Bayesian Linear Model

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Why do we need Bayesian models for spatial data

- The classical MLE based approach is limited in scope.
- For example, uncertainty quantification for the covariance parameters is tricky
    - Need to leverage asymptotic results
    - Increasing and fixed domain asymptotics for irregular sptial data
    - Parameters often not identifiable (Zhang 2006)
- The Bayesian approach expands the class of models and easily handles:
    - repeated measures or multiple data sources
    - unbalanced or missing data
    - spatial misalignment and change of support
    - varying coefficient models

  – and many other settings that are precluded (or much more complicated) in classical settings.

Basics of Bayesian inference

- We start with a model (likelihood) $f(y \mid \theta)$ for the observed data $y = (y_1, \ldots, y_n)'$ given unknown parameters θ (perhaps a collection of several parameters).
- Add a prior distribution $p(\theta \mid \lambda)$, where λ is a vector of hyper-parameters.

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- If λ are known/fixed, then the posterior distribution of θ is given by:

$$p(\theta \mid y, \lambda) = \frac{p(\theta \mid \lambda) \times f(y \mid \theta)}{p(y \mid \lambda)} = \frac{p(\theta \mid \lambda) \times f(y \mid \theta)}{\int f(y \mid \theta) p(\theta \mid \lambda) d\theta}.$$

  We refer to this formula as Bayes Theorem.

A simple example: Normal data and normal priors

- Example: Say $y = (y_1, \ldots, y_n)'$, where $y_i \overset{iid}{\sim} N(\theta, \sigma^2)$; assume σ is known.
- $\theta \sim N(\mu, \tau^2)$, i.e. $p(\theta) = N(\theta \,|\, \mu, \tau^2)$; μ, τ^2 are known.
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$$
\begin{aligned}
p(\theta|y) &\propto N(\theta \mid \mu, \tau^2) \times \prod_{i=1}^{n} N(y_i \mid \theta, \sigma^2) \\
&= N\left(\theta \mid \frac{\sigma^2}{\sigma^2 + n\tau^2}\mu + \frac{n\tau^2}{\sigma^2 + n\tau^2}\bar{y}, \frac{\sigma^2\tau^2}{\sigma^2 + n\tau^2}\right)
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\end{aligned}
$$

- When $\tau^2 \to \infty$ or $n \to \infty$, $\theta \,|\, y \sim N(\bar{y}, \sigma^2/n)$, i.e., same as the classical result

Improper priors

- In the previous example, $\theta \,|\, y \sim N(\bar{y}, \sigma^2/n)$ when $\tau^2 = \infty$
- However, $\tau^2 = \infty \Rightarrow p(\theta) \propto 1$ is not a valid density as $\int 1 = \infty$. So why is it that we are even discussing them?
- If the priors are improper (that's what we call them), as long as the resulting posterior distributions are valid we can still conduct legitimate statistical inference on them.

Basic of Bayesian inference

- Point estimation: simply choose an appropriate distribution summary: posterior mean, median or mode.
- Bayesian credible sets:. A $100(1-\alpha)\%$ credible set C for θ satisfies

$$P(\theta \in C \mid y) = \int_C p(\theta \mid y) d\theta \geq 1 - \alpha.$$

- The interval between the $\frac{\alpha}{2}^{th}$ and $(1-\frac{\alpha}{2})^{th}$ quantiles of $p(\theta \mid y)$ is a $100(1-\alpha)\%$ Bayesian *credible interval*.
- Often direct calculation of quantiles, modes and means are not straightforward.

Sampling-based inference:

- Approximate the posterior distribution $p(\theta \mid y)$ by drawing samples $\{\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(M)}\}$ from it.
- $p(\theta \mid y) \approx \frac{1}{M} \sum_{i=1}^{M} I(\theta = \theta^{(i)})$
- Numerical integration can be replaced by "Monte Carlo integration".

$$E_{\theta \mid y}(g(\theta)) \approx \frac{1}{M} \sum_{i=1}^{M} g(\theta^{(i)})$$

- Sample quantiles approximate posterior quantiles

Bayesian Linear Model

- $y_i \overset{\text{iid}}{\sim} N(x_i'\beta, \sigma^2)$,
- Assume prior $\beta \sim N(\mu, V)$
- $p(\beta \mid \sigma^2, y) \propto N(y \mid X\beta, \sigma^2 I) \times N(\beta \mid \mu, V)$

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- $p(\beta \,|\, \sigma^2, y) \propto N(y \,|\, X\beta, \sigma^2 I) \times N(\beta \,|\, \mu, V)$
- $\beta \sim N((X'X/\sigma^2 + V^{-1})^{-1} X'y/\sigma^2, (X'X/\sigma^2 + V^{-1})^{-1})$

Super useful result:

$p(\beta) \propto \prod_{i=1}^{n} \exp\left(-\frac{1}{2}(y_i - X_i\beta)' Q_i (y_i - X_i\beta)\right) \Rightarrow$
$\beta \sim N\left(B^{-1}b, B^{-1}\right)$ where $B = \sum_{i=1}^{n} X_i' Q_i X_i$ and
$b = \sum_{i=1}^{n} X_i' Q_i y_i$

Bayesian Linear Model

- $\beta \sim N((X'X/\sigma^2 + V^{-1})^{-1}X'y/\sigma^2, (X'X/\sigma^2 + V^{-1})^{-1})$
- If $V^{-1} = 0$, then
  $p(\beta \,|\, \sigma^2, y) = N(\beta \,|\, (X^T X)^{-1} X^T y,\, \sigma^2 (X^T X)^{-1})$.
- $V^{-1} = 0$ corresponds to $p(\beta) \propto 1$ (another example of an improper prior)

Basics of Bayesian inference

- If λ are unknown (hyperparameter), we assign a prior, $p(\lambda)$, and seek:

$$p(\theta, \lambda \,|\, y) = p(\lambda) p(\theta \,|\, \lambda) f(y \,|\, \theta) / p(y).$$

The proportionality constant does not depend upon θ or λ:

$$p(y) = \int p(\lambda) p(\theta \,|\, \lambda) f(y \,|\, \theta) d\lambda d\theta$$

- The above represents a joint posterior from a hierarchical model. The marginal posterior distribution for θ is:

$$p(\theta \,|\, y) \propto \int p(\lambda) p(\theta \,|\, \lambda) f(y \,|\, \theta) d\lambda.$$

Marginal and conditional distributions

- $\beta \mid \sigma^2, y \sim N((X'X/\sigma^2 + V^{-1})^{-1}X'y/\sigma^2, (X'X/\sigma^2 + V^{-1})^{-1})$

- $p(\beta \mid \sigma^2, y)$ would have been the desired posterior distribution had σ^2 been known.

- If σ^2 is unknown, $p(\beta \mid \sigma^2, y)$ is called the the conditional posterior distribution of β.

- The marginal posterior distribution by integrating out σ^2 is:

$$p(\beta \mid y) = \int p(\beta \mid \sigma^2, y) p(\sigma^2 \mid y) d\sigma^2$$

- Can we bypass the integration and still do inference on $\theta \mid y$?

Composition Sampling

- Suppose $\theta = (\theta_1, \theta_2)$ and we know how to sample from the marginal posterior distribution $p(\theta_2|y)$ and the conditional distribution $P(\theta_1 \mid \theta_2, y)$.
- Goals: Draw samples from the marginal posterior $p(\theta_1 \mid y)$ and from the joint distribution: $p(\theta_1, \theta_2 \mid y)$

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- Goals: Draw samples from the marginal posterior $p(\theta_1 \,|\, y)$ and from the joint distribution: $p(\theta_1, \theta_2 \,|\, y)$

- We do this in two stages using composition sampling:
  - First draw $\theta_2^{(j)} \sim p(\theta_2 \,|\, y),\ j = 1, \ldots M$.
  - Next draw $\theta_1^{(j)} \sim p\left(\theta_1 \,|\, \theta_2^{(j)}, y\right)$.

Composition Sampling

- Composition sampling:
  - First draw $\theta_2^{(j)} \sim p(\theta_2 \,|\, y),\ j = 1, \ldots M$.
  - Next draw $\theta_1^{(j)} \sim p\left(\theta_1 \,|\, \theta_2^{(j)}, y\right)$.
- This sampling scheme produces exact samples, $\{\theta_1^{(j)}, \theta_2^{(j)}\}_{j=1}^{M}$ from the posterior distribution $p(\theta_1, \theta_2 \,|\, y)$.
- Gelfand and Smith (JASA, 1990) demonstrated automatic marginalization: $\{\theta_1^{(j)}\}_{j=1}^{M}$ are samples from $p(\theta_1 \,|\, y)$ and (of course!) $\{\theta_2^{(j)}\}_{j=1}^{M}$ are samples from $p(\theta_2 \,|\, y)$.
- In effect, composition sampling has performed the following "integration":

$$p(\theta_1 \,|\, y) = \int p(\theta_1 \,|\, \theta_2, y) p(\theta_2 \,|\, y) d\theta.$$

Composition Sampling for Bayesian Linear Model

- $y_i \stackrel{\text{iid}}{\sim} N(x_i'\beta, \sigma^2)$, $p(\beta) \propto 1$
- Assume an Inverse Gamma ($IG(a, b)$) prior for σ^2, i.e.,

$$p(\sigma^2) \propto \left(\frac{1}{\sigma^2}\right)^{a+1} exp(-b/\sigma^2)$$

- Marginal posterior distribution of σ^2 is:

$$p(\sigma^2 \,|\, y) = IG\left(\sigma^2 \,|\, a + \frac{n-p}{2}, b + \frac{(n-p)s^2}{2}\right),$$

  where $s^2 = \hat{\sigma}^2 = \frac{1}{n-p} y^T (I - P_X) y$, $P_X = X(X'X)^{-1}X'$.
- If $a = b = 0$, i.e., $p(\sigma^2) \propto 1/\sigma^2$, then
  $\sigma^2 \,|\, y \sim IG(\sigma^2 \,|\, (n-p)/2, (n-p)s^2/2)$ and $E(\sigma^2 \,|\, y) = \hat{\sigma}^2$.
  Striking similarity with the classical result!

Composition sampling for Bayesian Linear Model

- Now we are ready to carry out composition sampling from $p(\beta, \sigma^2 \,|\, y)$ as follows:
    - Draw M samples from $p(\sigma^2 \,|\, y)$:
    $$\sigma^{2(j)} \sim IG\left(\frac{n-p}{2}, \frac{(n-p)s^2}{2}(n-p)\right),\ j = 1, \ldots M$$
    - For $j = 1, \ldots, M$, draw from $p(\beta \,|\, \sigma^{2(j)}, y)$:
    $$\beta^{(j)} \sim N\left((X^TX)^{-1}X^Ty,\ \sigma^{2(j)}(X^TX)^{-1}\right)$$
- The resulting samples $\{\beta^{(j)}, \sigma^{2(j)}\}_{j=1}^{M}$ represent M samples from $p(\beta, \sigma^2 \,|\, y)$.
- $\{\beta^{(j)}\}_{j=1}^{M}$ are samples from the marginal posterior distribution $p(\beta \,|\, y)$. This is a multivariate t density:

$$p(\beta \,|\, y) = \frac{\Gamma(n/2)}{(\pi(n-p))^{p/2}\Gamma((n-p)/2)|s^2(X^TX)^{-1}|}\left[1 + \frac{(\beta-\hat{\beta})^T(X^TX)(\beta-\hat{\beta})}{(n-p)s^2}\right]^{-n/2}.$$

Bayesian predictions

- To predict new observations $\tilde{y}$, based upon the observed data y, we specify a joint probability model $p(\tilde{y}, y \mid, \theta)$, which defines the conditional predictive distribution:

$$p(\tilde{y} \mid y, \theta) = \frac{p(\tilde{y}, y \mid, \theta)}{p(y \mid \theta)}.$$

- Posterior predictive distribution is $p(\tilde{y} \mid y) = \int p(\tilde{y} \mid y, \theta) p(\theta \mid y) d\theta$.
- This can be evaluated using composition sampling:
  - First obtain: $\theta^{(j)} \sim p(\theta \mid y),\ j = 1, \ldots M$
  - For $j = 1, \ldots, M$ sample $\tilde{y}^{(j)} \sim p(\tilde{y} \mid y, \theta^{(j)})$
- The $\{\tilde{y}^{(j)}\}_{j=1}^{M}$ are samples from the posterior predictive distribution $p(\tilde{y} \mid y)$.

Bayesian predictions from the linear model

- Suppose we have observed the new predictors $\tilde{X}$, and we wish to predict the outcome $\tilde{y}$. We specify $p(\tilde{y}, y \mid \theta)$ to be a normal distribution:

$$\begin{pmatrix} y \\ \tilde{y} \end{pmatrix} \sim N\left(\begin{bmatrix} X \\ \tilde{X} \end{bmatrix} \beta, \sigma^2 I \right)$$

- Note $p(\tilde{y} \mid y, \beta, \sigma^2) = p(\tilde{y} \mid \beta, \sigma^2) = N(\tilde{y} \mid \tilde{X}\beta, \sigma^2 I)$.
- The posterior predictive distribution:

$$\begin{aligned} p(\tilde{y} \mid y) &= \int p(\tilde{y} \mid y, \beta, \sigma^2) p(\beta,\, \sigma^2 \mid y) d\beta d\sigma^2 \\ &= \int p(\tilde{y} \mid \beta, \sigma^2) p(\beta,\, \sigma^2 \mid y) d\beta d\sigma^2. \end{aligned}$$

- By now we are comfortable evaluating such integrals:
  - First obtain: $(\beta^{(j)}, \sigma^{2(j)}) \sim p(\beta, \sigma^2 \mid y)$, $j = 1, \dots, M$
  - Next draw: $\tilde{y}^{(j)} \sim N(\tilde{X}\beta^{(j)}, \sigma^{2(j)} I)$.

Bayesian inference for spatial linear model

- $y(s) = x(s)'\beta + w(s) + \epsilon(s)$, $w(s) \sim GP(0, C(\cdot, \cdot \mid \phi))$, $\epsilon \overset{\text{iid}}{\sim} N(0, \tau^2)$
- For n locations, we have $y = N(X\beta + w, \tau^2 I)$, $w \sim N(0, C(\phi))$
- Assuming stationarity, $C(\phi) = \sigma^2 R(\phi)$ where $R(\phi)$ is the correlation matrix
- Marginalised model: $y \sim N(X\beta, \sigma^2 R + \tau^2 R(\phi))$
- Even if we assume ϕ is known and σ^2 and τ^2 are given Inverse Gamma priors, composition sampling does not help here
- Composition sampling still relies on marginal posteriors which involve complex integration
- How to do inference on the Bayesian parameters?