Chapter 4

- ▶ 4.1 Normal approximation (Laplace's method)
- ▶ 4.2 Large-sample theory
- ▶ 4.3 Counter examples
  - ▶ includes examples of difficult posteriors for MCMC, too
- ▶ 4.4 Frequency evaluation*
- ▶ 4.5 Other statistical methods*

Normal approximation (Laplace approximation)

▶ Often posterior converges to normal distribution when $n \to \infty$

▶ If posterior is unimodal and close to symmetric
  ▶ we can approximate $p(\theta|y)$ with normal distribution

$$p(\theta|y) \approx \frac{1}{\sqrt{2\pi}\sigma_\theta} \exp\left(-\frac{1}{2\sigma_\theta^2}(\theta - \hat{\theta})^2\right)$$

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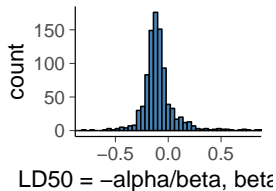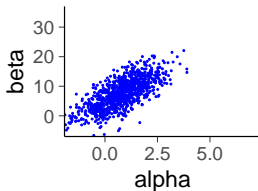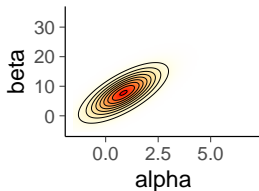$$p(\theta|y) \approx \frac{1}{\sqrt{2\pi}\sigma_\theta} \exp\left(-\frac{1}{2\sigma_\theta^2}(\theta - \hat{\theta})^2\right)$$

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  ▶ A most strict proof by LeCam in 1950's

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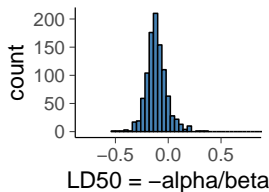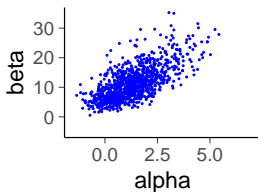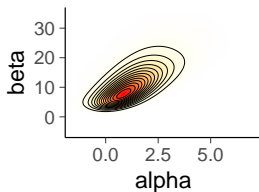
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$$f(\theta) = f(\hat{\theta}) + f'(\hat{\theta})(\theta - \hat{\theta}) + \frac{f''(\hat{\theta})}{2!}(\theta - \hat{\theta})^2 + \frac{f^{(3)}(\hat{\theta})}{3!}(\theta - \hat{\theta})^3 + \dots$$

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  ▶ if $\hat{\theta}$ is at mode, then $f'(\hat{\theta}) = 0$
  ▶ often when $n \to \infty$, $\frac{f^{(3)}(\hat{\theta})}{3!}(\theta - \hat{\theta})^3 + \dots$ is small

Multivariate Taylor series

▶ Multivariate series expansion

$$f(\theta) = f(\hat{\theta}) + \frac{df(\theta')}{d\theta'}\bigg|_{\theta'=\hat{\theta}}(\theta - \hat{\theta}) + \frac{1}{2!}(\theta-\hat{\theta})^T \frac{d^2 f(\theta')}{d\theta'^2}\bigg|_{\theta'=\hat{\theta}}(\theta-\hat{\theta}) + \dots$$
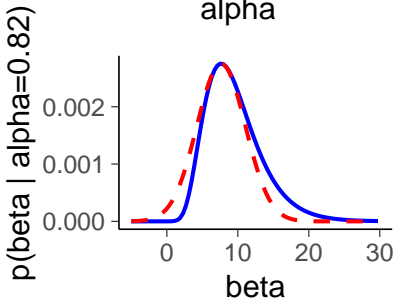
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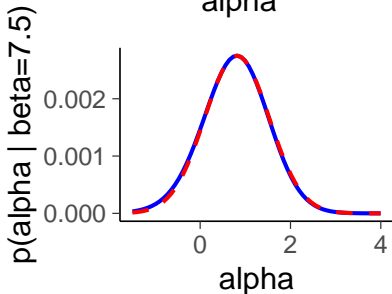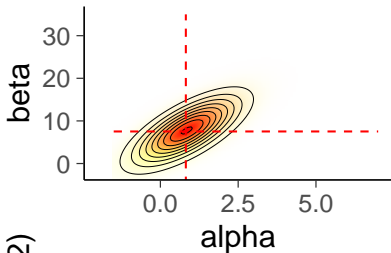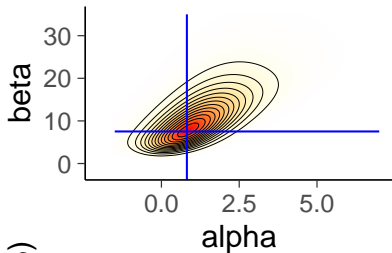
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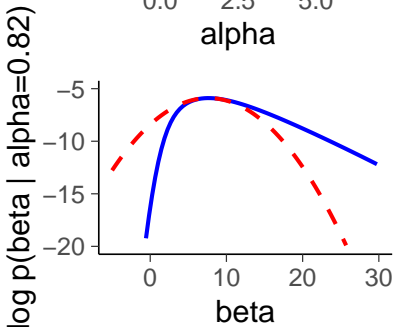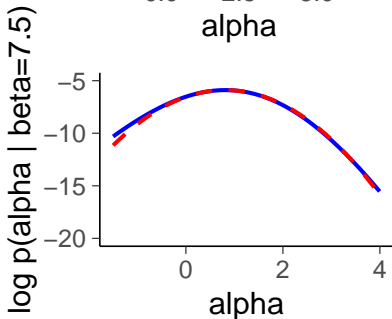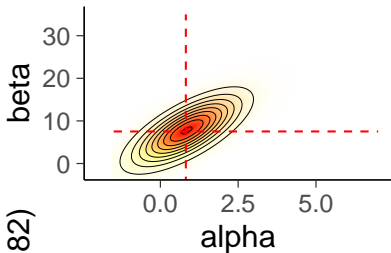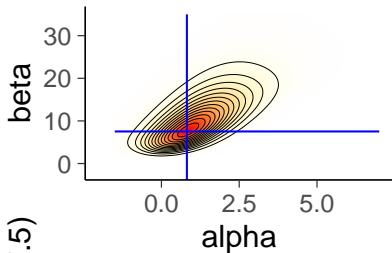
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▶ Normal approximation

$$p(\theta|y) \approx \mathrm{N}(\hat{\theta}, [I(\hat{\theta})]^{-1})$$

where $I(\theta)$ is called *observed information*

$$I(\theta) = -\frac{d^2}{d\theta^2} \log p(\theta|y)$$

Normal approximation

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  - $I(\hat{\theta})$ is the second derivatives at the mode and thus describes the curvature at the mode
  - if the mode is inside the parameter space, $I(\hat{\theta})$ is positive
  - if θ is a vector, then $I(\theta)$ is a matrix

Normal approximation

► BDA3 Ch 4 has an example where it is easy to compute first and second derivatives and there is easy analytic solution to find where the first derivatives are zero

Normal approximation – example

▶ Normal distribution, unknown mean and variance
  ▶ uniform prior $(\mu, \log \sigma)$
  ▶ normal approximation for the posterior of $(\mu, \log \sigma)$

$$\log p(\mu, \log \sigma | y) = \text{constant} - n \log \sigma - \frac{1}{2\sigma^2}[(n-1)s^2 + n(\bar{y} - \mu)^2]$$

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from which it is easy to compute the mode

$$(\hat{\mu}, \log \hat{\sigma}) = \left(\bar{y}, \frac{1}{2} \log \left(\frac{n-1}{n} s^2 \right) \right)$$

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$$
\frac{d^2}{d(\log \sigma)^2} \log p(\mu, \log \sigma | y) = -\frac{2}{\sigma^2}((n-1)s^2 + n(\bar{y} - \mu)^2)
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matrix of the second derivatives at $(\hat{\mu}, \log \hat{\sigma})$

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$$p(\mu, \log \sigma | y) \approx \mathsf{N} \left(\begin{pmatrix} \mu \\ \log \sigma \end{pmatrix} \middle| \begin{pmatrix} \bar{y} \\ \log \hat{\sigma} \end{pmatrix}, \begin{pmatrix} \hat{\sigma}^2/n & 0 \\ 0 & 1/(2n) \end{pmatrix} \right)$$

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  - ▶ e.g. in R, demo4_1.R:

```r
bioassayfun <- function(w, df) {
  z <- w[1] + w[2]*df$x
  -sum(df$y*(z) - df$n*log1p(exp(z)))
}

theta0 <- c(0,0)
optimres <- optim(w0, bioassayfun, gr=NULL, df1, hessian=T)
thetahat <- optimres$par
Sigma <- solve(optimres$hessian)
```

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    - ► second order autodiff coming to Stan

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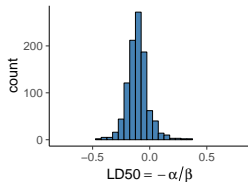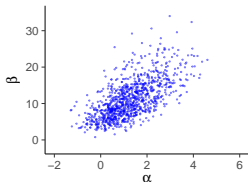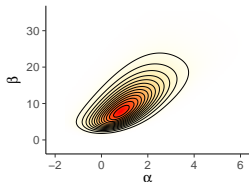- ▶ Accuracy can be improved by importance sampling (Ch 10)

Example: Importance sampling in Bioassay
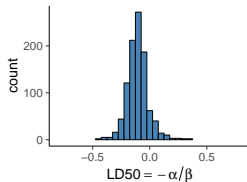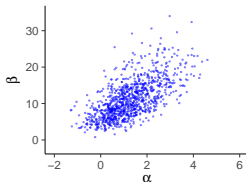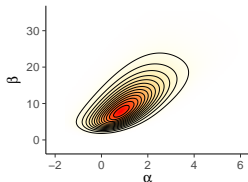
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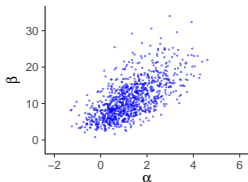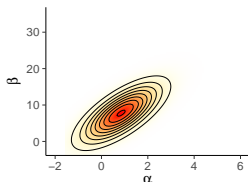
But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!
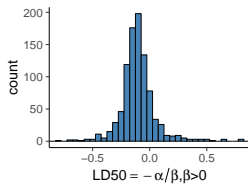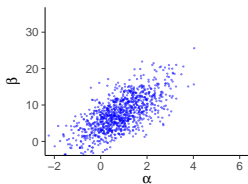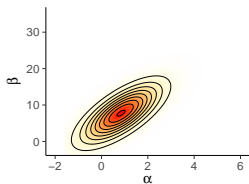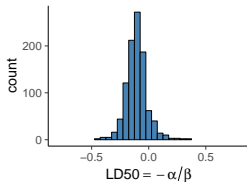
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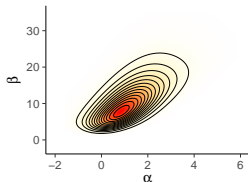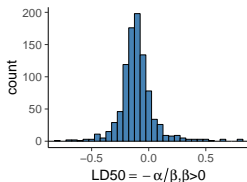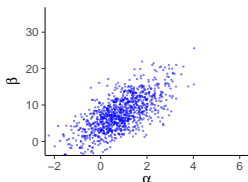
Example: Importance sampling in Bioassay
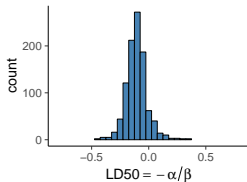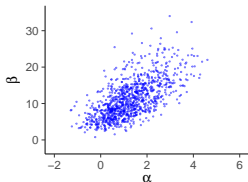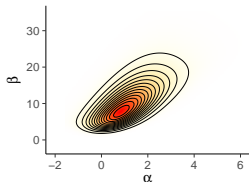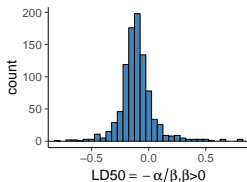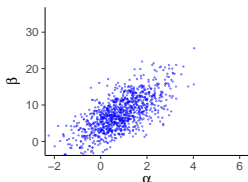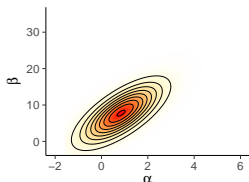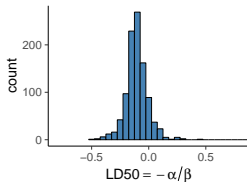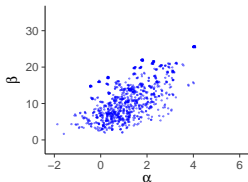
Grid sd(LD50) ≈ 0.1, IS sd(LD50) ≈ 0.1

Normal approximation

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- ▶ Pareto-k diagnostic of importance sampling weights can be used for diagnostic
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- ▶ RStanARM has an option `algorithm='optimizing'`
  - ▶ since version 2.19.2 (2019-10-03)
    - + Pareto-k diagnostic
    - + importance resampling (IR)

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▶ Other distributions can be used (e.g. *t*-distribution)
▶ Instead of mode and Hessian at mode, e.g.
  ▶ variational inference (Ch 13)
    ▶ CS-E4820 - Machine Learning: Advanced Probabilistic Methods
    ▶ Stan has an experimental ADVI algorithm
  ▶ expectation propagation (Ch 13)
  ▶ speed of these is usually between optimization and MCMC

Distributional approximations
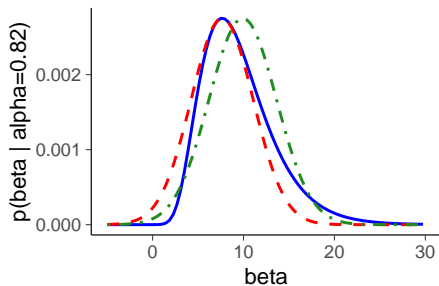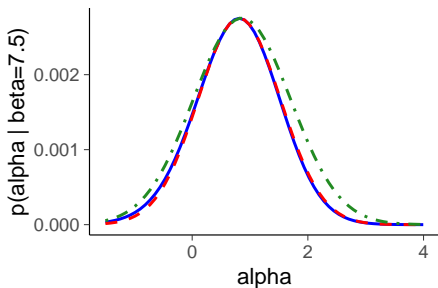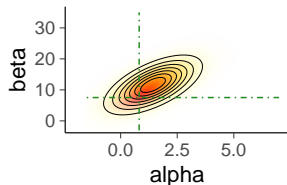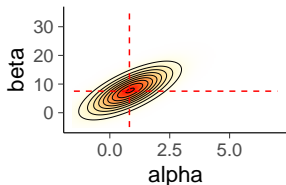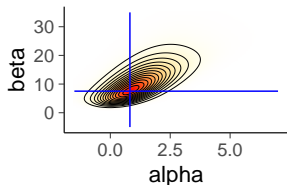
Exact, Normal at mode, Normal with variational inference

Distributional approximations

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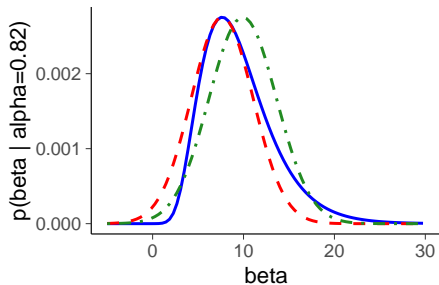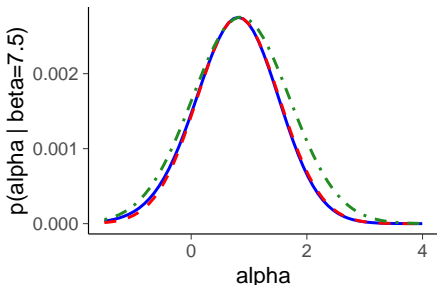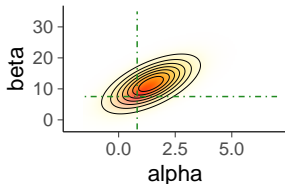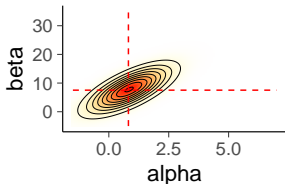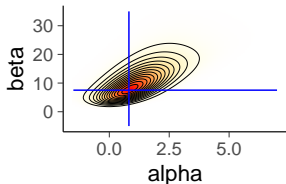
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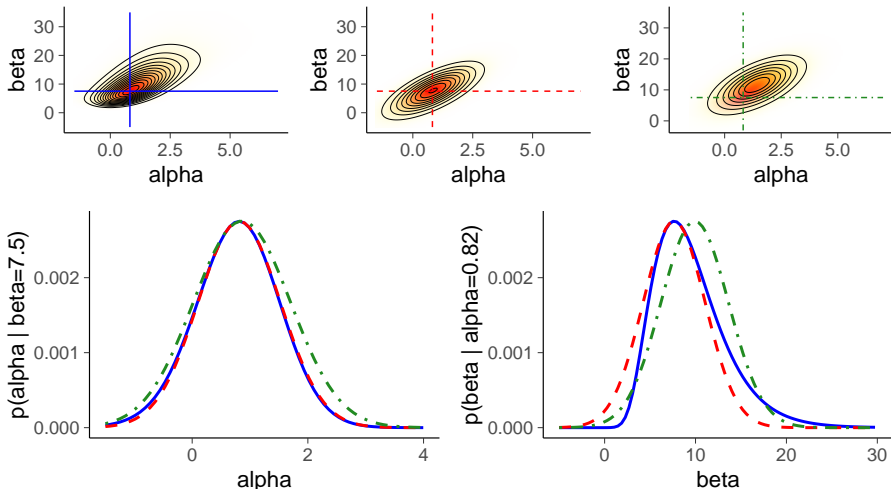
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Large sample theory

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    ▶ the higher order terms in Taylor series increase slower than the second order term
  ▶ see counter examples

Large sample theory

- ▶ Assume "true" underlying data distribution $f(y)$
    - ▶ observations $y_1, \ldots, y_n$ are independent samples from the joint distribution $f(y)$
    - ▶ "true" data distribution $f(y)$ is not always well defined
    - ▶ in the following we proceed as if there were true underlying data distribution
    - ▶ for the theory the exact form of $f(y)$ is not important as long at it has certain regularity conditions

Large sample theory

- ▶ Consistency
  - ▶ if true distribution is included in the parametric family, so that $f(y) = p(y|\theta_0)$ for some θ_0, then posterior converges to a point θ_0, when $n \to \infty$

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Large sample theory – counter examples

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- ▶ Problem also for other inference methods like MCMC

Large sample theory – counter examples

▶ If the number of parameter increases as the number of observation increases
  ▶ in some models number of parameters depends on the number of observations
  ▶ e.g. time series models $y_i \sim N(\theta_i, \sigma^2)$ and θ_i has prior in time
  ▶ posterior of θ_i does not converge to a point, if additional observations do not bring enough information

Large sample theory – counter examples

- ► Aliasing (FI: valetoisto)
    - ► special case of under-identifiability where likelihood repeats in separate points
    - ► e.g. mixture of normals

    $$p(y_i|\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \lambda) = \lambda \, \mathsf{N}(\mu_1, \sigma_1^2) + (1 - \lambda) \, \mathsf{N}(\mu_2, \sigma_2^2)$$

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- For MCMC makes the convergence diagnostics more difficult, as it is difficult to identify aliasing from other multimodality

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▶ Improper posterior
  ▶ asymptotic results assume that probability sums to 1
  ▶ e.g. Binomial model, with $\mathrm{Beta}(0, 0)$ prior and observation $y = n$
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- ▶ Should have a positive prior probability/density where needed

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  ▶ e.g. $y_i \sim N(\theta, 1)$ with a restriction $\theta \geq 0$ and assume that $\theta_0 = 0$
    ▶ posterior of θ is left truncated normal distribution with $\mu = \bar{y}$
    ▶ in the limit $n \to \infty$ posterior is half normal distribution
▶ Can be easy or difficult for MCMC

Large sample theory – counter examples

- ► Tails of the distribution
    - ► normal approximation may be accurate for the most of the posterior mass, but still be inaccurate for the tails
    - ► e.g. parameter which is constrained to be positive; given a finite *n*, normal approximation assumes non-zero probability for negative values

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    - ► Calibration
        - ► α%-posterior interval has the true value in α% cases
        - ► α%-predictive interval has the true future values in α% cases
        - ► approximate calibration with shorter intervals for likely true values more important than exact calibration with bad intervals for all possible values.