Computational Statistics II

Unit C.2: Data augmentation for probit and logit models

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Unit C.2

Main concepts

- Albert & Chib data augmentation for probit models;
- Pólya-gamma data augmentation for logit models;
- EM and MM algorithms for logit models.

- Associated **R** code is available on the website of the course
- Additional **R** code (EM tutorial): `https://github.com/tommasorigon/logisticVB`

Main references

- Albert, J. H., & Chib, S. (1993). Bayesian analysis of binary and polychotomous response data. *JASA*, **88**(422), 669–679.
- Durante, D., & Rigon, T. (2019). Conditionally conjugate mean-field variational Bayes for logistic models. *Statistical Science*, **34**(3), 472–485.
- Polson, N. G., Scott, J. G., & Windle, J. (2013). Bayesian inference for logistic models using Pólya-Gamma latent variables. *JASA*, **108**(504), 1339–1349.

Probit and logit regression models (recap)

- One of the first data augmentation success stories within the Bayesian framework is the highly influential Albert & Chib (1993) paper for probit regression.

- Although this approach is nowadays **sub-optimal** in several contexts, it is worth recalling it for historical purposes.

- Let $\mathbf{y} = (y_1, \dots, y_n)^\intercal$ be a vector of the observed **binary responses**.

- Let $\mathbf{X}$ be the corresponding **design matrix** whose generic row is $\mathbf{x}_i = (1, x_{i2}, \dots, x_{ip})^\intercal$, for $i = 1, \dots, n$.

- We consider a generalized linear model such that

$$(y_i \mid \pi_i) \overset{\text{ind}}{\sim} \text{Bern}(\pi_i), \qquad \pi_i = g(\eta_i), \qquad \eta_i = \boldsymbol{x}_i^\intercal \boldsymbol{\beta} = \beta_1 x_{i1} + \cdots + \beta_p x_{ip},$$

  where $g(\cdot)$ is either the inverse logit transform or the cdf of a standard normal $\Phi(\cdot)$.

Probit data-augmentation

- The **likelihood** function of a probit regression model is the following

$$\pi(\boldsymbol{y} \mid \beta) = \prod_{i=1}^{n} \Phi(\boldsymbol{x}_i^\intercal \beta)^{y_i}\{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}^{1-y_i}$$
$$= \prod_{i=1}^{n} [\mathbb{1}(y_i = 1)\Phi(\boldsymbol{x}_i^\intercal \beta) + \mathbb{1}(y_i = 0)\{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}].$$

- Let us assume a multivariate Gaussian prior $\pi(\beta)$, leading to the posterior

$$\pi(\beta \mid \boldsymbol{y}) = \frac{\pi(\beta)\prod_{i=1}^{n} \Phi(\boldsymbol{x}_i^\intercal \beta)^{y_i}\{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}^{1-y_i}}{\int_{\mathbb{R}^d} \pi(\beta)\prod_{i=1}^{n} \Phi(\boldsymbol{x}_i^\intercal \beta)^{y_i}\{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}^{1-y_i} \mathrm{d}\beta},$$

whose normalizing constant is often (but not always!) **hard to approximate**.

- Whenever computations of the normalizing constant are numerically unstable, we may seek a suitable data augmentation strategy that enables Gibbs sampling and EM.

Probit data-augmentation

- We introduce a vector of latent variables $\boldsymbol{z} = (z_1, \dots, z_n)^\intercal$ taking values $z_i \in \mathbb{R}$.
- Let us consider the following generative mechanism:

$$z_i = \boldsymbol{x}_i^\intercal \boldsymbol{\beta} + \epsilon_i, \qquad \epsilon_i \overset{\text{iid}}{\sim} \mathrm{N}(0,1), \qquad i = 1, \dots, n.$$

  and transform the scores into binary variables $y_i = \mathbb{1}(z_i > 0)$, for $i = 1, \dots, n$.
- The augmented likelihood, therefore, is given by

$$\pi(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\beta}) = \prod_{i=1}^n \phi(z_i \mid \boldsymbol{x}_i^\intercal \boldsymbol{\beta}, 1)\{\mathbb{1}(z_i > 0)\mathbb{1}(y_i = 1) + \mathbb{1}(z_i \le 0)\mathbb{1}(y_i = 0)\}.$$

- **Exercise**. Prove that the marginal distribution of $\pi(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\beta})$ coincides with $\pi(\boldsymbol{y} \mid \boldsymbol{\beta})$.

Gibbs sampling for probit models

- It is easy to show (try that as an **exercise**) that the full conditional distribution can be obtained in closed form, and they can be easily simulated.

- The full conditional distribution of β is **conjugate** under a Gaussian prior $\beta \sim \mathrm{N}(\boldsymbol{b}, \boldsymbol{B})$, so that

$$(\beta \mid \boldsymbol{y}, \boldsymbol{z}) \sim \mathrm{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad \boldsymbol{\mu} = \boldsymbol{\Sigma}(\boldsymbol{X}^\intercal \boldsymbol{z} + \boldsymbol{B}^{-1}\boldsymbol{b}), \quad \boldsymbol{\Sigma} = (\boldsymbol{X}^\intercal \boldsymbol{X} + \boldsymbol{B}^{-1})^{-1}.$$

- The elements of the full conditional distribution $(\boldsymbol{z} \mid \boldsymbol{y}, \beta)$ are independent and having density

$$\pi(z_i \mid y_i = 1, \beta) \propto \phi(z_i \mid \boldsymbol{x}_i^\intercal \beta, 1)\mathbb{1}(z_i > 0)$$

  and

$$\pi(z_i \mid y_i = 0, \beta) \propto \phi(z_i \mid \boldsymbol{x}_i^\intercal \beta, 1)\mathbb{1}(z_i \leq 0).$$

  In other words, the z_i's follow a **truncated normal distribution**.

- **Homework 2**. Implement this Gibbs sampling using the Pima Indian dataset.

Yes, but what about skew-normals?

- Recently, it has been recognized that the "intractable" posterior density

$$\pi(\beta \mid \boldsymbol{y}) = \frac{\pi(\beta) \prod_{i=1}^{n} \Phi(\boldsymbol{x}_i^\intercal \beta)^{y_i} \{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}^{1-y_i}}{\int_{\mathbb{R}^d} \pi(\beta) \prod_{i=1}^{n} \Phi(\boldsymbol{x}_i^\intercal \beta)^{y_i} \{1 - \Phi(\boldsymbol{x}_i^\intercal \beta)\}^{1-y_i} \mathrm{d}\beta},$$

  is actually a **known distribution**!

- Indeed, the distribution of $(\beta \mid \boldsymbol{y})$ is a **unified skew normal** ($\textsc{sun}$).

- Do we still need data-augmentation steps? Depending on the context, iid sampling from a $\textsc{sun}$ distribution is relatively easy (large p) or problematic (large n).

Reference

- Durante, D. (2019). Conjugate Bayes for probit regression via unified skew-normal distributions. *Biometrika*, 106(4), 765–779.

The logit regression model

- The logit regression model is often termed the **canonical choice** for binary regression; see, e.g., the classic monograph by McCullagh and Nelder (1986).

- The first key reason is its improved **interpretability**, as the regression coefficients β can be nicely interpreted as log-odds ratios.

- The second reason is its analytical tractability since the logit case is an **exponential family** of distributions.

- The latter property has many implications, both within the frequentist and Bayesian framework; see, e.g., the classic paper by Diaconis and Ylvisaker (1979).

- The **likelihood** function of a logit regression model is the following

$$\pi(\boldsymbol{y} \mid \beta) = \prod_{i=1}^{n} \frac{\exp(y_i \boldsymbol{x}_i^\intercal \beta)}{1 + \exp(\boldsymbol{x}_i^\intercal \beta)}.$$

The Pólya-gamma distribution

- In a relatively recent paper, Polson et al. (2013) described a data-augmentation scheme for logistic regression based on the Pólya-gamma distribution.

- **Definition (Pólya-gamma)**. A positive random variable Z has a Pólya-gamma distribution with parameters $\alpha > 0$ and $\gamma \in \mathbb{R}$ denoted as $Z \sim \mathrm{PG}(\alpha, \gamma)$, if

$$Z \overset{d}{=} \frac{1}{2\pi^2} \sum_{k=1}^{\infty} \frac{G_k}{(k - 1/2)^2 + \gamma^2/(4\pi^2)},$$

  where $G_k \sim \mathrm{GA}(\alpha, 1)$ are independent random variables.

- **Remark**. The density $\pi(z \mid \alpha, \gamma)$ of a Pólya-gamma random variable $Z \sim \mathrm{PG}(\alpha, \gamma)$ is expressed in terms of an infinite summation, but it can be **easily simulated**.

- In **R** this can be done using the `rpg.devroye` function of the `BayesLogit` **R** package.

Technical results about the Pólya-gamma distribution

- **Technical lemma 1.** The Laplace transform characterizing the law of $V \sim \text{PG}(\alpha, 0)$ for any $\lambda > 0$ is readily available as

$$\mathbb{E}\{\exp(-\lambda V)\} = \prod_{k=1}^{\infty}\left(1 + \frac{\lambda}{2\pi^2(k-1/2)^2}\right)^{-\alpha} = \cosh(\sqrt{\lambda/2})^{-\alpha}.$$

- **Technical lemma 2.** The general family of distributions $Z \sim \text{PG}(\alpha, \gamma)$ is generated through the exponential tilting of $V \sim \text{PG}(\alpha, 0)$, since

$$\pi(z \mid \alpha, \gamma) = \frac{e^{-z\gamma^2/2}\pi(z \mid \alpha, 0)}{\mathbb{E}\{\exp(-\gamma^2/2V)\}} = \cosh(\gamma/2)^{\alpha} e^{-z\gamma^2/2}\pi(z \mid \alpha, 0).$$

  This can be again proved using the Laplace transform and appealing to the Weierstrass factorization theorem.

- **Intriguing idea?** The Pólya-gamma is also infinitely divisible $\implies$ CRM / NRMI can be constructed. The characterizing Lévy-intensity is available as an infinite series.

The data augmentation

- Let $\boldsymbol{z} = (z_1, \dots, z_n)^\intercal$ be a vector of latent iid random variables following a $\text{PG}(1, 0)$.
- Then, we define the following **augmented likelihood**

$$\pi(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\beta}) = \prod_{i=1}^{n} \frac{1}{2} \pi(z_i \mid 1, 0) \exp\{(y_i - 1/2)\boldsymbol{x}_i^\intercal \boldsymbol{\beta} - z_i(\boldsymbol{x}_i^\intercal \boldsymbol{\beta})^2/2\}.$$

- Thanks to the **technical lemma 1**, we immediately recognize that this is a valid data augmentation since

$$\pi(\boldsymbol{y} \mid \boldsymbol{\beta}) = \int_{\mathbb{R}^n} \pi(\boldsymbol{y}, \boldsymbol{z} \mid \boldsymbol{\beta}) \mathrm{d}\boldsymbol{z}.$$

- The augmented log-likelihood is **quadratic** in $\boldsymbol{\beta}$, as in the probit case, facilitating posterior computations.

Gibbs sampling for logit models

- The full conditional distribution of β is **conjugate** under a Gaussian prior $\beta \sim \mathrm{N}(\boldsymbol{b}, \boldsymbol{B})$, so that

$$(\beta \mid \boldsymbol{y}, \boldsymbol{z}) \sim \mathrm{N}_p(\boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad \boldsymbol{\mu} = \boldsymbol{\Sigma}\{\boldsymbol{X}^\intercal(\boldsymbol{y} - 1/2) + \boldsymbol{B}^{-1}\boldsymbol{b}\}, \quad \boldsymbol{\Sigma} = (\boldsymbol{X}^\intercal \boldsymbol{Z}\boldsymbol{X} + \boldsymbol{B}^{-1})^{-1},$$

  where $\boldsymbol{Z} = \mathrm{diag}(z_1, \dots, z_n)$.

- Using the **technical lemma 2**, we recognize that the elements of the full conditional distribution $(\boldsymbol{z} \mid \boldsymbol{y}, \beta)$ are independent and such that

$$(z_i \mid \boldsymbol{y}, \beta) \sim \mathrm{PG}(1, \boldsymbol{x}_i^\intercal \beta), \qquad i = 1, \dots, n.$$

  Note that z_i is independent on $\boldsymbol{y}$ given β.

- This enables a straightforward Gibbs sampling strategy, provided we can efficiently sample the Pólya-gamma random variables.

- Improved strategies can be devised if $y_i \sim \mathrm{Bin}(n_i, \pi_i)$.

R implementation

```r
logit_Gibbs <- function(R, burn_in, y, X, B, b) {
  p <- ncol(X); n <- nrow(X)
  out <- matrix(0, R, p) # Initialize an empty matrix to store the values
  P <- solve(B) # Prior precision matrix
  Pb <- P %*% b; Xy <- crossprod(X, y - 1 / 2) # Terms appearing in the Gibbs sampling
  beta <- rep(0, p)   # Initialization

  # Gibbs sampling
  for (r in 1:(R + burn_in)) {
    eta <- c(X %*% beta)
    omega <- rpg.devroye(num = n, h = 1, z = eta) # Sampling the Pólya-gamma latent variables

    eig <- eigen(crossprod(X * sqrt(omega)) + P, symmetric = TRUE)
    Sigma <- crossprod(t(eig$vectors) / sqrt(eig$values))
    mu <- Sigma %*% (Xy + Pb)
    A1 <- t(eig$vectors) / sqrt(eig$values)
    beta <- mu + c(matrix(rnorm(1 * p), 1, p) %*% A1)  # Sampling beta

    if (r > burn_in) {
        out[r - burn_in, ] <- beta # Store the values after the burn-in period
    }
  }
  out
}
```

The Pima Indian dataset

- We consider once again the Pima Indian dataset example of **unit B.2**.
- The Pólya-gamma Gibbs sampler has excellent mixing and it requires **no tuning**.

```
# Running the MCMC (R = 30000, burn_in = 5000)
fit_MCMC <- as.mcmc(logit_Gibbs(R, burn_in, y, X, B, b))

summary(effectiveSize(fit_MCMC)) # Effective sample size (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  10018   13592   15411   15182   17369   18900

summary(R / effectiveSize(fit_MCMC)) # Integrated autocorrelation time (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#  1.587   1.728   1.950   2.051   2.209   2.995

summary(1 - rejectionRate(fit_MCMC)) # Acceptance rate (beta)
#   Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
#      1       1       1       1       1       1
```

The Newton-Raphson algorithm (recap)

- The Pólya-gamma data augmentation is also useful also for **maximization** purposes.
- For the sake of clarity, let us focus on the MLE, which is defined as

$$\hat{\beta} = \arg\max_{\beta \in \mathbb{R}^p} \left[\sum_{i=1}^{n} y_i(\boldsymbol{x}_i^\intercal \beta) - \log\{1 + \exp(\boldsymbol{x}_i^\intercal \beta)\} \right].$$

- Extensions to the MAP case (penalized MLE) is often straightforward.
- The textbook approach for this problem is the **Newton-Raphson** method, which gives

$$\beta^{(r+1)} = \beta^{(r)} + (\boldsymbol{X}^\intercal \boldsymbol{H}^{(r)} \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal (\boldsymbol{y} - \boldsymbol{\pi}^{(r)}),$$

with $\boldsymbol{H}^{(r)} = \text{diag}\{\pi_1^{(r)}(1 - \pi_1^{(r)}), \ldots, \pi_n^{(r)}(1 - \pi_n^{(r)})\}$.

Potential pitfalls

- The Newton-Raphson iterative scheme does not guarantee a monotonic sequence, implying that the algorithm could **fail**.

```r
y <- c(rep(0,50), 1, rep(0,50), 0, rep(0, 5), rep(1, 10))          # Binary outcomes
X <- cbind(1, c(rep(0, 50), 0, rep(0.001, 50), 100, rep(-1, 15))) # Design matrix
```

- The MLE is $\hat{\beta} = (-4.603, -5.296)$ and $\log \pi(\boldsymbol{y} \mid \hat{\beta}) = -15.156$.

- However, the `glm` **R** command, which uses Newton-Raphson, does not reach the correct value and raises a warning.

```r
coef(glm(y ~ X[, -1], family = "binomial")) # Estimation using Newton-Raphson.

## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
##   (Intercept)       X[, -1]
## -3.372166e+15 -2.085057e+13
```

The EM algorithm for logistic regression

- An EM strategy automatically leads to much higher numerical stability due to the monotonic property.

- **Expectation step**. In the first place, note that

$$\mathcal{Q}(\beta \mid \beta^{(r)}) = \sum_{i=1}^{n} (y_i - 1/2)\boldsymbol{x}_i^\intercal \beta - \frac{1}{2}\mathbb{E}(z_i)(\boldsymbol{x}_i^\intercal \beta)^2 + \text{const},$$

where the expectation is taken w.r.t. Pólya-gamma density, $\pi(z_i \mid \boldsymbol{y}, \beta^{(r)})$ whose expectation is known:

$$\mathbb{E}(z_i) = \hat{z}_i^{(r)} = \frac{\tanh(\boldsymbol{x}_i^\intercal \beta^{(r)}/2)}{2\boldsymbol{x}_i^\intercal \beta^{(r)}}.$$

- **Maximization step**. Hence, we aim at maximizing $\mathcal{Q}(\beta \mid \beta^{(r)})$, obtaining

$$\beta^{(r+1)} = \arg\max_{\beta \in \mathbb{R}^p} \mathcal{Q}(\beta \mid \beta^{(r)}) = (\boldsymbol{X}^\intercal \hat{\boldsymbol{Z}}^{(r)} \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal (\boldsymbol{y} - 1/2),$$

where $\hat{\boldsymbol{Z}}^{(r)} = \text{diag}(\hat{z}_1^{(r)}, \ldots, \hat{z}_n^{(r)})$.

The EM for logistic regression

- It turns out that the Pólya-gamma data augmentation not only leads to a stable algorithm but also has a **sharp connection** with the Newthon-Rapson method.

- With some algebraic manipulation, we can show that

$$\beta^{(r+1)} = (\boldsymbol{X}^\intercal \hat{\boldsymbol{Z}}^{(r)} \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal (\boldsymbol{y} - 1/2) = \beta^{(r)} + (\boldsymbol{X}^\intercal \hat{\boldsymbol{Z}}^{(r)} \boldsymbol{X})^{-1} \boldsymbol{X}^\intercal (\boldsymbol{y} - \boldsymbol{\pi}^{(r)}),$$

- In other terms, the Pólya-gamma EM coincides with a Newton-Rapshon step, having replaced the diagonal matrix $\boldsymbol{H}^{(r)}$ with $\hat{\boldsymbol{Z}}^{(r)}$.

- Interestingly, the following inequalities hold true

$$\pi_i^{(r)}(1 - \pi_i^{(r)}) \le \frac{\tanh(\boldsymbol{x}_i^\intercal \beta^{(r)}/2)}{2\boldsymbol{x}_i^\intercal \beta^{(r)}} \le \frac{1}{4}.$$

- The first inequality implies that the EM will perform **smaller but safer** steps compared to the Newton-Rapshon algorithm.

Implementation in R

```
logit_EM <- function(X, y, tol = 1e-16, beta_start = NULL, maxiter = 10000) {

  # Initialization
  loglik <- numeric(maxiter)
  Xy <- crossprod(X, y - 0.5)
  eta <- c(X %*% beta)
  w <- tanh(eta / 2) / (2 * eta); w[is.nan(w)] <- 0.25
  loglik[1] <- sum(y * eta - log(1 + exp(eta)))

  # Iterative procedure
  for (t in 2:maxiter) {
    beta <- solve(qr(crossprod(X * w, X)), Xy)
    eta <- c(X %*% beta)
    w <- tanh(eta / 2) / (2 * eta); w[is.nan(w)] <- 0.25

    loglik[t] <- sum(y * eta - log(1 + exp(eta)))
    if (loglik[t] - loglik[t - 1] < tol) {
      return(list(beta = beta, Convergence = cbind(Iteration = (1:t) - 1,
        Loglikelihood = loglik[1:t])))
    }
  }
  stop("The algorithm has not reached convergence")
}
```

Solving the pitfalls of Newton-Raphson

- We compare the value of $\log \pi(\boldsymbol{y} \mid \beta^{(r)})$ obtained through the two algorithms and using the previously considered dataset.

- Both the EM and Newton-Raphson are initialized at $\beta^{(0)} = (0, 0)$. Moreover, this means that $\pi_i^{(0)}(1 - \pi_i^{(0)}) = 1/4$, implying that the first iteration will coincide.

Iteration	0	1	2	3	4	5
Newton-Raphson	-81.098	-38.814	-36.271	-35.433	-26.314	-733.671
EM	-81.098	-38.814	-36.778	-36.332	-36.168	-36.064

- At the 5th iteration, the Newton-Raphson **diverges**, leading to a failure. Conversely, the EM slowly yet steadily increases the log-likelihood.

The MM algorithm for logistic regression

- We finally consider a MM algorithm for finding the MLE of a logistic regression, which is based on the following **minorize** function

$$g(\beta \mid \beta^{(r)}) = \log \pi(\boldsymbol{y} \mid \beta^{(r)}) + (\boldsymbol{y} - \boldsymbol{\pi}^{(r)})^\intercal \boldsymbol{X}(\beta - \beta^{(r)}) + \frac{1}{2}(\beta - \beta^{(r)})^\intercal \boldsymbol{W}(\beta - \beta^{(r)}),$$

with $\boldsymbol{W} = 0.25\boldsymbol{X}^\intercal \boldsymbol{X}$.

- The minorize function indeed satisfies $g(\beta \mid \beta^{(r)}) \leq \log \pi(\boldsymbol{y} \mid \beta)$.

- The maximization of leads to the following MM **monotonic** iterative procedure

$$\beta^{(r+1)} = \beta^{(r)} + 4(\boldsymbol{X}^\intercal \boldsymbol{X})^{-1}\boldsymbol{X}^\intercal(\boldsymbol{y} - \boldsymbol{\pi}^{(r)}).$$

- This leads to an algorithm that makes even smaller steps than the EM, but it has the advantage of not requiring a matrix inversion at every iteration.

Implementation in R

```
logit_MM <- function(X, y, tol = 1e-16, beta_start = NULL, maxiter = 10000) {

  # Initialization
  loglik <- numeric(maxiter)
  B <- 4 * solve(crossprod(X)) # Bohning and Lindsay matrix
  eta <- c(X %*% beta)
  prob <- 1 / (1 + exp(- eta))
  loglik[1] <- sum(y * eta - log(1 + exp(eta)))

  # Iterative procedure
  for (t in 2:maxiter) {
    beta <- beta + B %*% crossprod(X, y - prob))
    eta <- c(X %*% beta)
    prob <- 1 / (1 + exp(- eta))
    loglik[t] <- sum(y * eta - log(1 + exp(eta)))
    if (loglik[t] - loglik[t - 1] < tol) {
      return(list(beta = beta, Convergence = cbind(Iteration = (1:t) - 1,
        Loglikelihood = loglik[1:t])))
    }
  }
  stop("The algorithm has not reached convergence")
}
```

EM and MM comparison (simulated data)