

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)

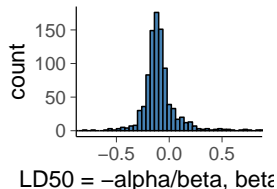
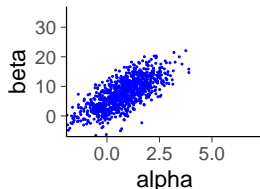
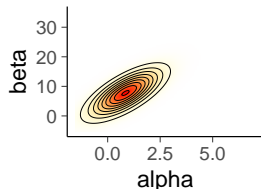
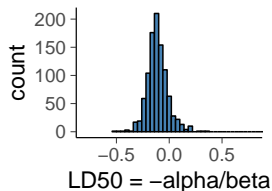
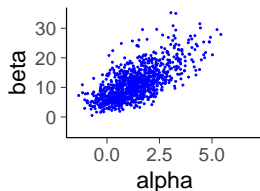
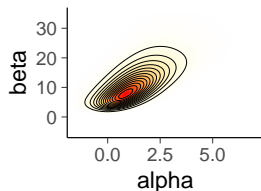
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 - we can then approximate $p(\theta|y)$ with normal distribution

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 - Laplace used this (before Gauss) to approximate the posterior of binomial model to infer ratio of girls and boys born

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Taylor series

- 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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- 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

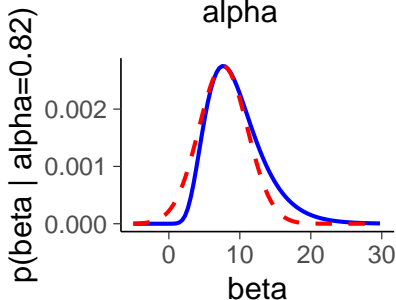
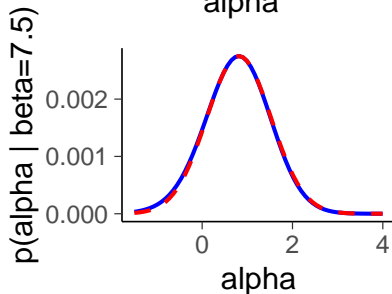
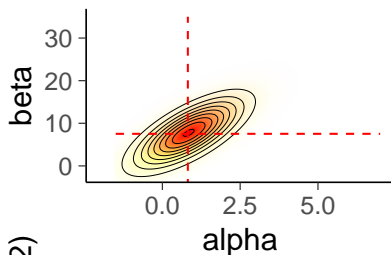
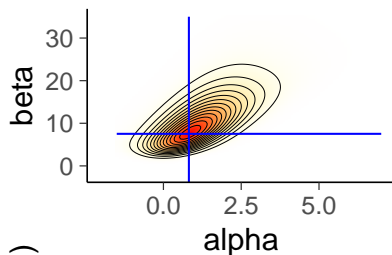
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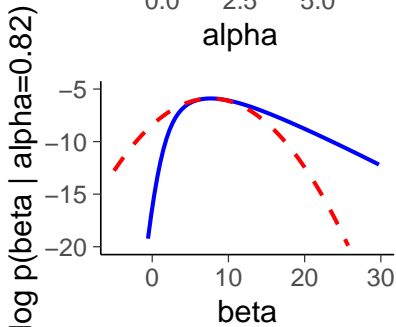
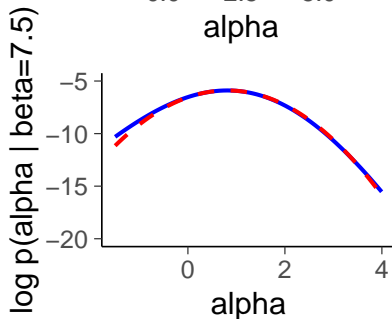
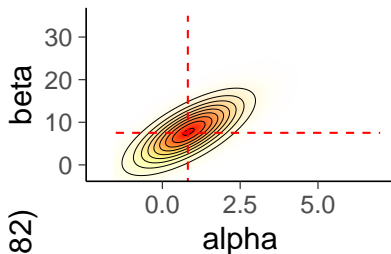
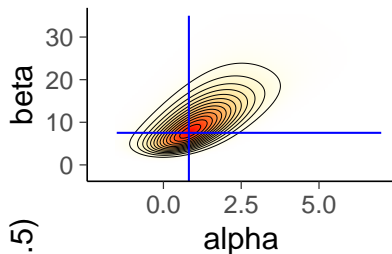
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$$\text{Hessian } H(\theta) = -I(\theta)$$

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

- $I(\hat{\theta})$ 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

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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, hessi  
thetahat <- optimres$par  
Sigma <- solve(optimres$hessian)
```

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 - second order autodiff in progress

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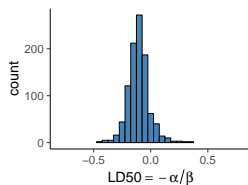
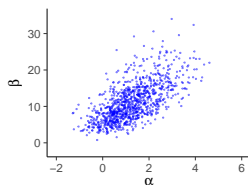
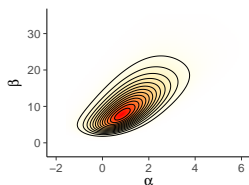
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- In some cases accuracy for a conditional distribution is sufficient (Ch 13)
 - e.g. Gaussian latent variable models, such as Gaussian processes (Ch 21) and Gaussian Markov random fields
 - Rasmussen & Williams: Gaussian Processes for Machine Learning
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- Accuracy can be improved by importance sampling (Ch 10)

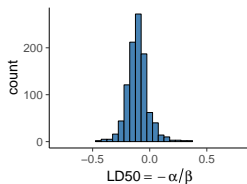
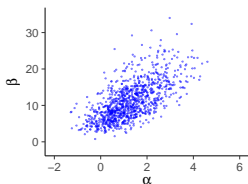
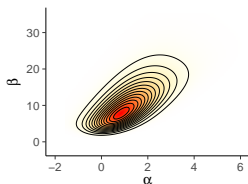
Example: Importance sampling in Bioassay

Grid

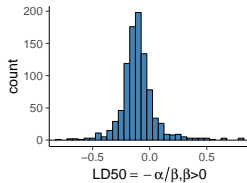
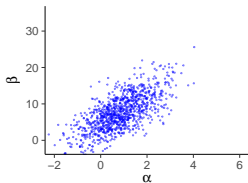
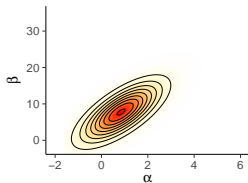


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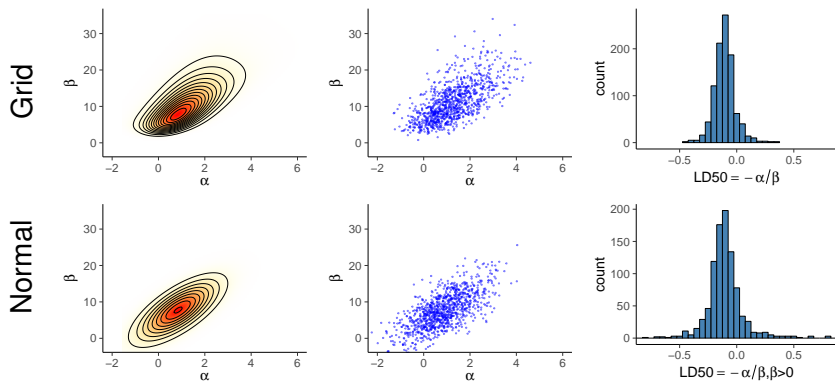
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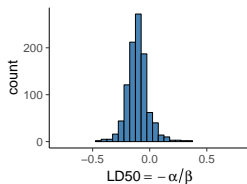
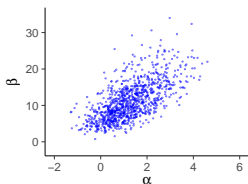
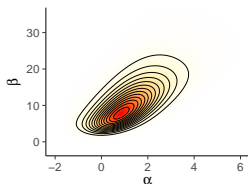


But the normal approximation is not that good here:

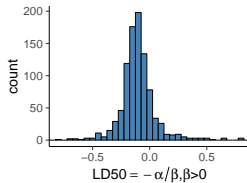
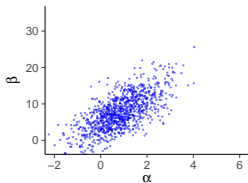
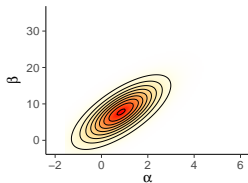
Grid $sd(LD50) \approx 0.1$, Normal $sd(LD50) \approx .75$!

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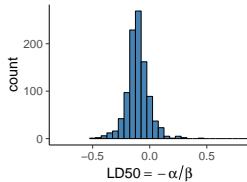
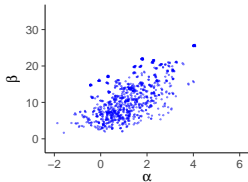
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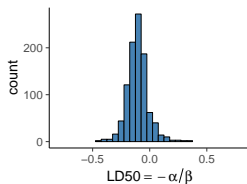
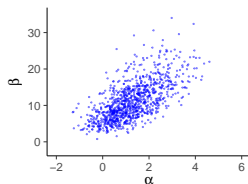
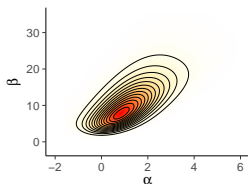


IS

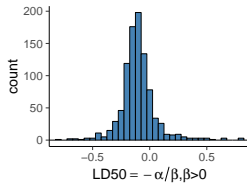
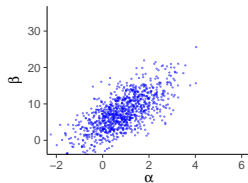
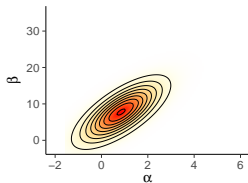


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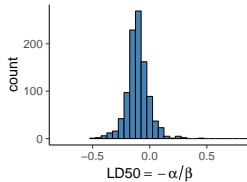
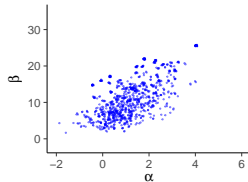
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Normal approximation

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 - in Bioassay example $k = 0.57$, which is ok
- CmdStan(R) has Laplace algorithm
 - since version 2.33 (2023)
 - + Pareto- k diagnostic via posterior package
 - + importance resampling (IR) via posterior package

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Normal approximation and parameter transformations

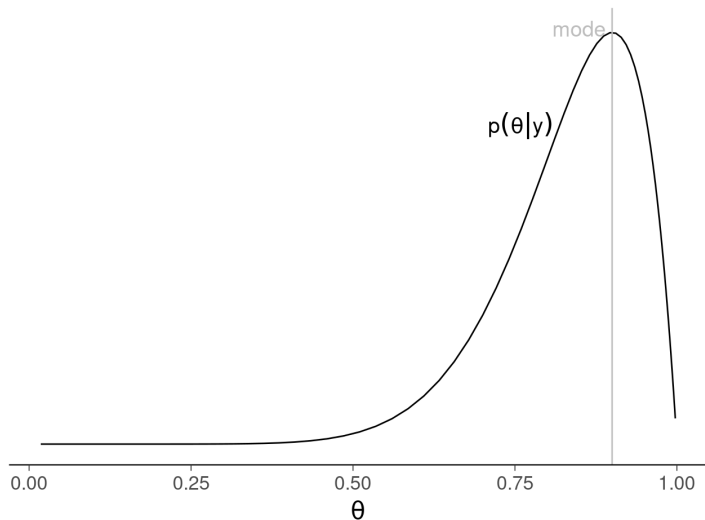
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 - density of the transformed parameter needs to include Jacobian of the transformation (BDA3 p. 21)

Normal approximation and parameter transformations

Binomial model $y \sim \text{Bin}(\theta, N)$, with data $y = 9, N = 10$

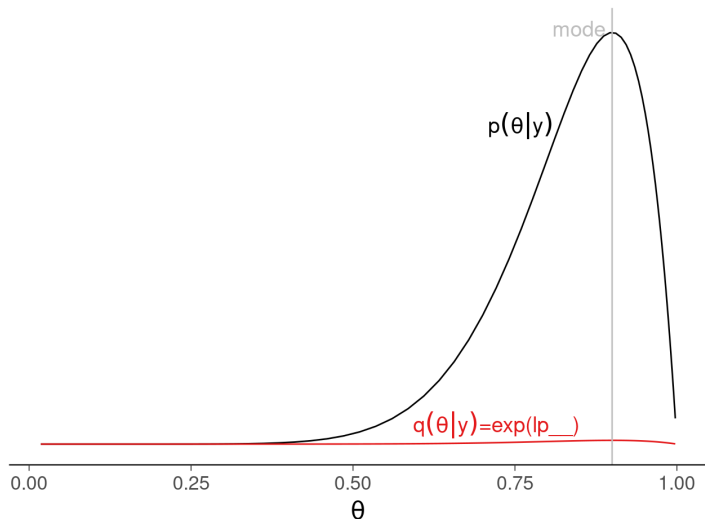
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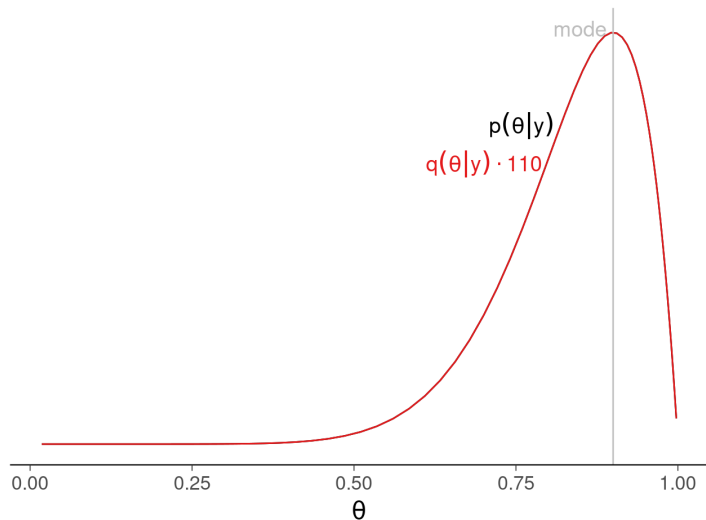
Stan computes only the unnormalized posterior $q(\theta|y)$



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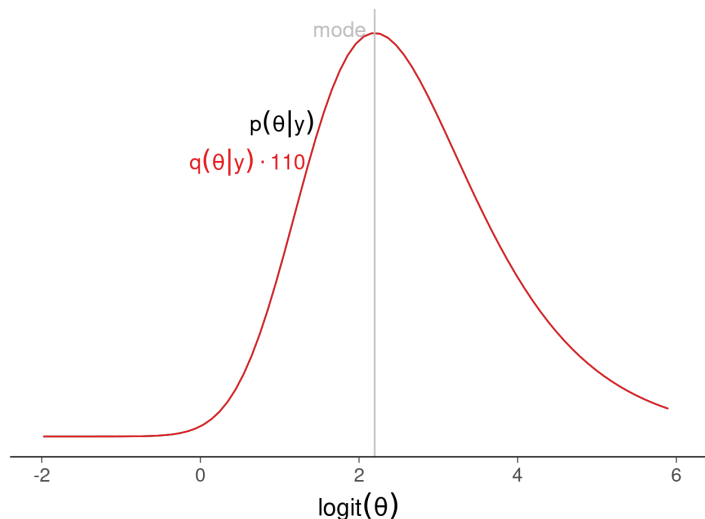
For illustration purposes we normalize Stan result $q(\theta|y)$



Normal approximation and parameter transformations

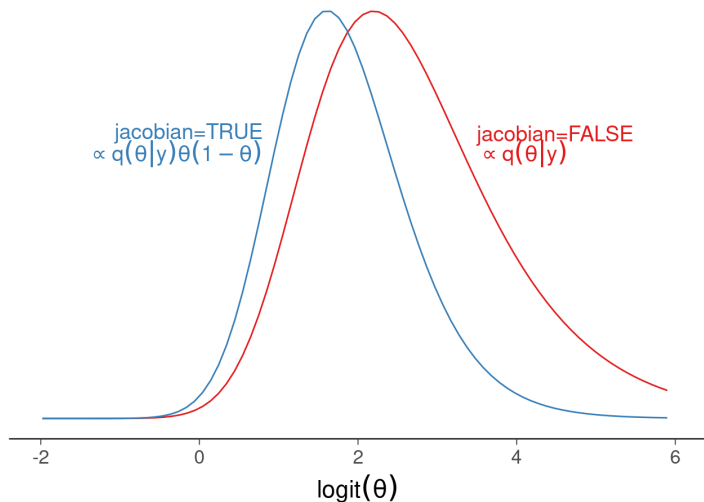
With $\text{Beta}(1, 1)$ prior, the posterior is $\text{Beta}(9 + 1, 1 + 1)$

$\text{Beta}(9 + 1, 1 + 1)$, but x-axis shows the unconstrained $\text{logit}(\theta)$



Normal approximation and parameter transformations

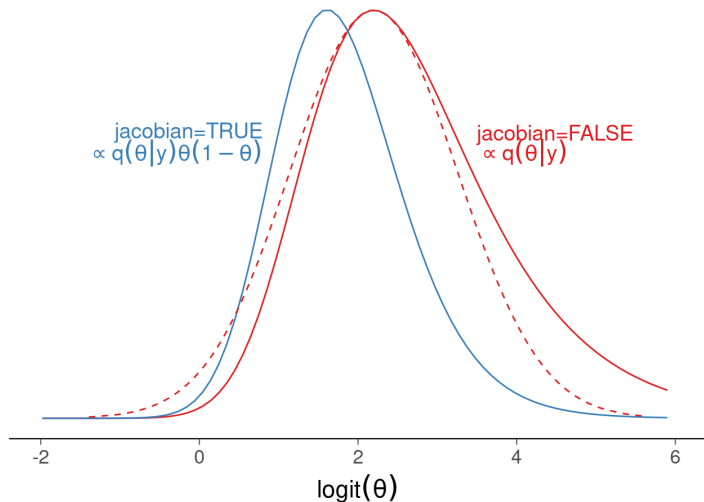
...but we need to take into account the absolute value of the determinant of the Jacobian of the transformation $\theta(1 - \theta)$



Normal approximation and parameter transformations

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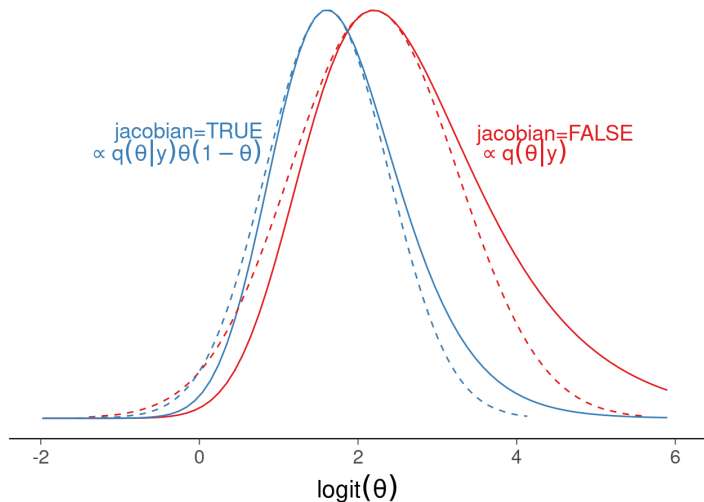
Let's compare a wrong normal approximation...



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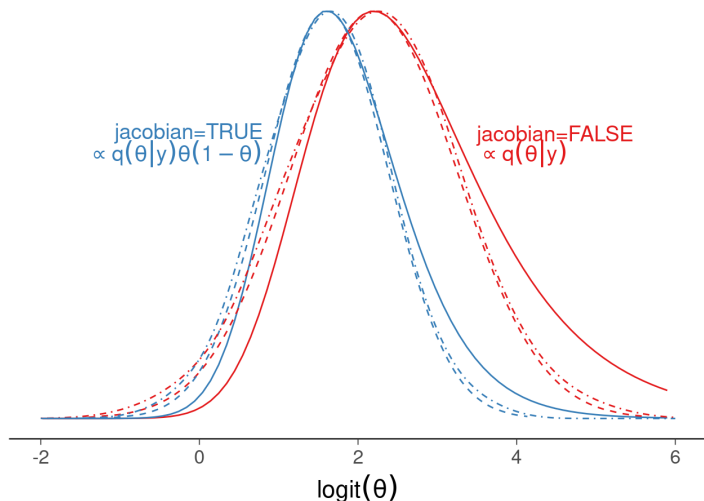
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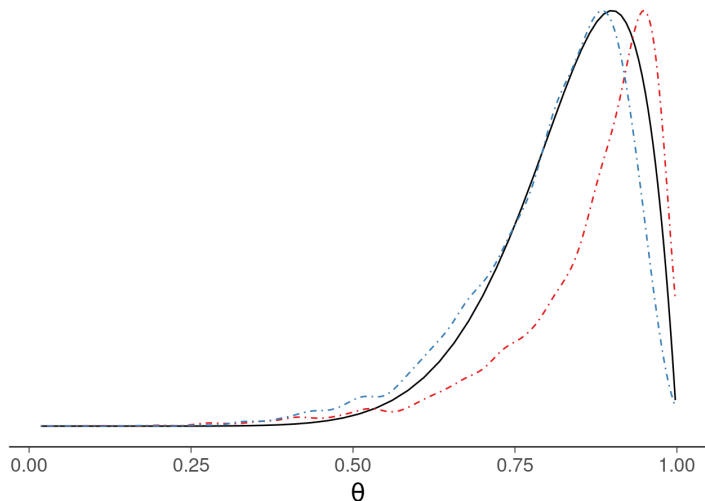
Sample from both approximations and show KDEs for draws



Normal approximation and parameter transformations

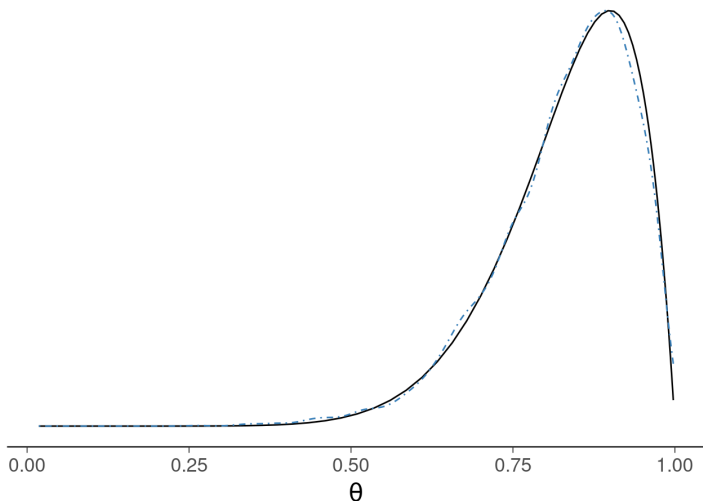
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Inverse transform draws and show KDEs



Normal approximation and parameter transformations

Laplace approximation can be further improved with importance resampling



Other distributional approximations

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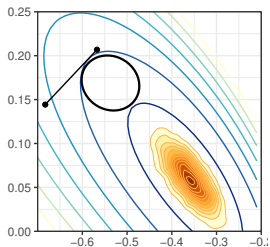
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- Other distributions can be used (e.g. t -distribution)

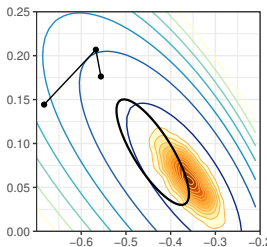
Other distributional approximations

- Higher order derivatives at the mode can be used
- Split-normal and split- t by Geweke (1989) use additional scaling along different principal axes
- 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
 - CS-E4895 - Gaussian Processes
 - Stan has the ADVI algorithm (not very good implementation)
 - Stan has Pathfinder algorithm (CmdStanR, brms)
 - instead of normal, methods with flexible flow transformations
 - expectation propagation (Ch 13)
 - speed of these is usually between optimization and MCMC
 - stochastic variational inference can be even slower than MCMC

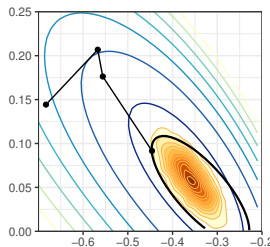
Pathfinder: Parallel quasi-Newton variational inference.



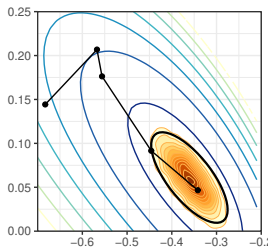
iteration 3
estimated ELBO: -340.5



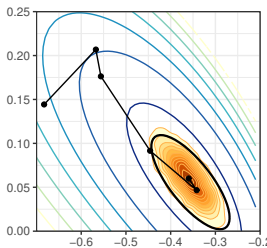
iteration 4
estimated ELBO: -332.2



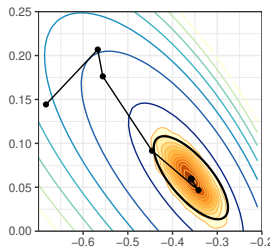
iteration 5
estimated ELBO: -329.7



iteration 6
estimated ELBO: -329.6



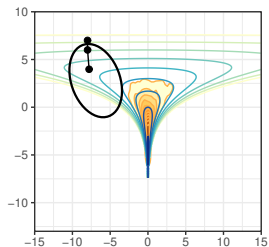
iteration 7
estimated ELBO: -329.6



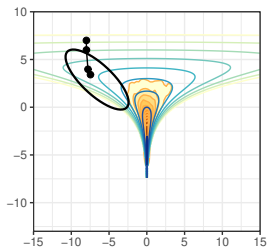
iteration 8
estimated ELBO: -329.7

Zhang, Carpenter, Gelman, and Vehtari (2022). Pathfinder: Parallel quasi-Newton variational inference. *Journal of Machine Learning Research*, 23(306):1–49.

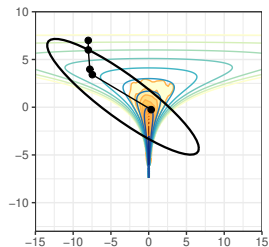
Pathfinder: Parallel quasi-Newton variational inference.



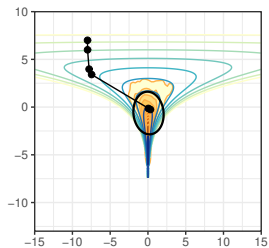
iteration 3
estimated ELBO: -4.3



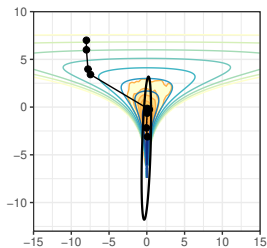
iteration 4
estimated ELBO: -0.4



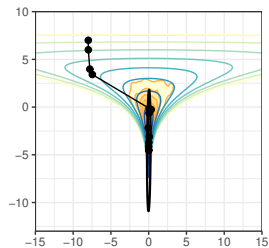
iteration 5
estimated ELBO: -132.1



iteration 6
estimated ELBO: 1.4



iteration 9
estimated ELBO: -579.9



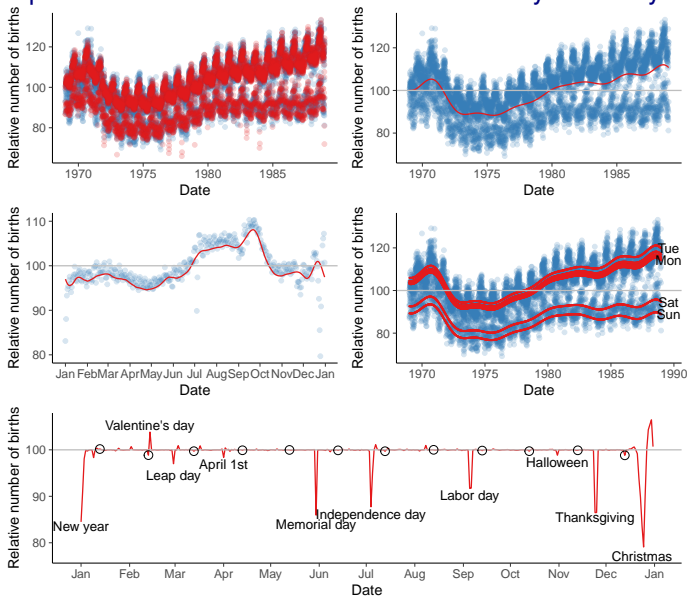
iteration 13
estimated ELBO: -5.7

Zhang, Carpenter, Gelman, and Vehtari (2022). Pathfinder: Parallel quasi-Newton variational inference. *Journal of Machine Learning Research*, 23(306):1–49.

Pathfinder: Parallel quasi-Newton variational inference.

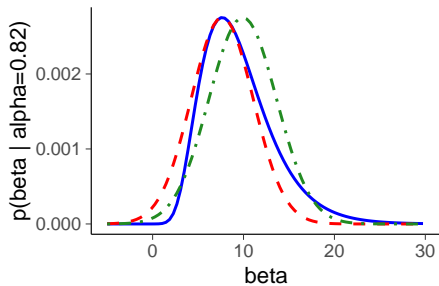
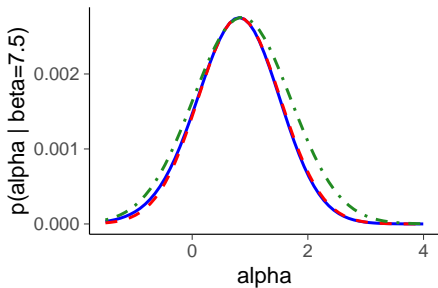
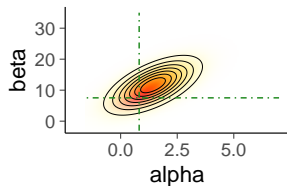
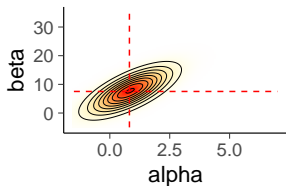
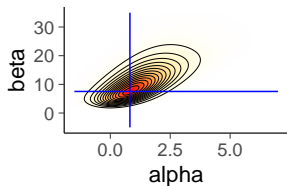
Birthdays case study uses Pathfinder to speed up workflow

<https://users.aalto.fi/~ave/casestudies/Birthdays/birthdays.html>



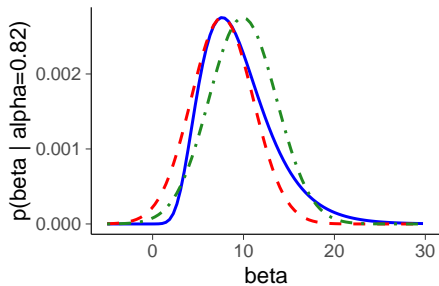
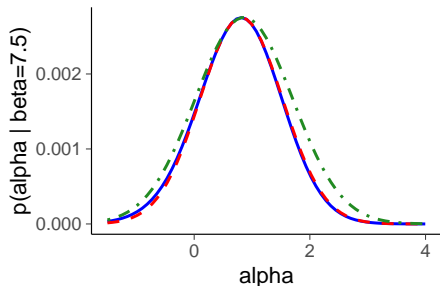
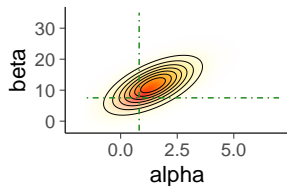
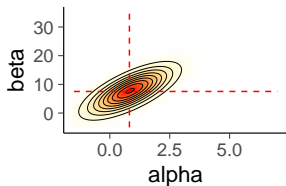
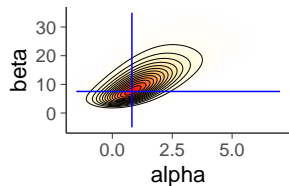
Distributional approximations

Exact, Normal at mode, Normal with variational inference



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Exact, Normal at mode, Normal with variational inference

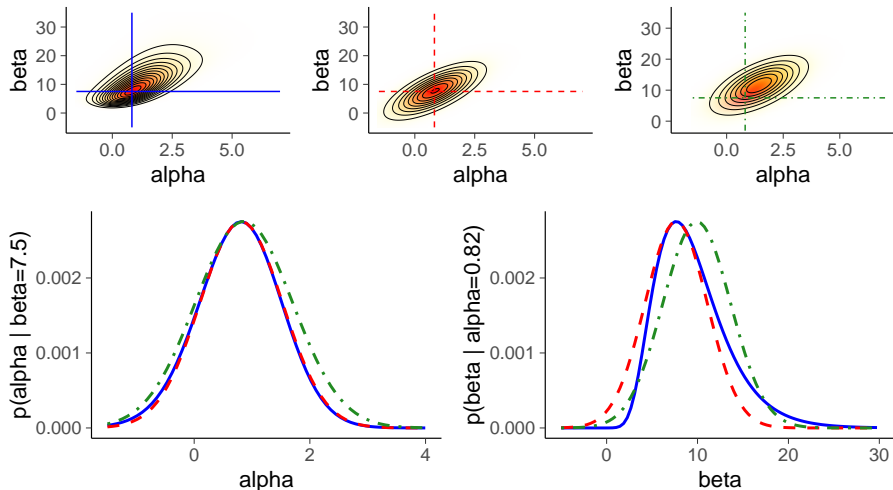


Grid $\text{sd}(\text{LD50}) \approx 0.090$,

Normal $\text{sd}(\text{LD50}) \approx .75$, Normal + IR $\text{sd}(\text{LD50}) \approx 0.096$ (Pareto- $k = 0.57$)

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VI $\text{sd}(\text{LD50}) \approx 0.13$, VI + IR $\text{sd}(\text{LD50}) \approx 0.095$ (Pareto- $k = 0.17$)

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 - with increasing number of posterior dimensions, the stochastic divergence estimate gets worse and flows have problems, too (Dhaka, Catalina, Andersen, Welandawe, Huggins, and Vehtari, 2021)

brms supports Laplace / Pathfinder / ADVI

These might be useful for initializing MCMC or big data. The ADVI implementation is not very good.

```
fit1 <- brm(..., algorithm = "laplace")
```

```
fit1 <- brm(..., algorithm = "pathfinder")
```

```
fit1 <- brm(..., algorithm = "meanfield")
```

```
fit1 <- brm(..., algorithm = "fullrank")
```