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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  - A most strict proof by LeCam in 1950's

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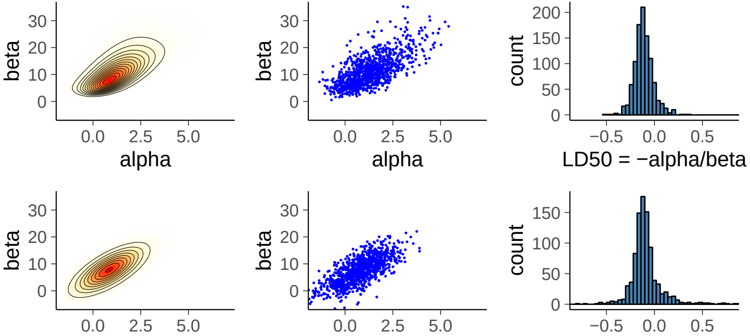

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  - often when $n \to \infty$, $\frac{f^{(3)}(\hat{\theta})}{3!}(\theta - \hat{\theta})^3 + \ldots$ is small

Multivariate Taylor series

- Multivariate series expansion

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

Normal approximation

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

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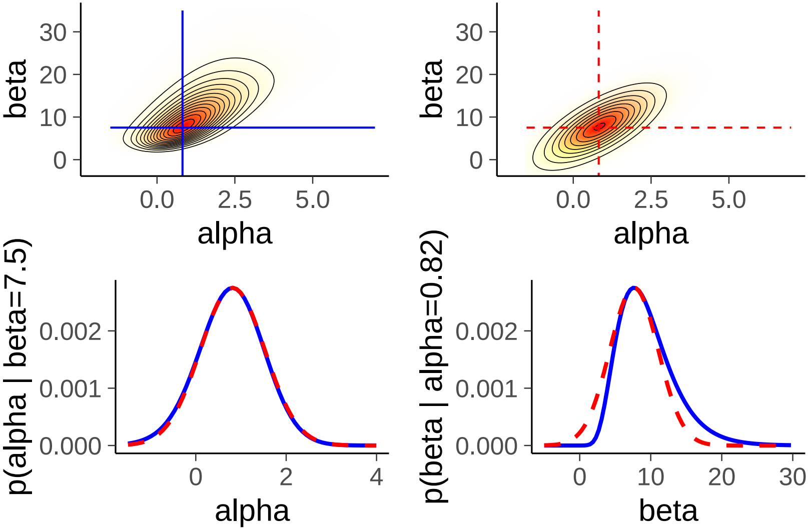

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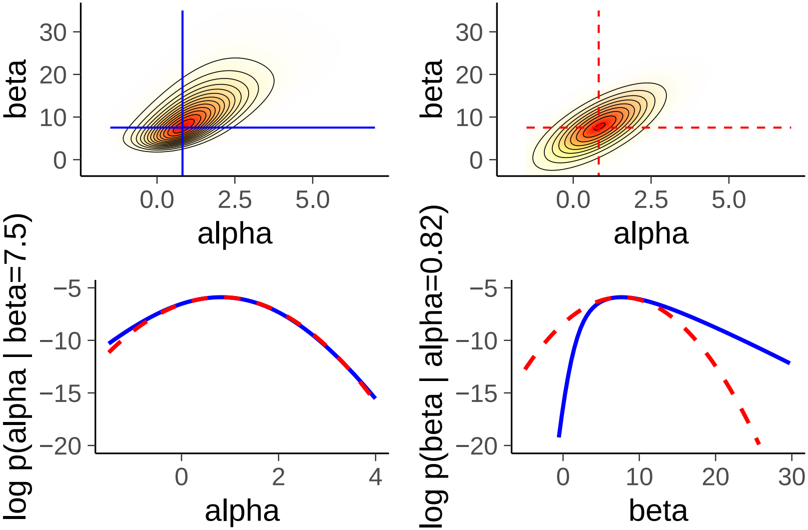

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- Normal approximation

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

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

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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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\end{aligned}$$

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 – example

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  posterior mode

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  normal approximation

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

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  - iterative optimization to find a mode (maye use gradients)
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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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    - second order autodiff coming to Stan

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- In some cases accuracy for a conditional distribution is sufficient (Ch 13)
  - e.g. Gaussian latent variable models, such as Gaussian processes (Ch 21)
    - CS-E4070 - Special Course in Machine Learning and Data Science: Gaussian processes - theory and applications

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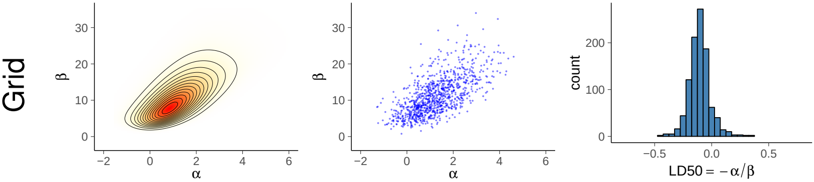
  - e.g. Gaussian latent variable models, such as Gaussian processes (Ch 21)
    - CS-E4070 - Special Course in Machine Learning and Data Science: Gaussian processes - theory and applications
- Accuracy can be improved by importance sampling (Ch 10)

Example: Importance sampling in Bioassay



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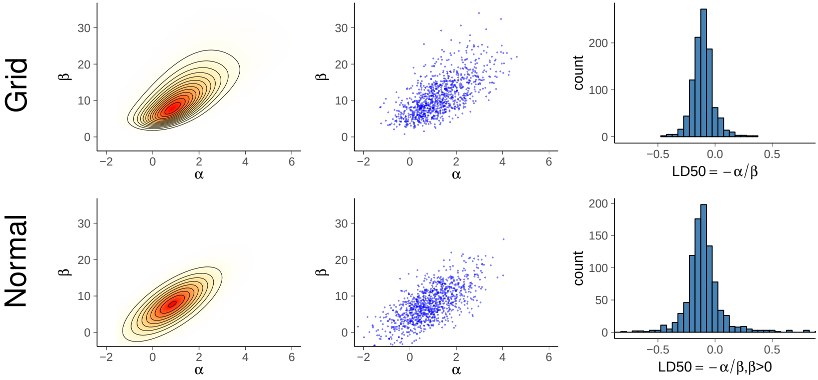

Normal approximation is discussed more in BDA3 Ch 4

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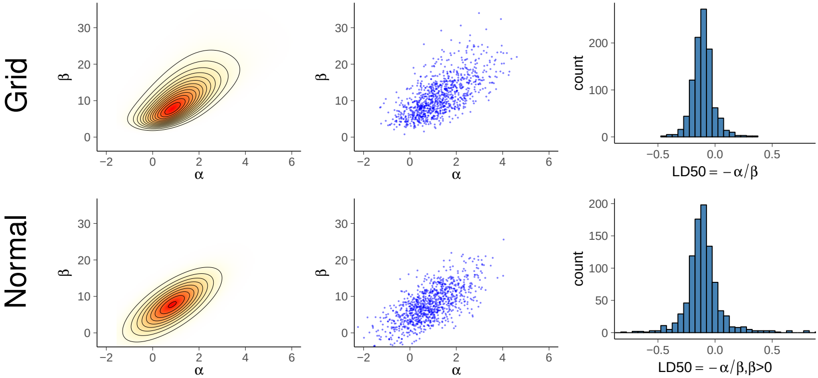

Normal approximation is discussed more in BDA3 Ch 4
But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

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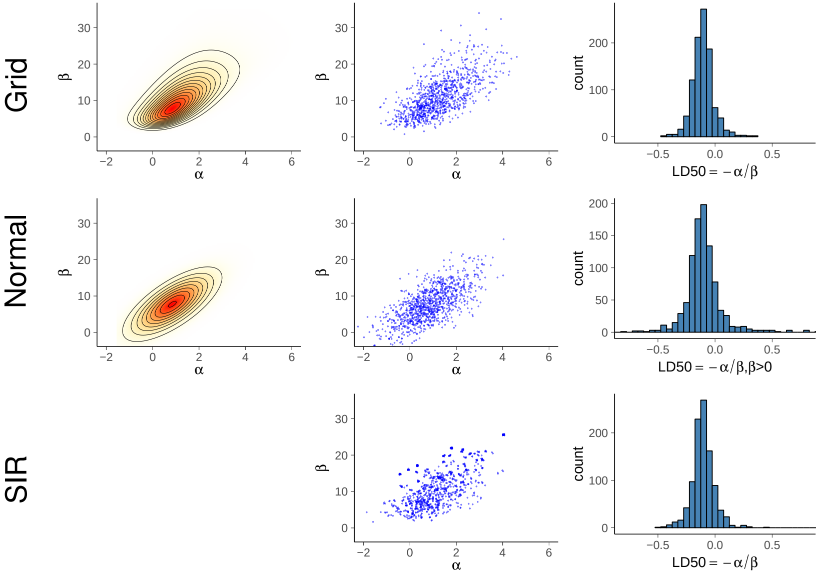

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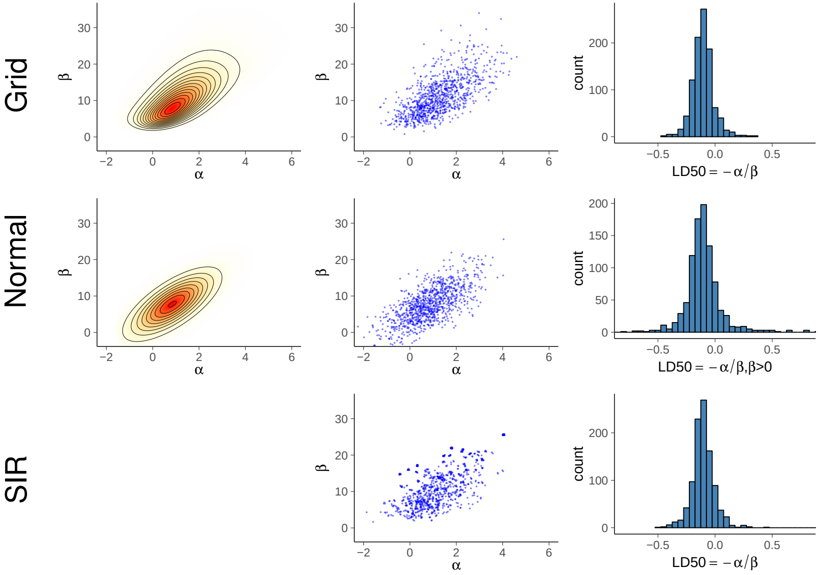

Grid sd(LD50) $\approx$ 0.1, SIR sd(LD50) $\approx$ 0.1

Normal approximation

- Accuracy can be improved by importance sampling
- Pareto-k diagnostic of importance sampling weights can be used for diagnostic
    - in Bioassay example $k = 0.57$, which is ok

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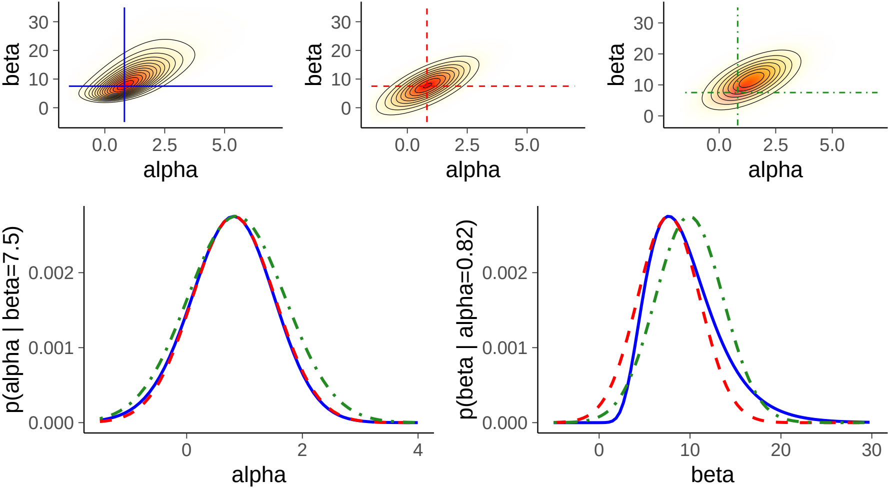
- Split-normal and split-*t* by Geweke use additional scaling along different principal axes
- Other distributions can be used
- Instead of mode and Hessian at mode, e.g.
    - variational inference (Ch 13)
        - CS-E4820 - Machine Learning: Advanced Probabilistic Methods
        - Stan has an experimental 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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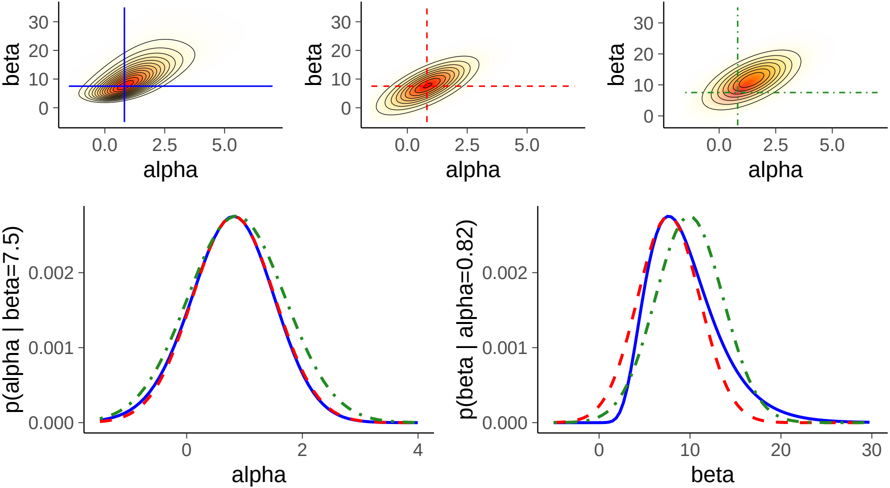

Grid sd(LD50) ≈ 0.090,
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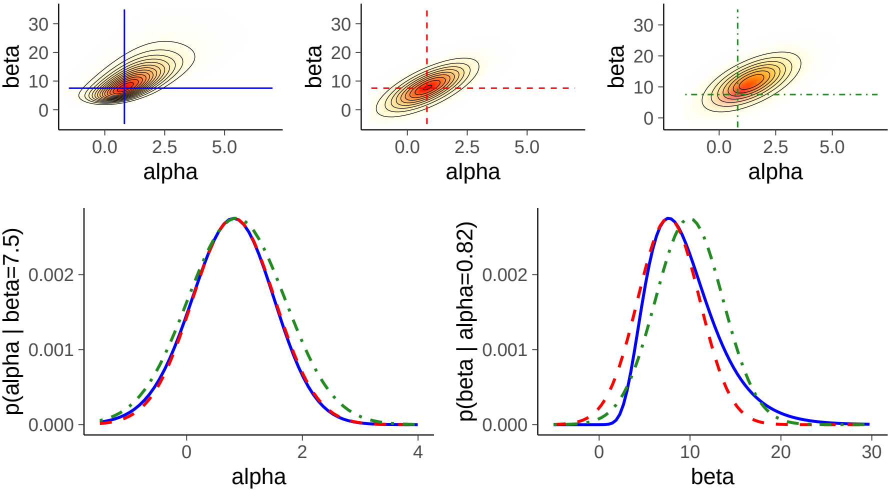

Grid sd(LD50) $\approx$ 0.090,
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VI sd(LD50) $\approx$ 0.13, VI + SIR sd(LD50) $\approx$ 0.095 (Pareto-k = 0.17)

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  - 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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- If true distribution is not included in the parametric family, then there is no true θ_0
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Large sample theory – counter examples

- Under- and non-identifiability
  - a model is under-identifiable, if the model has parameters or parameter combinations for which there is no information in the data
  - then there is no single point θ_0 where posterior would converge

Large sample theory – counter examples

- Under- and non-identifiability
  - a model is under-identifiable, if the model has parameters or parameter combinations for which there is no information in the data
  - then there is no single point θ_0 where posterior would converge
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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 $y_i \sim \mathrm{N}(\theta_i, \sigma^2)$ 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

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

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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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  - note that a prior close to a prior allowing unbounded posterior may produce almost unbounded posterior

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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 $y = n$
        - posterior $p(\theta|n, 0) = \theta^{n-1}(1-\theta)^{-1}$
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  - if in discrete case $p(\theta_0) = 0$ or in continuous case $p(\theta) = 0$ in the neighborhood of θ_0, then the convergence results based on the dominance of the likelihood do not hold

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  - if in discrete case $p(\theta_0) = 0$ or in continuous case $p(\theta) = 0$ in the neighborhood of θ_0, then the convergence results based on the dominance of the likelihood do not hold
- Should have a positive prior probability/density where needed

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- Convergence point at the edge of the parameter space
  - if θ_0 is on the edge of the parameter space, Taylor series expansion has to be truncated, and normal approximation does not necessarily hold

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  - if θ_0 is on the edge of the parameter space, Taylor series expansion has to be truncated, and normal approximation does not necessarily hold
  - e.g. $y_i \sim \mathrm{N}(\theta, 1)$ 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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    - no other point estimate with smalle squared error
  - Calibration
    - α%-posterior interval has the true value in α% cases
    - α%-predictive interval has the true future values in α% cases