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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  - bounded, non-singular, the number of parameters don't grow with n
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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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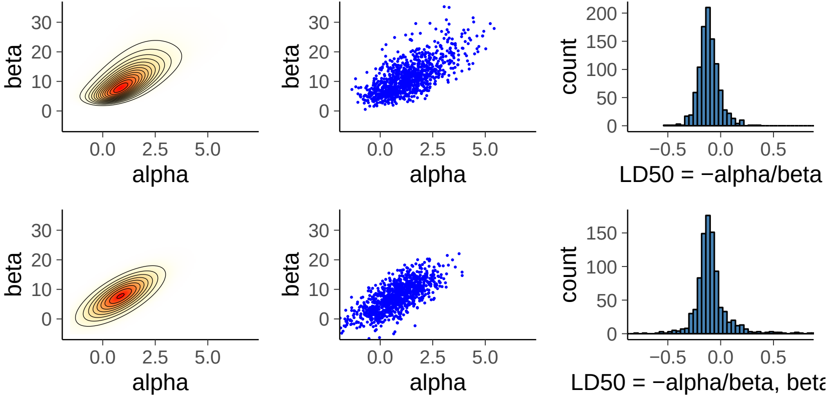

Taylor series

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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

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

Normal approximation

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$$\log p(\theta|y) = \log p(\hat{\theta}|y) + \frac{1}{2}(\theta - \hat{\theta})^T \left[\frac{d^2}{d\theta^2} \log p(\theta'|y)\right]_{\theta'=\hat{\theta}} (\theta - \hat{\theta}) + \ldots$$

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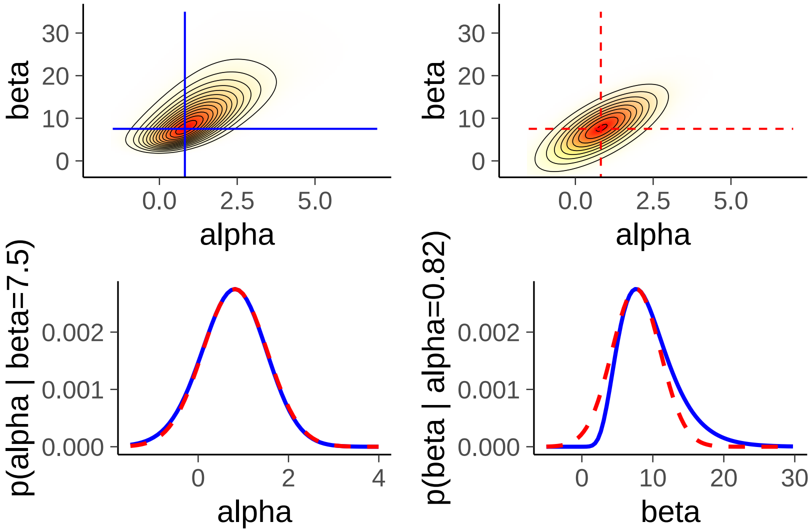

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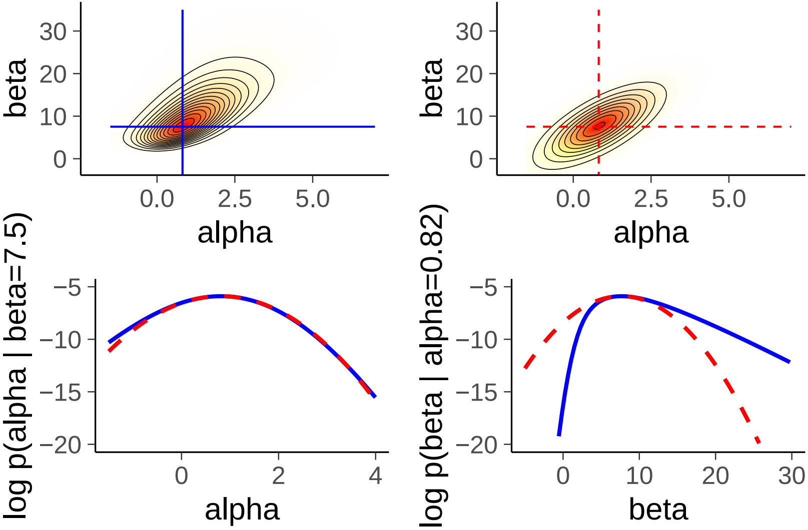

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Hessian $H(\theta) = -I(\theta)$

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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

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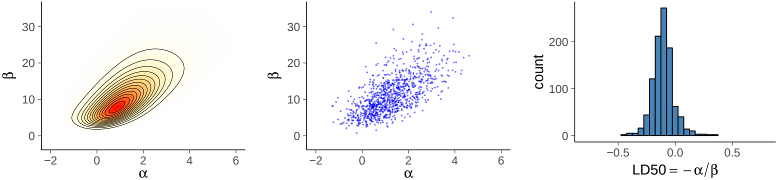
- Accuracy can be improved by importance sampling (Ch 10)

Example: Importance sampling in Bioassay

Grid



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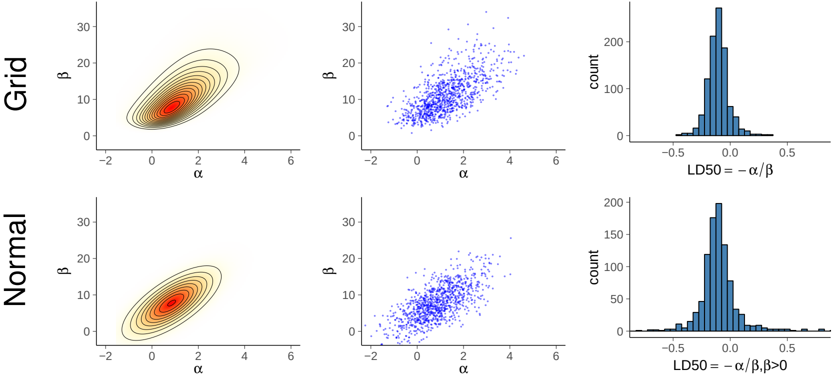

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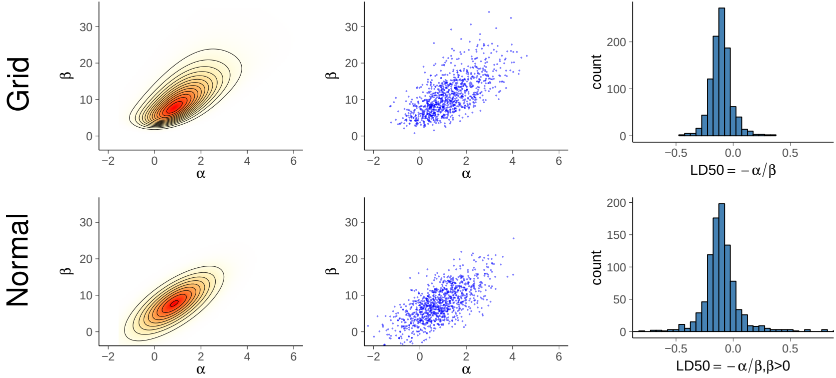
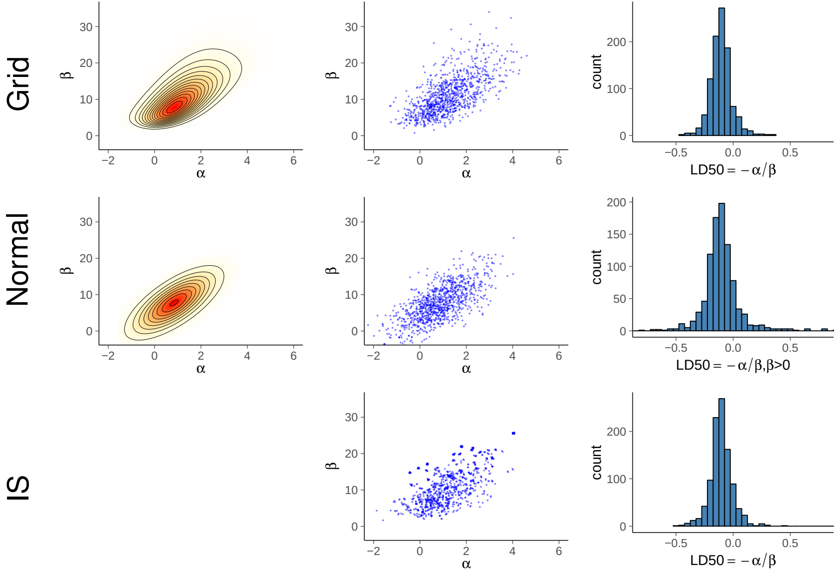


But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

Example: Importance sampling in Bioassay



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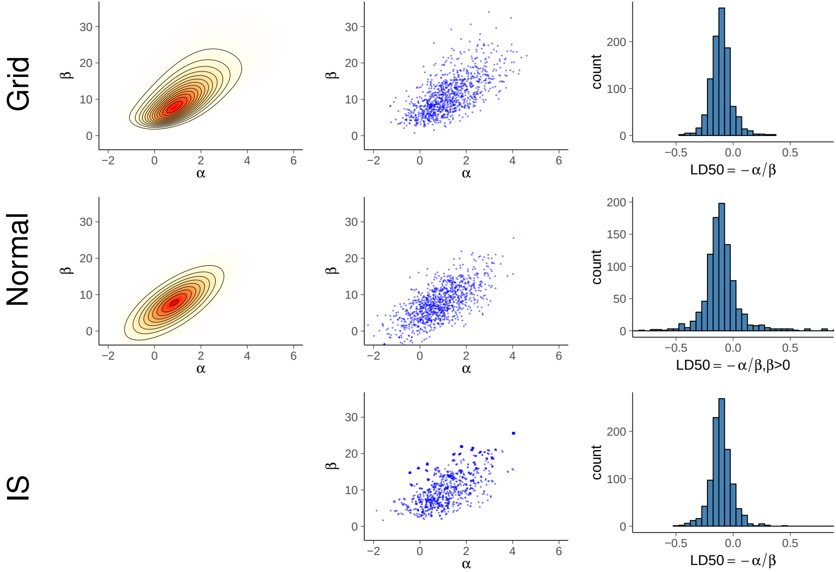

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  - in Bioassay example $k = 0.57$, which is ok
- CmdStan(R) has Laplace algorithm
  - since version 2.33 (2023)
    - + Pareto-*k* diagnostic via posterior package
    - + importance resampling (IR) via posterior package

Normal approximation and parameter transformations

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  - e.g. $\theta \in [0, 1]$ presenting probability

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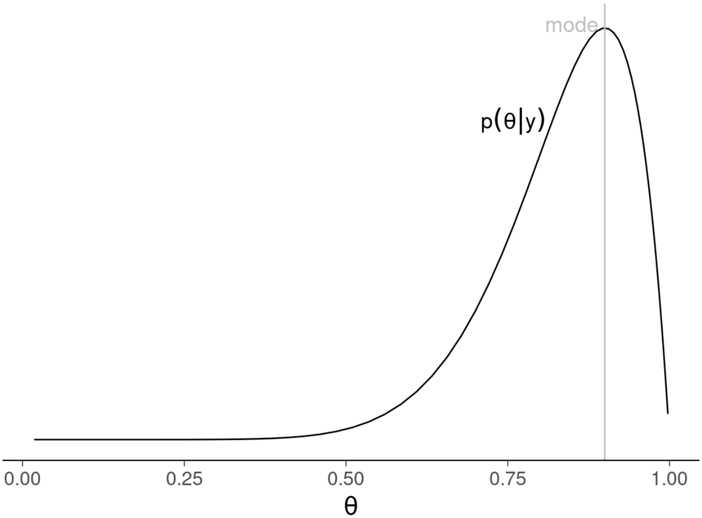
  - density of the transformed parameter needs to include Jacobian of the transformation (BDA3 p. 21)

Normal approximation and parameter transformations

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

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



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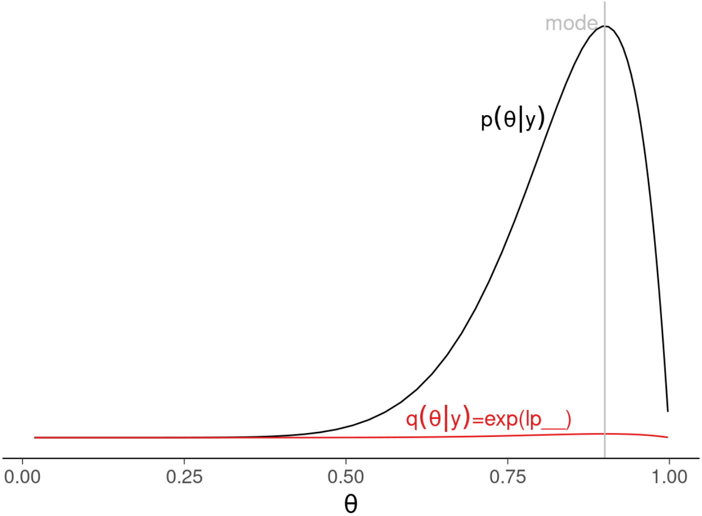
Stan computes only the unnormalized posterior $q(\theta|y)$



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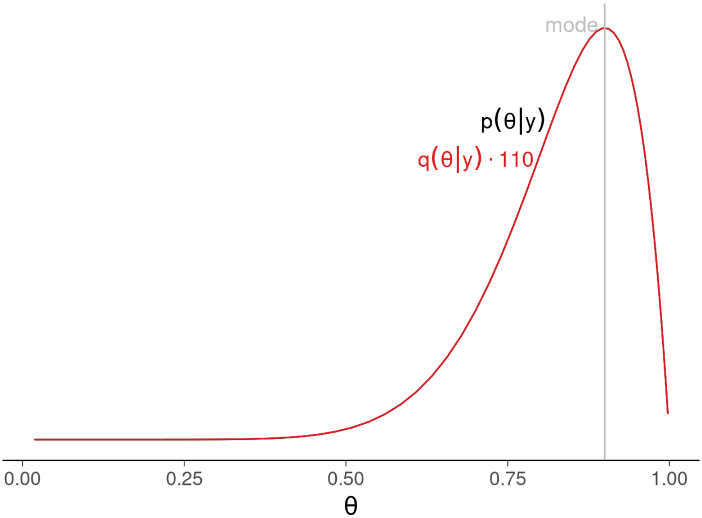
For illustration purposes we normalize Stan result $q(\theta|y)$



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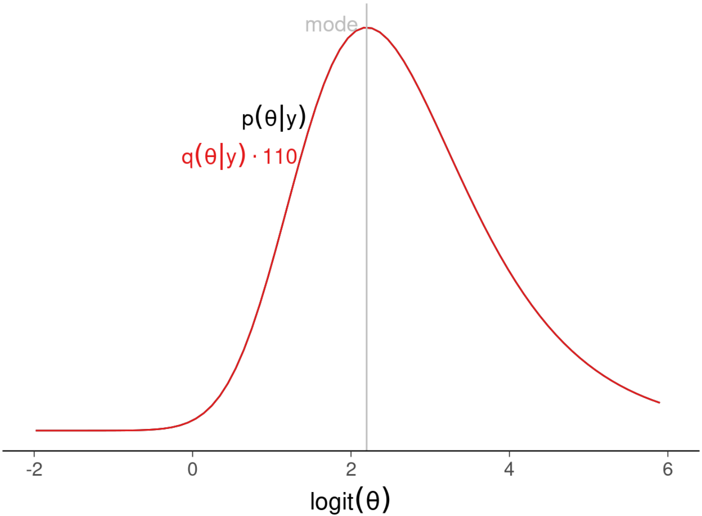
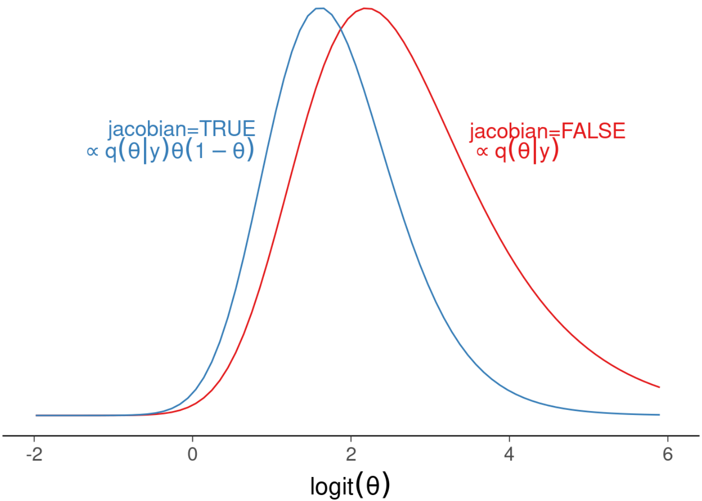
$\text{Beta}(9 + 1, 1 + 1)$, but x-axis shows the unconstrained $\text{logit}(\theta)$



Normal approximation and parameter transformations

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



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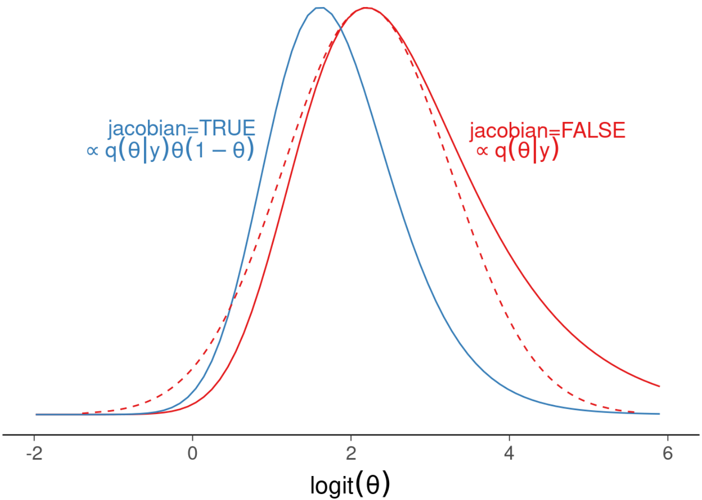

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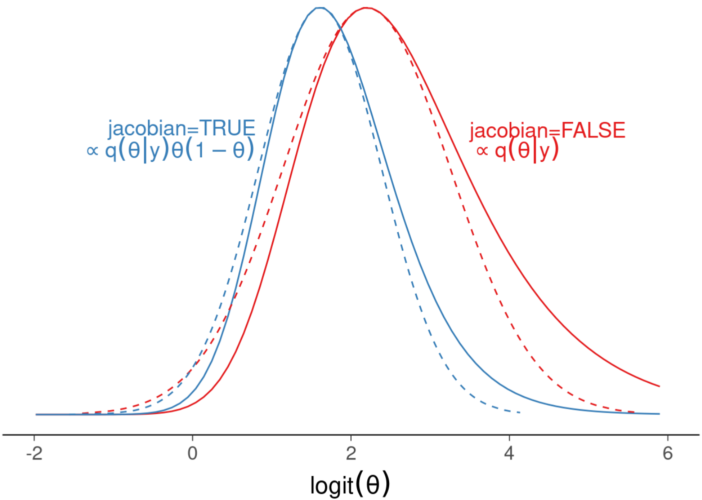

Normal approximation and parameter transformations

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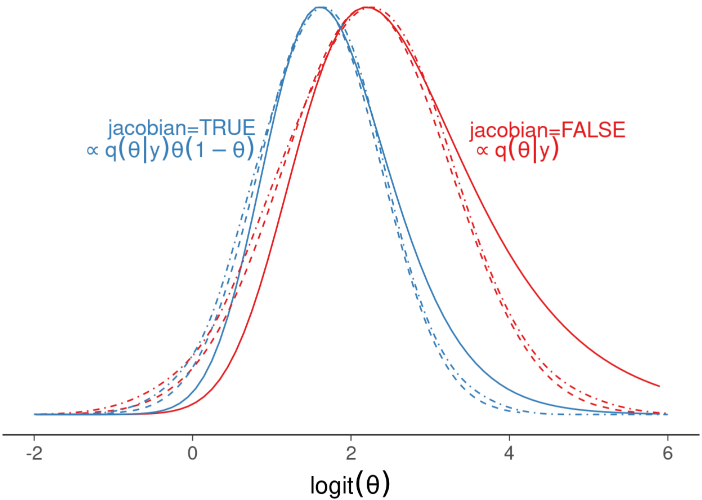
Sample from both approximations and show KDEs for draws



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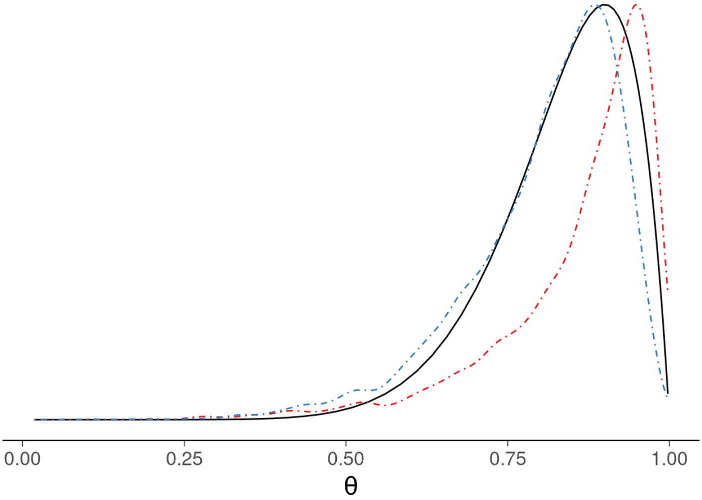
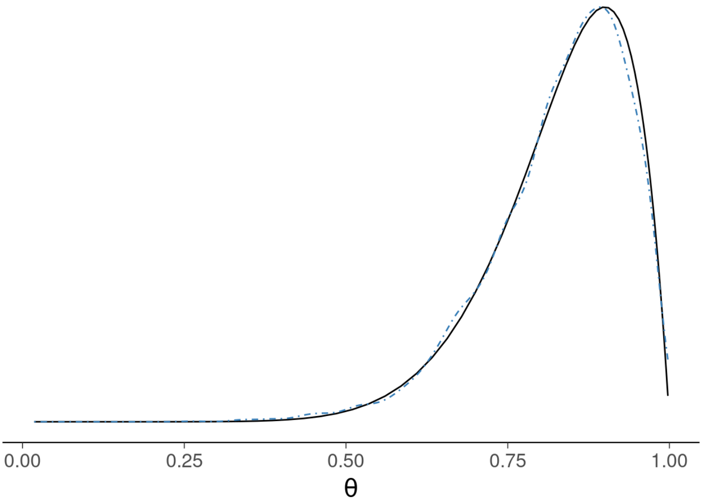
Inverse transform draws and show KDEs



Normal approximation and parameter transformations

Laplace approximation can be further improved with importance resampling



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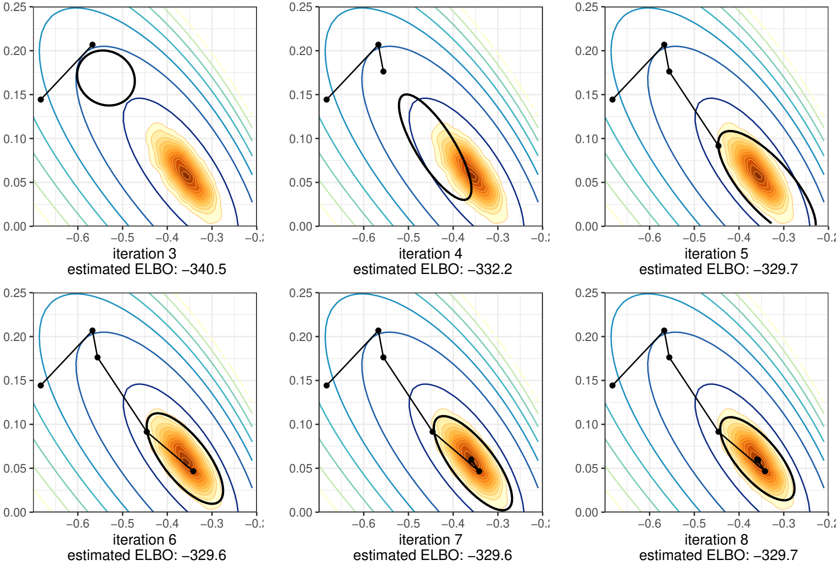
- Instead of mode and Hessian at mode, e.g.
  - variational inference (Ch 13)
    - CS-E4820 - Machine Learning: Advanced Probabilistic Methods
    - CS-E4895 - Gaussian Processes
    - Stan has the ADVI algorithm (not very good implementation)
    - Stan has Pathfinder algorithm (CmdStanR, brms)
    - 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.



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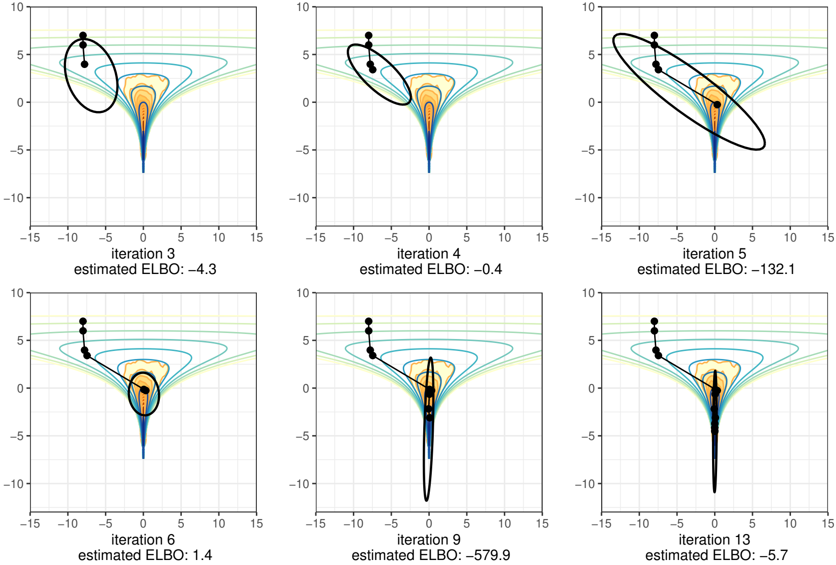

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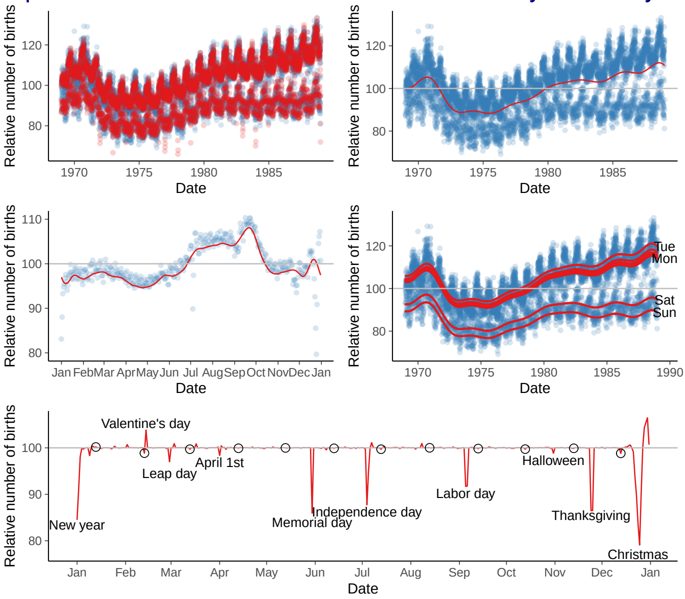
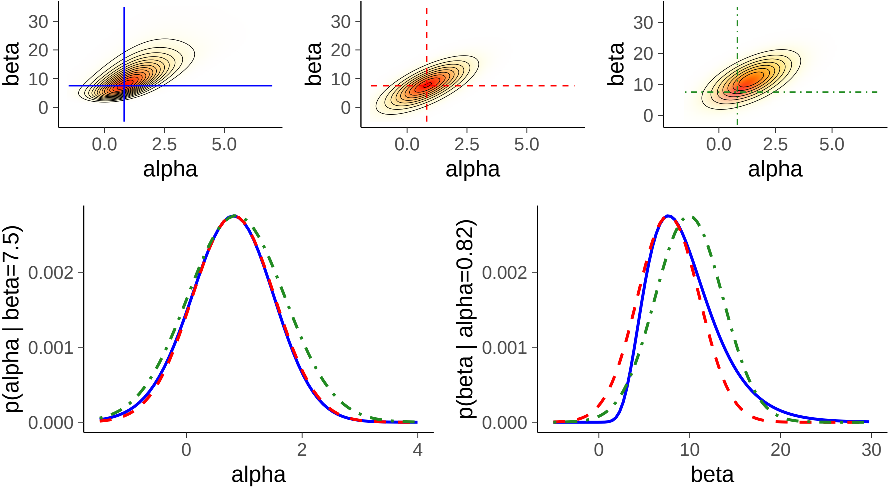
Birthdays case study uses Pathfinder to speed up workflow

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



Distributional approximations

Exact, Normal at mode, Normal with variational inference



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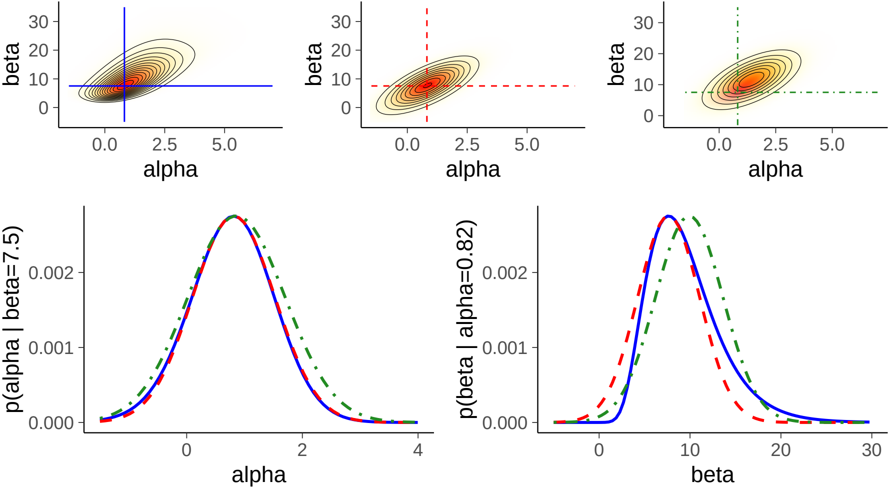

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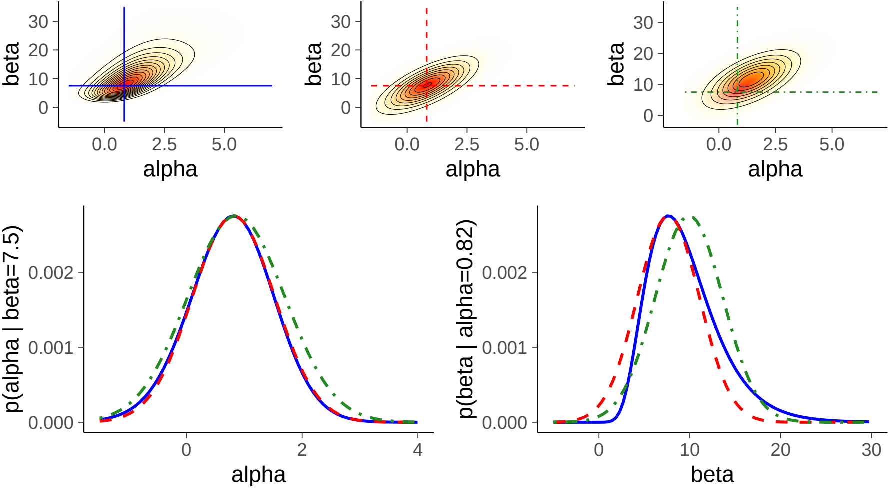

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  - with increasing number of posterior dimensions, the stochastic divergence estimate gets worse and flows have problems, too (Dhaka, Catalina, Andersen, Welandawe, Huggins, and Vehtari, 2021)

brms supports Laplace / Pathfinder / ADVI

These might be useful for initializng 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")
```