# STATISTICAL COMPUTATIONS

Integration: It is performed to evaluate integrals of the type

$$E(g(\theta)|\mathbf{x}) = \int_{\Theta} g(\theta)p(\theta|\mathbf{x})d\theta$$

Examples of commonly considered functions g are: A power of  $\theta$ , for the posterior moments; An indicator function, for posterior probabilities and HPDs; A loss function, in decision theoretic settings;  $p(z|\mathbf{x},\theta)$  for predictions.

The most common methods are: Numerical approximations; Direct sampling; Rejection sampling; Markov Chain Monte Carlo Methods.

### ANALYTIC APPROXIMATIONS

A Bayesian Central Limit Theorem, allowing normal approximations to the posterior distribution, is given by the following result.

Result: (Berger, p. 224) Let  $X_1, \ldots, X_n$  be an i.i.d. sample from the density  $p(X|\theta)$  and  $\pi(\theta)$  the prior. Then for large n and some regularity conditions,  $p(\theta|\mathbf{x})$  can be approximated as

- 1.  $N(\mu(\boldsymbol{x}), V(\boldsymbol{x}))$  where  $\mu(\boldsymbol{x})$  and  $V(\boldsymbol{x})$  are the posterior mean and covariance matrix, or
- 2.  $N(\hat{\theta}, \mathbf{I}(x)^{-1})$  where  $\hat{\theta}$  is the posterior mode and

$$\mathbf{I}_{ij}(\boldsymbol{x}) = -\left[\frac{\partial^2}{\partial \theta_i \partial \theta_j} \log(p(\boldsymbol{x}|\theta)p(\theta))\right]_{\theta = \hat{\theta}}$$

## ANALYTIC APPROXIMATIONS

A Taylor series expansion gives

$$\log p(\theta|\boldsymbol{x}) = \log p(\hat{\theta}|\boldsymbol{x}) + \frac{1}{2}(\theta - \hat{\theta})' \left[ \frac{d^2}{d\theta^2} \log p(\theta|\boldsymbol{x}) \right]_{\theta = \hat{\theta}} (\theta - \hat{\theta}) + \dots$$

The first term in the Taylor expansion is a constant. The second term vanishes and the third term corresponds to the log of a normal density.

Approximation are usually improved by transforming the parameters to have support in  $\mathbb{R}$ . They are also improved by looking at marginal distributions or even conditional distributions. See Appendix B for the scheme of a proof.

### Counterexamples

There are a number of cases when a normal approximation would not work:

- Non identified parameters.
- Number of parameters increasing with sample size.
- Aliasing.
- Unbounded likelihoods.
- Improper posterior distributions.
- Prior distribution that exclude the MLE.
- $\hat{\theta}$  on the boundary of the domain.
- Tail of the distribution.

#### COMPUTATIONS

Obtaining the normal approximation for the posterior distribution requires: (a) transforming the parameters; (b) calculating the posterior mode. So we face an optimization problem. For parameter spaces of large dimension, this is can be a difficult problem in itself. For small to moderate dimensionality the method of choice is Newton's method.

Given an initial iterate  $\theta^0$ , we compute the sequence

$$\theta^{t} = \theta^{t-1} - \left[ \frac{d^{2}}{d\theta^{2}} \log p(\theta|\boldsymbol{x}) \right]_{\theta=\theta^{t-1}}^{-1} \left[ \nabla \log p(\theta|\boldsymbol{x}) \right]_{\theta=\theta^{t-1}}^{-1}$$

until convergence. Notice that scheme will provide both the estimate of the maximum and its covariance matrix.

Table 5.1 of Albert (2007) contains 20 pairs of observations, one for each of 20 cities. These correspond to  $(y_j, n_j)$  being the numbers of cancer deaths and the numbers at risk. The data are available from the R package LearnBayes.

An initial model is  $y_j \sim Bin(n_j, \theta_j)$ . From this we can fit a Bayesian model using a beta prior. With a uniform prior, the posterior mean of  $\theta_j$  would be  $(y_j + 1)/(n_j + 2)$ .

Note that in a binomial model

$$E(y_j) = n_j \theta_j$$
 and  $var(y_j) = n_j \theta_j (1 - \theta_j)$ .

So the variance depends on the mean.

If we clump the data together we have  $\hat{\theta} = 9.92 * 10^{-4}$ . This implies that the variance is estimated as 70.92. But an empirical estimate of the variance of  $Y = (y_1, \dots, y_{20})$  yields 141.94, twice as much.

Thus, the data show more dispersion than is obtained by fitting such a binomial model. Write he beta density as

$$p(\theta) = \frac{1}{B(\mu\tau, \tau(1-\mu))} \theta^{\mu\tau-1} (1-\theta)^{\tau(1-\mu)-1} \ \theta \in (0,1)$$

Here  $E(\theta) = \mu \in (0,1), \ \tau > 0$  and

$$B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)}$$

Using the beta prior and the binomial likelihood we obtain

$$p(y_j | \mu, \tau) = \binom{n_j}{y_j} \frac{B(\mu \tau + y_j, \tau(1 - \mu) + n_j - y_j)}{B(\mu \tau, \tau(1 - \mu))}$$

This is the marginal density of the observations. It depends of two parameters:  $\mu$  and  $\tau$ . We can use it as the likelihood for the data. Thus,

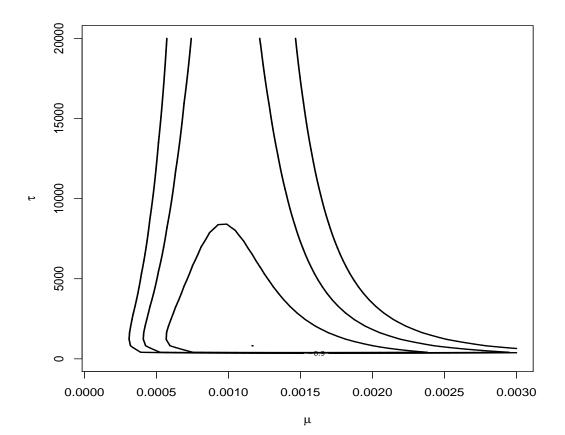
$$\prod_{j=1}^{20} \frac{B(\mu\tau + y_j, \tau(1-\mu) + n_j + y_j)}{B(\mu\tau, \tau(1-\mu))}$$

This is known as the beta-binomial model.

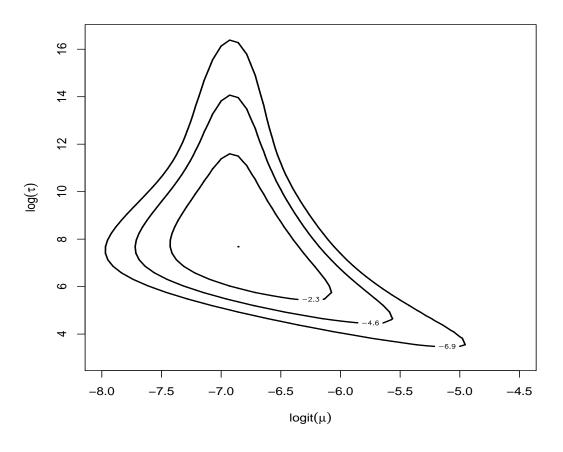
To complete the model we need to specify a prior for the two parameters  $\mu$  and  $\tau$ . We use the prior

$$p(\mu, \tau) \propto \frac{1}{\mu(1-\mu)} \frac{1}{(1+\tau)^2} \quad \mu \in (0, 1) \quad \tau > 0$$

Contour of the log-posterior of  $\mu$  and  $\tau$ .



Contour of the log-posterior of  $\theta_1 = \log\left(\frac{\mu}{1-\mu}\right)$  and  $\theta_2 = \log(\tau)$ .



Contour of the normal approximation to the 4 log-posterior of  $\theta_1$  and  $\theta_2$ . The mode is § 10 (-6.82, 7.57)and the covariance matrix is -7.5 -7.0 -6.5 -6.0 -5.5 -5.0 -4.5 $logit(\mu)$ 

#### APPROXIMATING WITH MIXTURES

If the posterior distribution is multimodal, suppose that  $\hat{\theta}_1, \dots, \hat{\theta}_K$  are the posterior modes, then the posterior can be approximated as

$$\sum_{k=1}^{K} \omega_k N(\hat{\theta}_k, \mathbf{I}_k(\boldsymbol{x}))$$

When the posterior modes are fairly widely separated, we use  $\omega_k = q(\hat{\theta}_k | \boldsymbol{x}), k = 1, \dots, K$ , where q is the un-normalized posterior density.

For small samples, a more conservative approximation is given by a mixture of Student densities:

$$\sum_{k=1}^{K} q(\hat{\theta}_k | \boldsymbol{x}) \left[ \alpha + (\theta - \hat{\theta}_k)' \mathbf{I}_k(\boldsymbol{x})^{-1} (\theta - \hat{\theta}_k) \right]^{-(d+\alpha)/2}$$

## LAPLACE APPROXIMATION

Laplace approximations are useful to approximate expressions of the form

$$\int_{\Theta} g(\theta) \exp\{-nh(\theta)\} d\theta$$

The approximation is given by

$$g(\hat{\theta})(2\pi/n)^{d/2}|\hat{\Sigma}|^{1/2}\exp\{-nh(\hat{\theta})\}, \quad \hat{\Sigma} = \left[\frac{\partial^2}{\partial\theta\partial\theta'}h(\theta)\right]_{\theta=\hat{\theta}}^{-1}$$

and  $\hat{\theta}$  is the value that minimizes h.

It can be seen that these approximations are  $o(n^{-1})$ .

### LAPLACE APPROXIMATION

For posterior inference we consider a non-negative  $g(\theta)$  and define

$$-nh(\theta) = \log(p(\boldsymbol{x}|\theta)) + \log(p(\theta))$$
 and  $nh^*(\theta) = nh(\theta) - \log(g(\theta))$ 

Denoting by  $\theta^*$  the value that minimizes  $h^*$  and  $\Sigma^*$  the corresponding matrix of second derivatives, we have that

$$E(g(\theta)) \approx \frac{g(\theta^*)|\Sigma^*|^{1/2} \exp\{-nh^*(\theta^*)\}}{|\hat{\Sigma}|^{1/2} \exp\{-nh(\hat{\theta})\}}$$

Due to cancellations between the numerator and denominator, this approximation is of order  $o(n^{-2})$ .