

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 $n \rightarrow \infty$
- 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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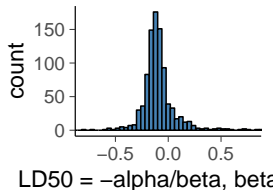
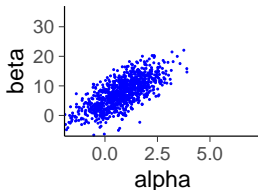
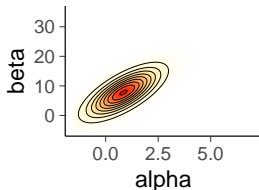
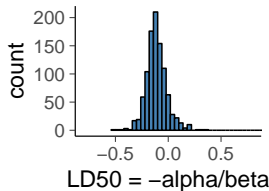
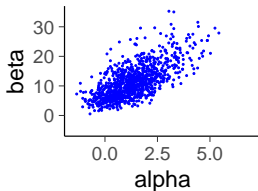
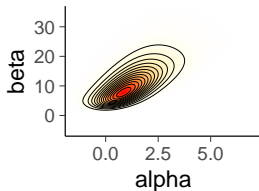
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- A most strict proof by LeCam in 1950's

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

Multivariate Taylor series

- Multivariate series expansion

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

Normal approximation

- Taylor series expansion of the log posterior around the posterior mode $\hat{\theta}$

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Normal approximation

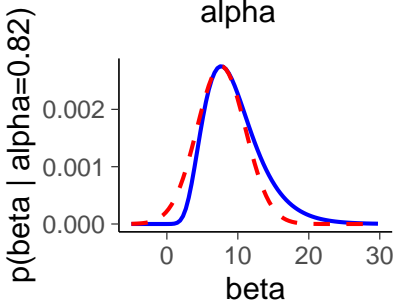
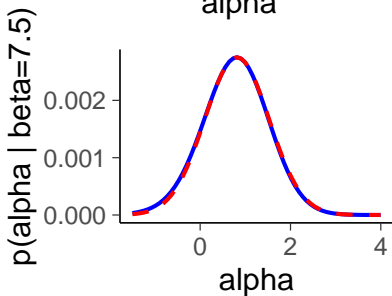
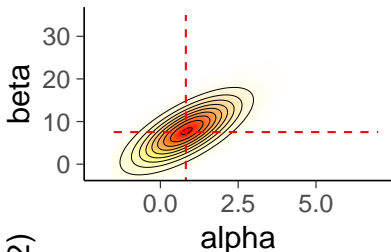
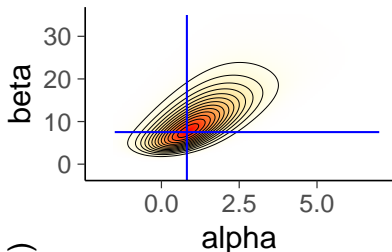
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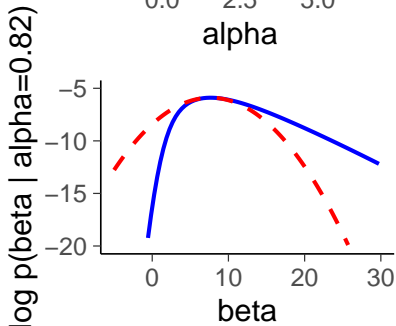
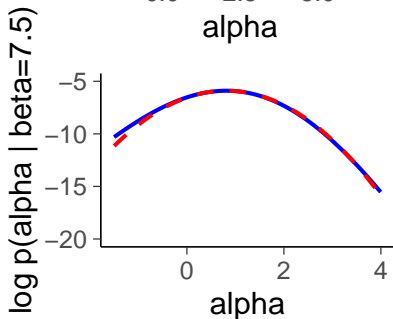
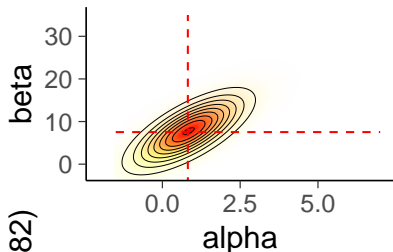
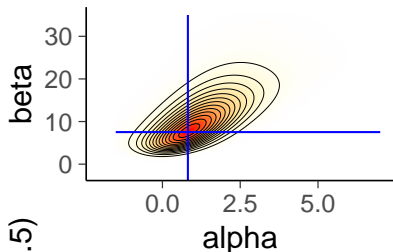
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- Normal approximation

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

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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matrix of the second derivatives at $(\hat{\mu}, \log \hat{\sigma})$

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normal approximation

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

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 - e.g. in R, demo4_1.R:

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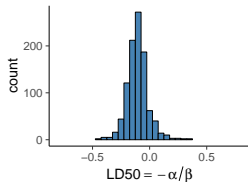
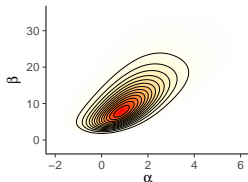
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- Accuracy can be improved by importance sampling (Ch 10)

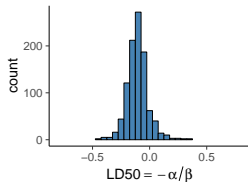
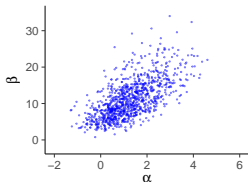
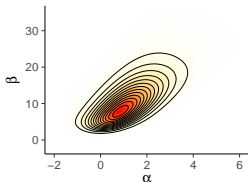
Example: Importance sampling in Bioassay

Grid

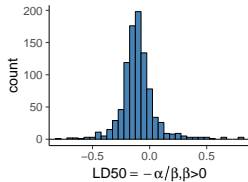
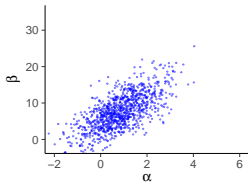
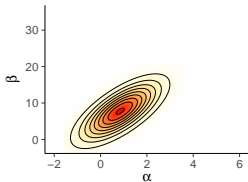


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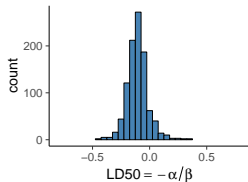
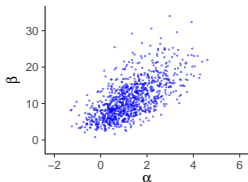
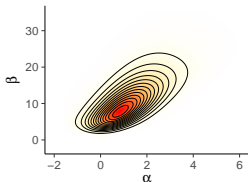


Normal

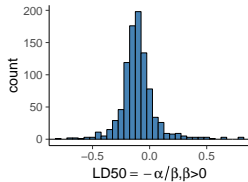
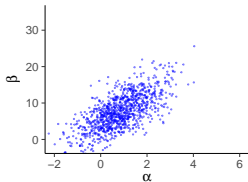
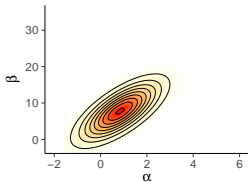


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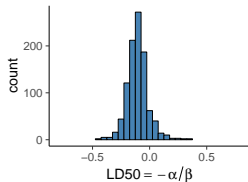
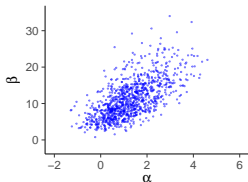
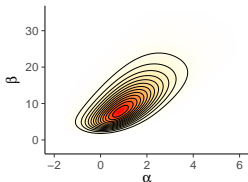


But the normal approximation is not that good here:

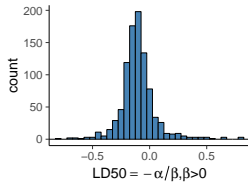
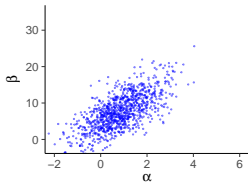
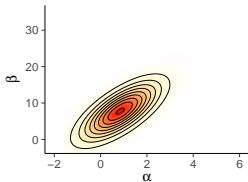
Grid $sd(LD50) \approx 0.1$, Normal $sd(LD50) \approx .75!$

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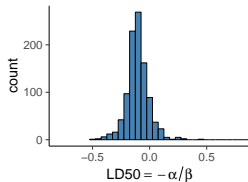
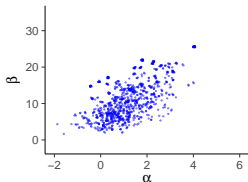
Grid



Normal

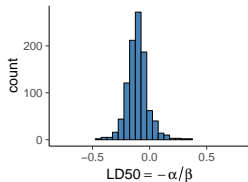
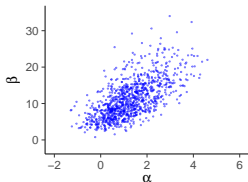
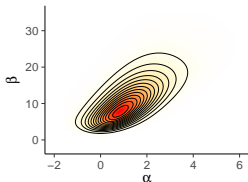


IS

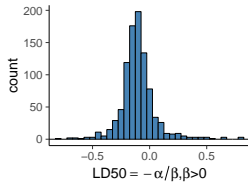
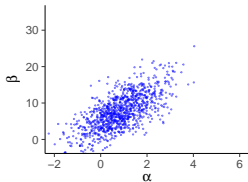
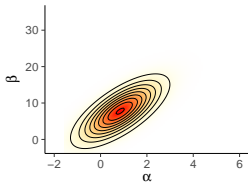


Example: Importance sampling in Bioassay

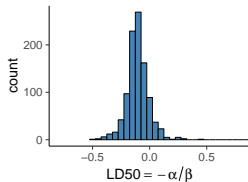
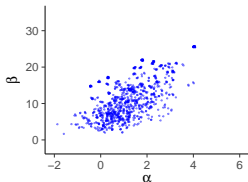
Grid



Normal



IS



Grid $sd(LD50) \approx 0.1$, IS $sd(LD50) \approx 0.1$

Normal approximation

- Accuracy can be improved by importance sampling
- Pareto- k diagnostic of importance sampling weights can be used for diagnostic
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 - in Bioassay example $k = 0.57$, which is ok
- RStanARM has an option `algorithm='optimizing'`
 - since version 2.19.2 (2019-10-03)
 - + Pareto- k diagnostic
 - + importance resampling (IR)

Other distributional approximations*

- Higher order derivatives at the mode can be used

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- Split-normal and split- t by Geweke use additional scaling along different principal axes

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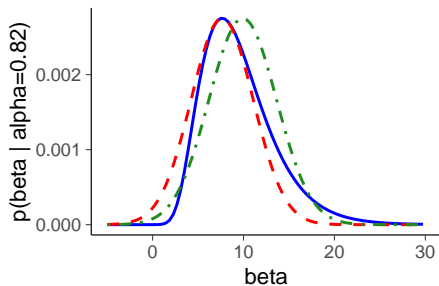
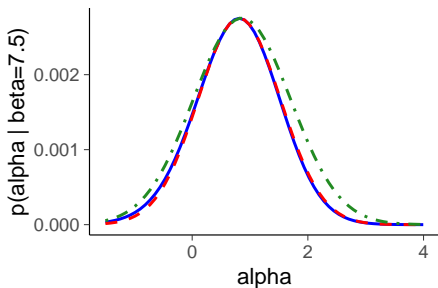
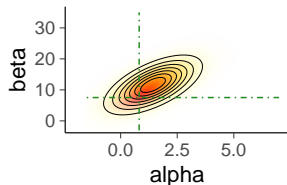
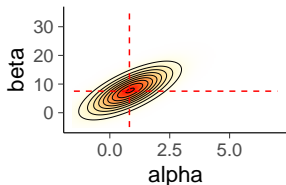
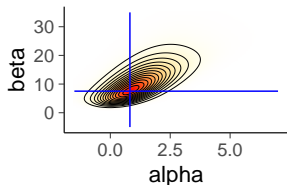
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- Higher order derivatives at the mode can be used
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- Other distributions can be used (e.g. t -distribution)
- Instead of mode and Hessian at mode, e.g.
 - variational inference (Ch 13)
 - CS-E4820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

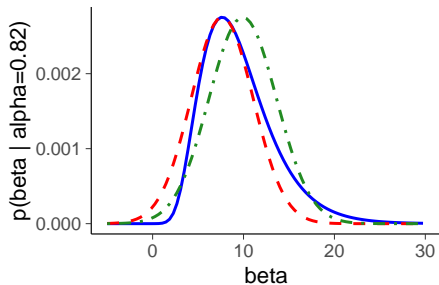
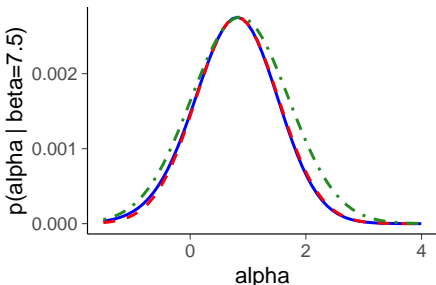
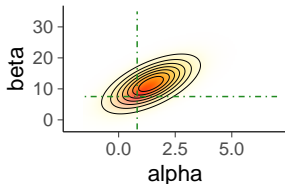
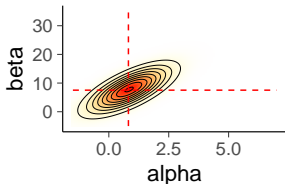
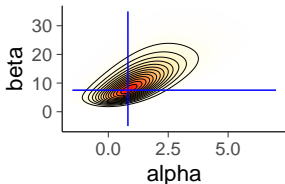
Distributional approximations

Exact, Normal at mode, Normal with variational inference



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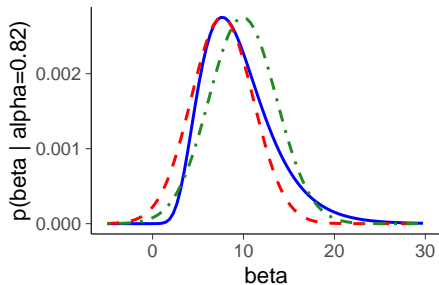
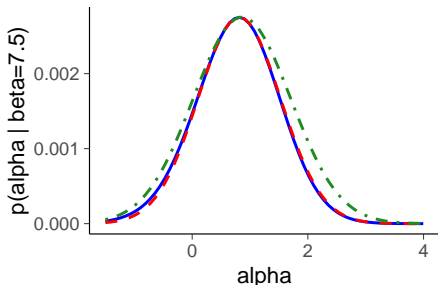
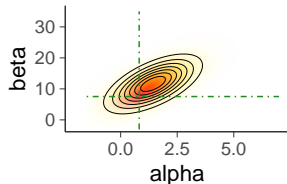
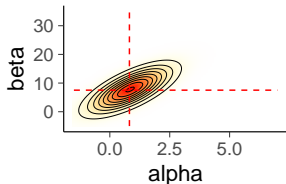
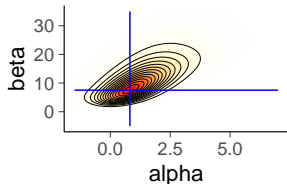
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Large sample theory

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 - see counter examples

Large sample theory

- Assume "true" underlying data distribution $f(y)$
 - observations y_1, \dots, 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 as it has certain regularity conditions

Large sample theory

- Consistency
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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

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

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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 $\text{Beta}(0, 0)$ prior and observation $y = n$
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- Should have a positive prior probability/density where needed

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- Convergence point at the edge of the parameter space
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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 $n \rightarrow \infty$ 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
 - $\alpha\%$ -posterior interval has the true value in $\alpha\%$ cases
 - $\alpha\%$ -predictive interval has the true future values in $\alpha\%$ cases
 - approximate calibration with shorter intervals for likely true values more important than exact calibration with bad intervals for all possible values.