mathbf{y}$ was bivariate normal with mean $\boldsymbol{\mu} = (\mu_1, \mu_2)$ and variance-covariance matrix $\sigma^2\mathbf{R}$, where $\mathbf{R}$ is a correlation matrix. However we did not estimate ρ at the very beginning.

Potential impact?

- What do you think is the potential impact of using an empirical Bayes, rather than a fully Bayesian approach?
  - If we reduce the dimensionality of the problem, which is what we are doing when using Empirical Bayes estimation, we would
    - artificially reduce the level of uncertainty in parameter estimation. In Bayesian inference, this would imply narrower posterior distributions.
  - To confirm this, let's re-examine some of the plots from the Bivariate normal example in Lecture 12.

Bivariate Normal Example in Lecture 13

In this example, assume $\mathbf{y}_i = (y_{1i},\ y_{2i})'$, $i = 1, \cdots, n$, are drawn from a bivariate normal distribution where each component marginally has the same variance.

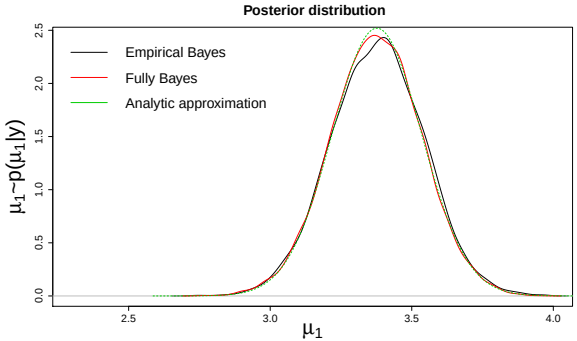
$$p(\mathbf{y}|\boldsymbol{\mu}, \sigma^2, \rho) = \frac{1}{2\pi\sigma^2\sqrt{(1-\rho^2)}} e^{-\frac{(\mathbf{y}-\boldsymbol{\mu})'\mathbf{R}^{-1}(\mathbf{y}-\boldsymbol{\mu})}{2\sigma^2}},$$

where $\boldsymbol{\mu} = (\mu_1,\ \mu_2)'$, $\mathbf{R} = \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \Rightarrow \mathbf{R}^{-1} = \frac{1}{1-\rho^2}\begin{pmatrix} 1 & -\rho \\ -\rho & 1 \end{pmatrix}$.

In the following, we first assume that the parameters requiring estimating are μ_1, μ_2, σ^2, and ρ is given. We then consider the situation where ρ also needs to be estimated. We use Gibbs (possibly plus MH) sampling to perform Bayesian analysis. Note if ρ is known, Bayesian analysis can be performed analytically. We will consider a flat prior for μ_1, μ_2 and assume $p(\sigma^2) \propto (\sigma^2)^{-1}$.

Example 1: μ_1

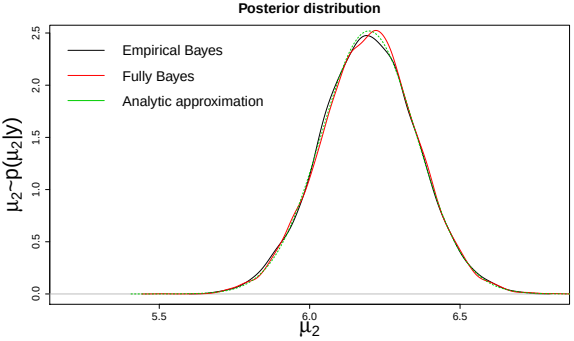
- In the following slides, we display the estimated posterior pdf's of μ_1, μ_2 and σ^2 obtained by
  - using Gibbs sampling with ρ fixed,
  - using Gibbs sampling with a Metropolis step to sample from the posterior of ρ.



- For μ_1, there appears to be little difference between empirical Bayes (ρ fixed) and full Bayesian (ρ estimated) estimates of the marginal posterior.

Example 1: μ_2

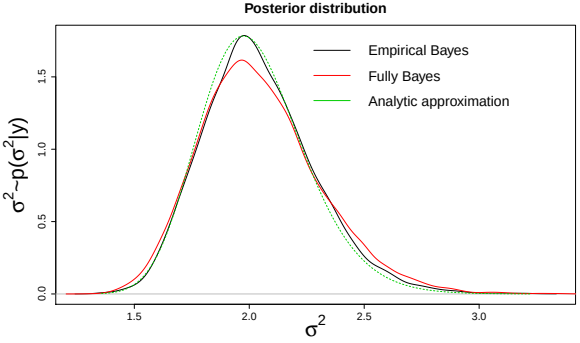
- In the following slides, we display the estimated posterior pdf's of μ_1, μ_2 and σ^2 obtained by
  - using Gibbs sampling with ρ fixed,
  - using Gibbs sampling with a Metropolis step to sample from the posterior of ρ.



- For μ_2, again there appears to be little difference between empirical Bayes (ρ fixed) and full Bayesian (ρ estimated) estimates of the marginal posterior.

Example 1: σ^2

- In the following slides, we display the estimated posterior pdf's of μ_1, μ_2 and σ^2 obtained by
  - using Gibbs sampling with ρ fixed,
  - using Gibbs sampling with a Metropolis step to sample from the posterior of ρ.



- For σ^2, fixing ρ has a noticeable impact on the posterior inference. The estimated posterior from the full Bayesian approach is less peaked with wider tails than the empirical Bayes counterpart.

Comparing chains

- We have considered a binomial likelihood with a Beta prior before. We have seen that different proposal distributions all lead to chains that converged to $p(\theta|y)$.

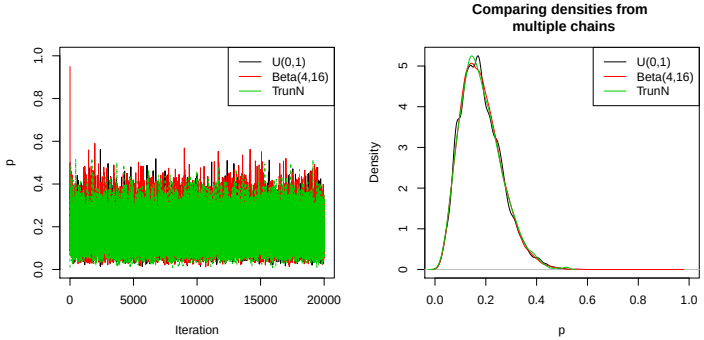


Figure: Comparison the chains using good $J(\theta^*|\cdot)$'s.

- Despite using different proposal distributions (resulting in different transitional pdf's $J(\theta^*|\cdot)$), all chains converge to $p(\theta|y)$. Cf. the Figure. Note the left plot is more commonly used.

Example 2: Poisson likelihood, Gamma prior

- Consider an example where we know the exact posterior. Assume we have count data for which a plausible likelihood is Poisson,

$$p(y_1, \dots y_n|\lambda) = \prod_{i=1}^{n} p(y_i|\lambda) = \prod_{i=1}^{n} \frac{\lambda^{y_i} e^{-\lambda}}{y_i!} = \frac{\lambda^{n\bar{y}} e^{-n\lambda}}{\prod_{i=1}^{n} y_i!}.$$

If we assume a Gamma prior for λ

$$p(\lambda) = \frac{\beta^{\alpha}}{\Gamma(\alpha)} \lambda^{\alpha-1} e^{-\beta\lambda},$$

we can show the posterior is Gamma $(\alpha + n\bar{y},\ \beta + n)$ by finding the kernel of the joint distribution,

$$p(y_1, \dots y_n, \lambda) = p(y_1, \dots y_n|\lambda)p(\lambda) \propto \lambda^{n\bar{y}} e^{-n\lambda} \times \lambda^{\alpha-1} e^{-\beta\lambda}$$

Example 2: Poisson likelihood, Gamma prior

- Now pretend you cannot sample directly from the exact posterior, and you decide to implement a Metropolis Hastings algorithm to get around this, which requires us to determine a proposal distribution.
- You decide that a good proposal distribution is

$$J(\lambda^*|\lambda^{(t-1)}) = \log \mathcal{N}(\hat{\mu}, c^2\hat{\sigma}^2/n),$$

where $\hat{\mu}$ is the sample mean of $\log(y_i + 0.1); i = 1, \ldots, n$, $\hat{\sigma^2}$ is the sample variance of $\log(y_i + 0.1); i = 1, \ldots, n$, and c is some constant.

  - Though by default the proposal distribution of λ^* depends on $\lambda^{(t-1)}$, it does not have to, as in this example.

- On the next slide, you will find the effect of using different proposal distributions.

Example 2: Poisson likelihood, Gamma prior

- Effect of poorly chosen proposal distributions.

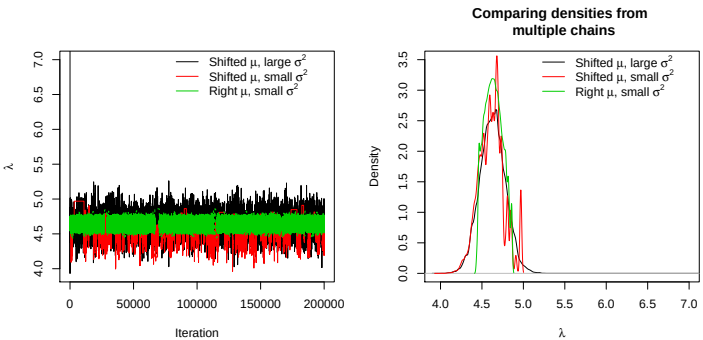


Figure: Comparing chains with poorly chosen $J(\theta^*|\cdot)$.

- Iteration plots of the three chains do not completely overlap, unlike the previous Binomial+Beta case.
- Determining the best proposal distribution is often very difficult. Instead, people generate multiple chains using the same proposal distribution but with different initial values.

A numerical criteria for convergence

- Would you trust visual inspection that chains have converged and/or mixed?
  - Would your answer change with the dimension of $\boldsymbol{\theta}$?

- To provide a numerical measure of convergence/mixing, Gelman and Rubin (1992) proposed the following diagnostic method, where for each element θ_j of the parameter vector $\boldsymbol{\theta}$ (notation $\boldsymbol{\theta}_{ijk}$ is used here, representing the j-th element in $\boldsymbol{\theta}$ in the k-th chain and i-th iteration), calculate

$$\hat{R}_j = \frac{(n-1)W_j/n + B_j/n}{W_j}$$

where $W_j = \frac{\sum_{k=1}^{m} s_{jk}^2}{m}$, $s_{jk}^2 = \frac{\sum_{i=1}^{n}(\psi_{ijk}-\bar{\psi}_{jk})^2}{n-1}$, $B_j = \frac{n\sum_{k=1}^{m}(\bar{\psi}_{jk}-\bar{\psi}_j)^2}{m-1}$, m is the number of chains, n is the number of iterations per chain, and $\psi_{ijk} = f(\boldsymbol{\theta}_{ijk})$.

- But what do we learn from this.

A numerical criteria for convergence

- In the formula for $\hat{R}_j$, s_{jk}^2 is the estimated posterior variance of parameter ψ_j in chain k, meaning W_j is the average within-chain posterior variance. B_j is the estimated variance between chain posterior chain. When the chains have converged to the posterior distribution, we would expect ...
  - The between and within chain variances to be the same $\Rightarrow \hat{R}_j \to 1$.
- If this is not the case, for instance if initial values were over-dispersed, we would expect $B_j > W_j \Rightarrow \hat{R}_j > 1$.
  - Note: Using multiple chains slit from one long chain may mitigate the over-dispersion effect.
  - The formula for $\hat{R}_j$ is motivated by ANOVA like problems. One ANOVA assumption is normally distributed errors. Hence the function f in $\psi_{ijk} = f(\boldsymbol{\theta}_{ijk})$, is often chosen to transform a highly non-normal parameter to something approximately normal.

Example of convergence diagnostic

- For p in the binomial likelihood, we use the transformation $\text{logit}(p)$. For λ in the Poisson likelihood, we use the transformation $\log(\lambda)$. We will discard the first 5 % of iterations from analysis, split the remaining chains exactly in half and perform no thinning.

Table: Gelman-Rubin diagnostic for two examples

Model	Parameter	$\hat{R}$	Upper limit C.I.
Binomial likelihood, Beta prior	p	1.0001	1.0002
(Well chosen $J(p\|\cdot)$, 20000 iterations)	$\text{logit}(p)$	1.0015	1.0019
Poisson likelihood, Gamma prior	λ	1.0203	1.0412
(Poorly chosen $J(\lambda\|\cdot)$, 200000 iterations)	$\log(\lambda)$	1.0206	1.0418

- The Gelman-Rubin diagnostics suggests that the chains of p converge to $p(p|\mathbf{y})$ more quickly than the chains of λ converge to $p(\lambda|\mathbf{y})$.

Effective sample size

- Because of auto-correlation, the number of iterations is not a measure of the true sample size. The effective sample size is defined as

$$n_{\text{eff}} = \frac{mn}{1 + 2\sum_{t=1}^{\infty} \rho_t},$$

  where m is the number of chains, n is the number of iterations per chain, and ρ_t is the auto-correlation at lag t. In order to estimate n_{eff}, the infinite sum is truncated at T, where T is the first positive integer such that $\hat{\rho}_{T+1} + \hat{\rho}_{T+2} \leq 0$.
- This means that the estimated effective sample size, $\hat{n}_{\text{eff}}$ is:

$$\hat{n}_{\text{eff}} = \frac{mn}{1 + 2\sum_{t=1}^{T} \hat{\rho}_t}.$$

Example Effective sample size

- Let's now calculate the effective sample size for each chain of the two examples.

Table: Effective sample size for two examples

Model	Parameter	$\hat{n}_{\text{eff}}$		
		Chain 1	Chain 2	Chain 3
Binomial likelihood, Beta prior	p	5408.63	5637.29	12599.14
(Well chosen $J(p\|\cdot)$, 20000 iterations)	$\text{logit}(p)$	6055.75	6774.92	11232.21
Poisson likelihood, Gamma prior	λ	1441.92	3405.03	431.44
(Poorly chosen $J(\lambda\|\cdot)$, 200000 iterations)	$\log(\lambda)$	1443.56	3424.521	438.76

Note for Binomial likelihood, $J(|)$ was $U(0,1)$ (chain 1), $\text{Be}(4,16)$ (chain 2), and truncated normal (chain 3). For Poisson likelihood, $J(|)$ was lognormal with shifted mean and large variance (chain 1), shifted mean and small variance (chain 2), and correct mean and small variance (chain 3).

- $\hat{n}_{\text{eff}}$ is lower than the number of iterations, especially in the Poisson case.
- Note the effective sample size and Gelman-Rubin diagnostics were calculated using the functions `effectiveSize` and `gelman.diag` from the `R` package `coda`.