# 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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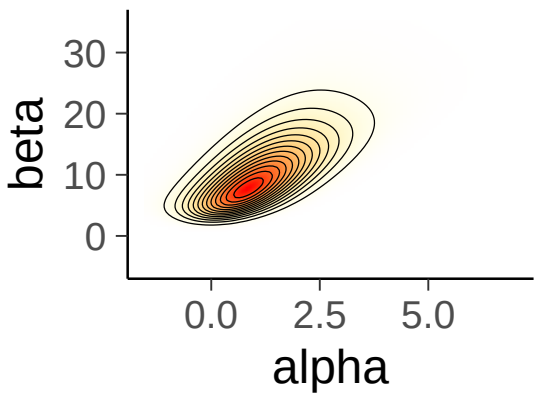


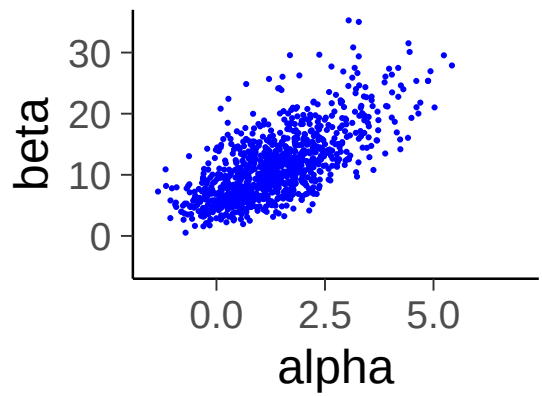


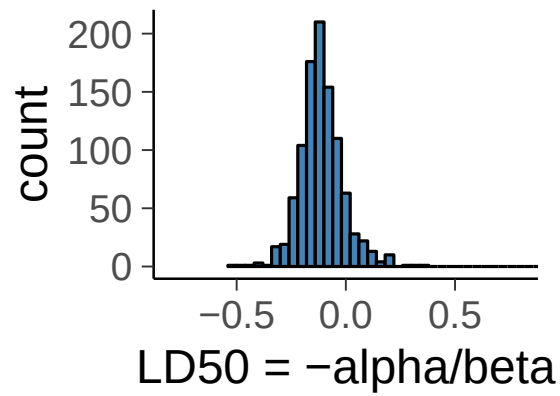


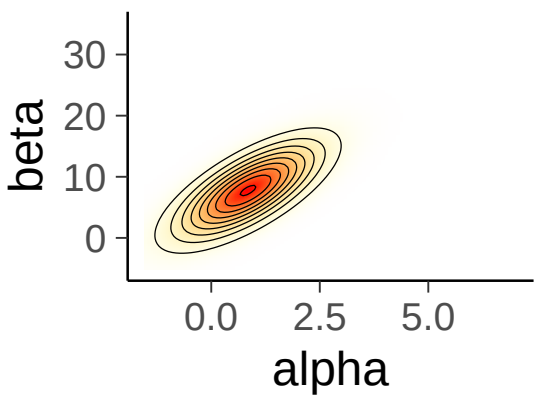


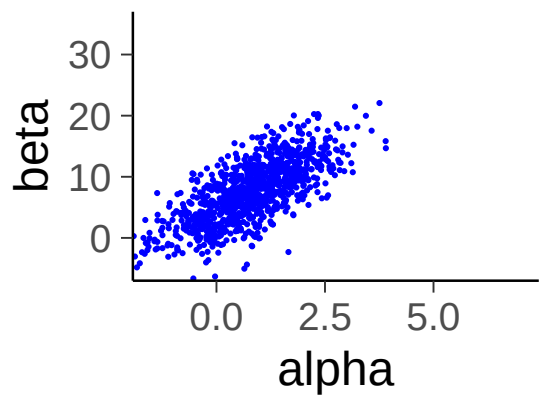


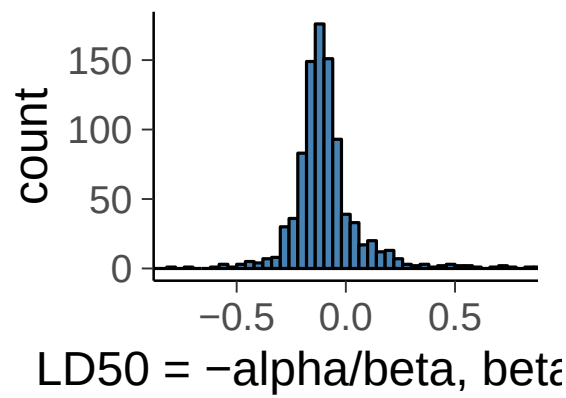

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  - if $\hat{\theta}$ is at mode, then $f'(\hat{\theta}) = 0$
  - often when $n \to \infty$, $\frac{f^{(3)}(\hat{\theta})}{3!}(\theta - \hat{\theta})^3 + \dots$ is small

# Multivariate Taylor series

- Multivariate series expansion

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

# Normal approximation

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

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

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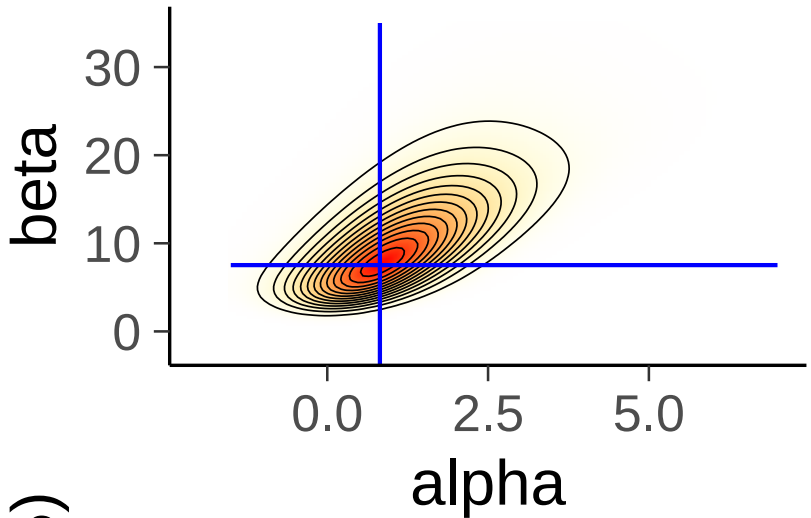


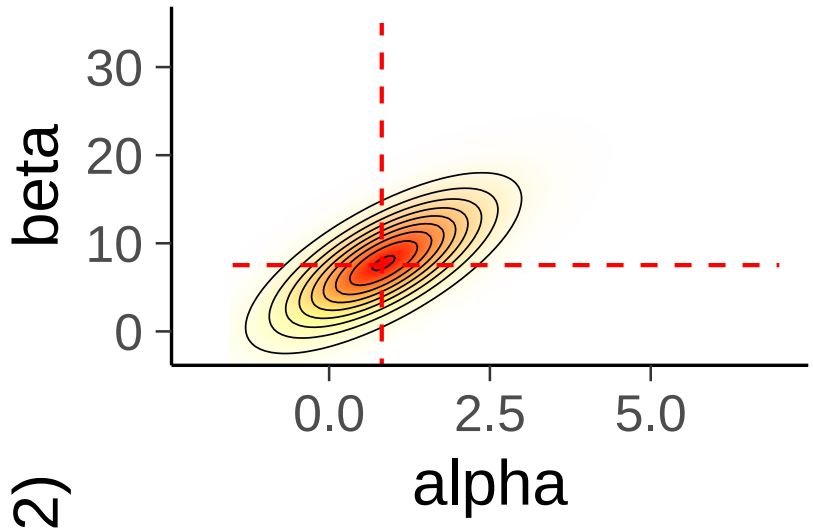


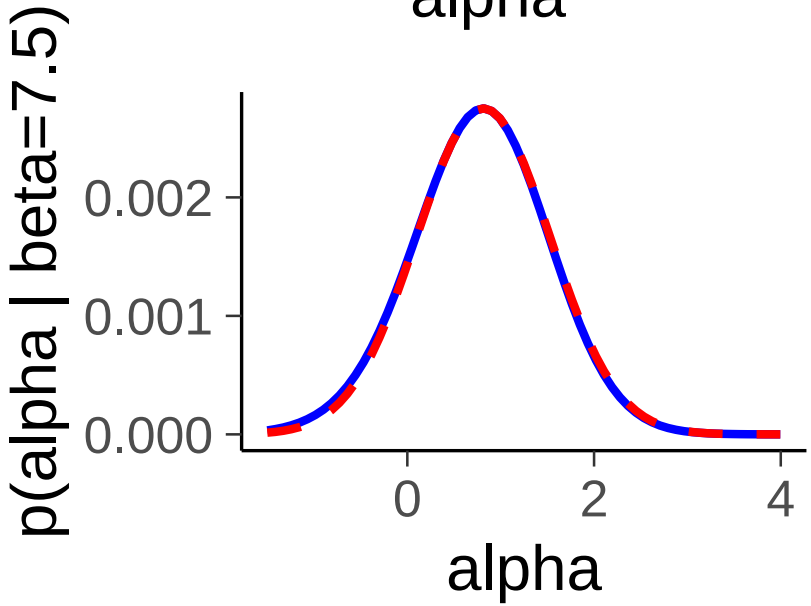


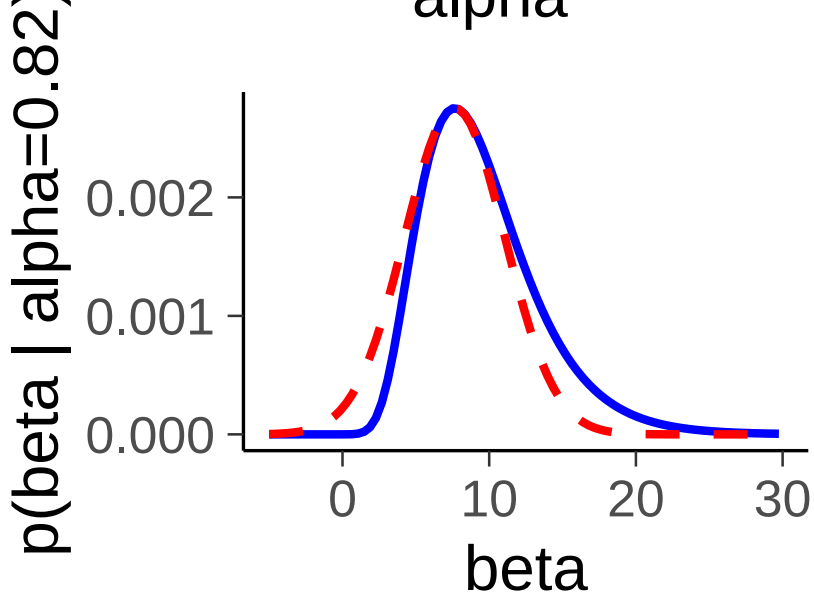

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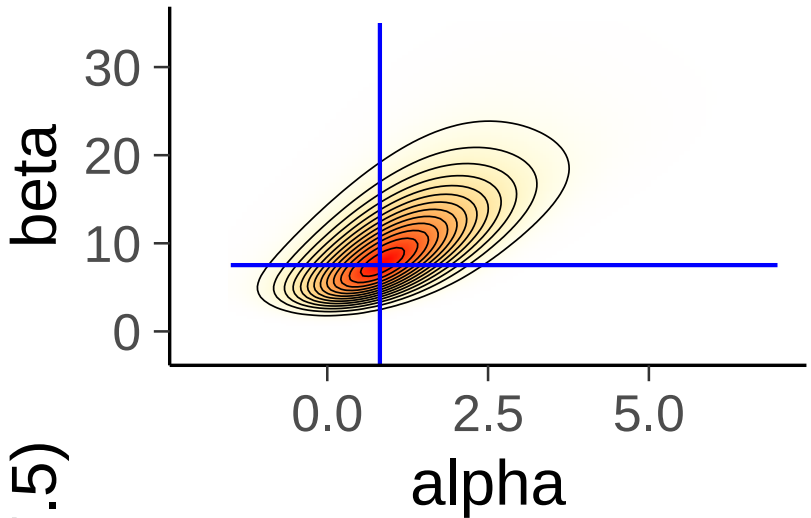


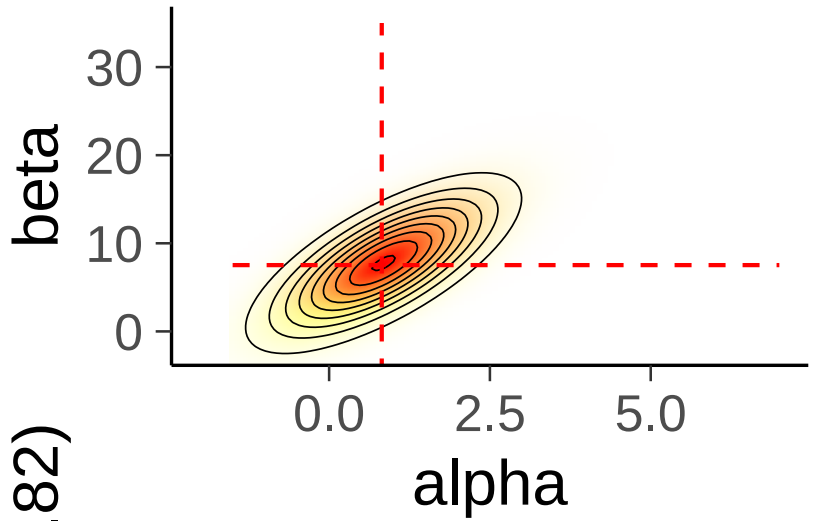


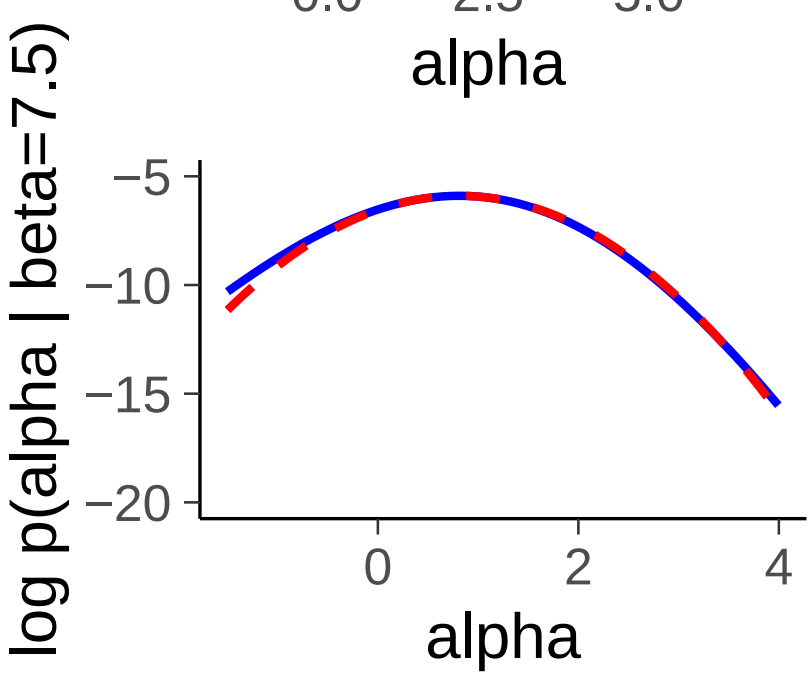


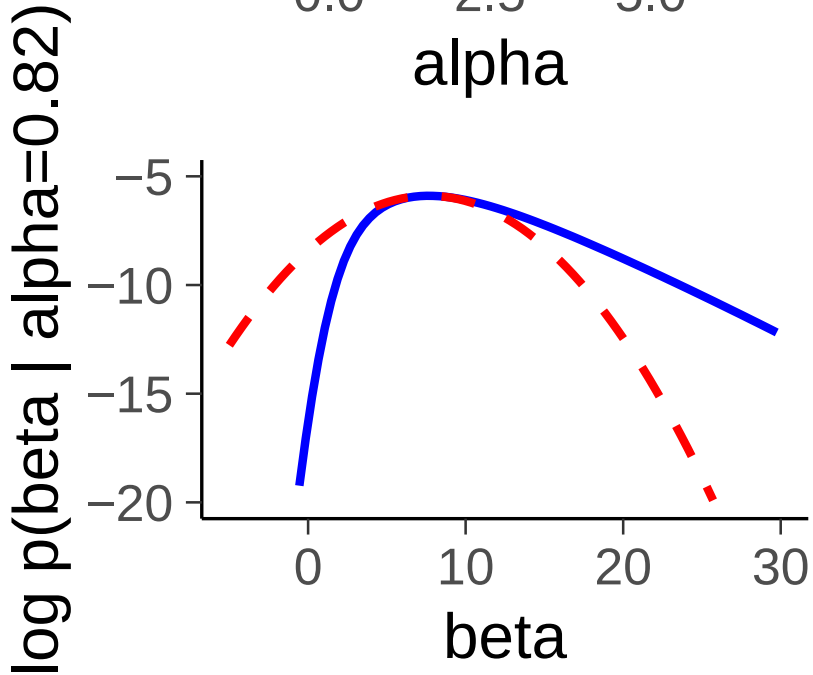

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$$p(\theta|y) \approx \mathrm{N}(\hat{\theta}, [I(\hat{\theta})]^{-1})$$

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

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

# Normal approximation

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

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

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

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

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  - 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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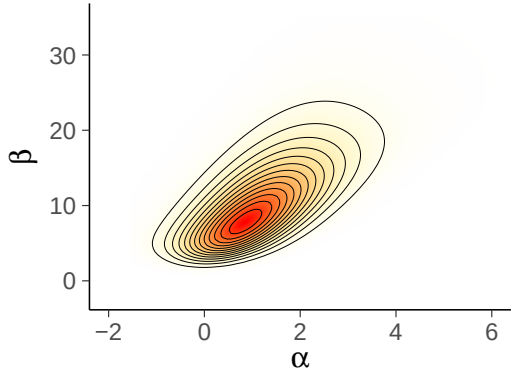
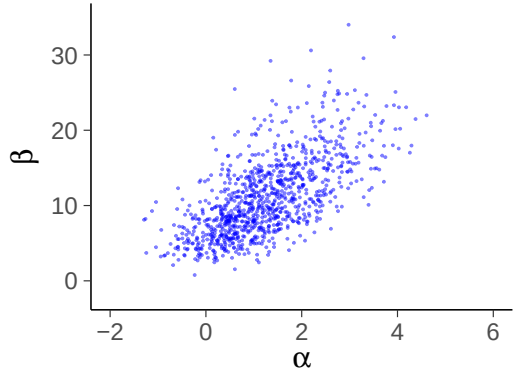
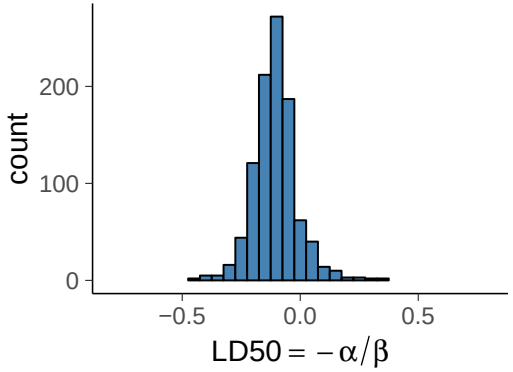
  - Rasmussen & Williams: Gaussian Processes for Machine Learning
- Accuracy can be improved by importance sampling (Ch 10)

# Example: Importance sampling in Bioassay

Grid



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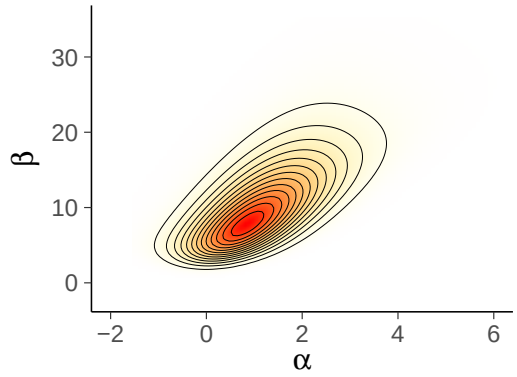
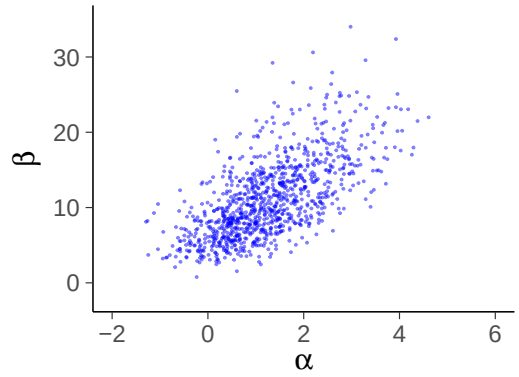
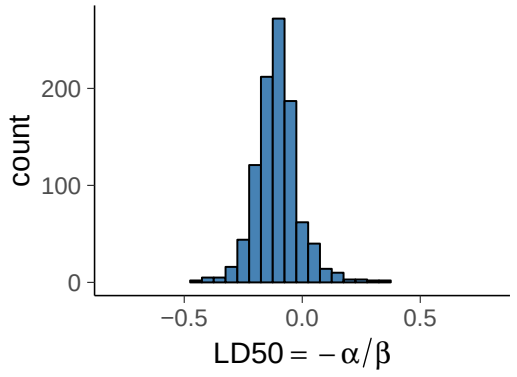
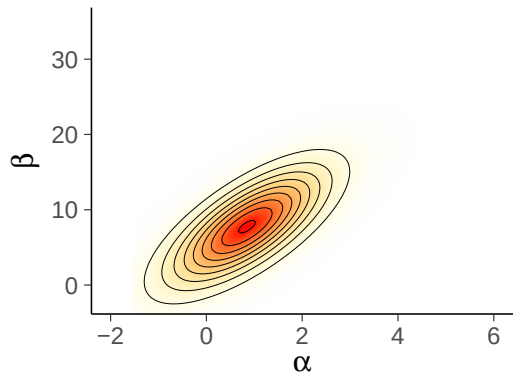
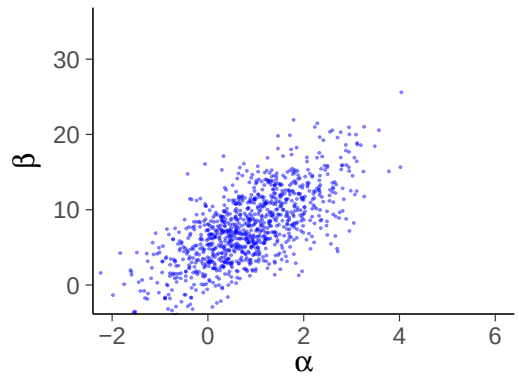


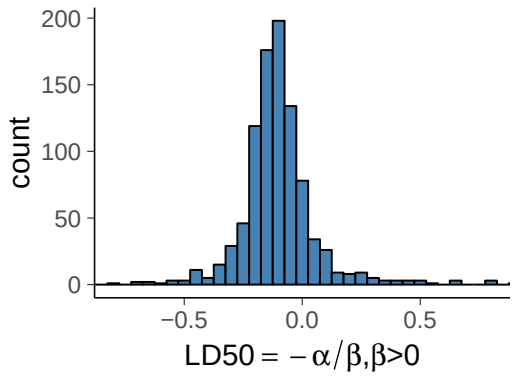




Normal

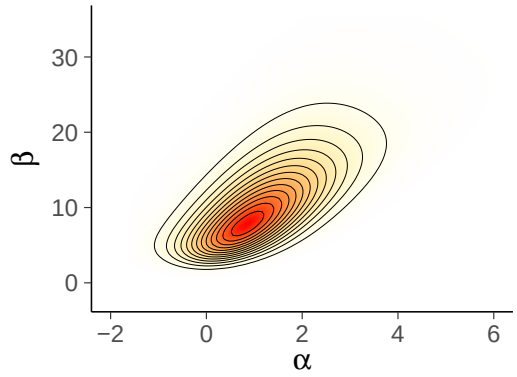


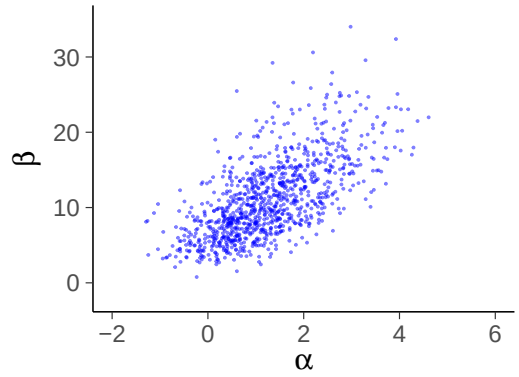



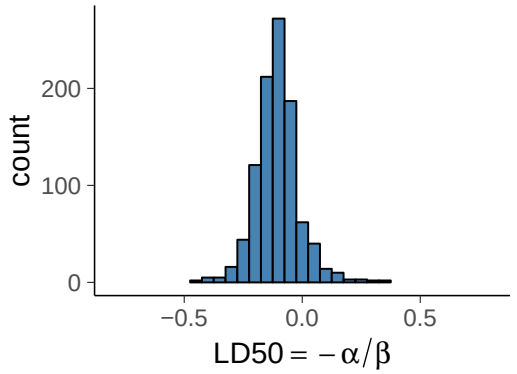



# Example: Importance sampling in Bioassay

Grid

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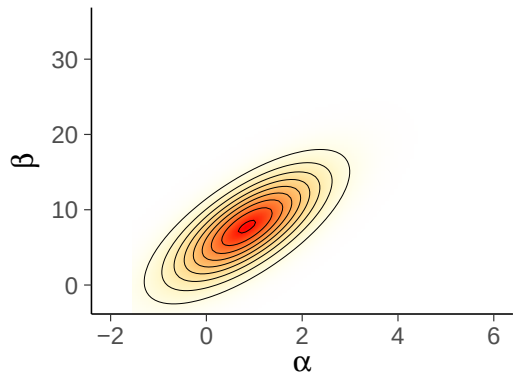


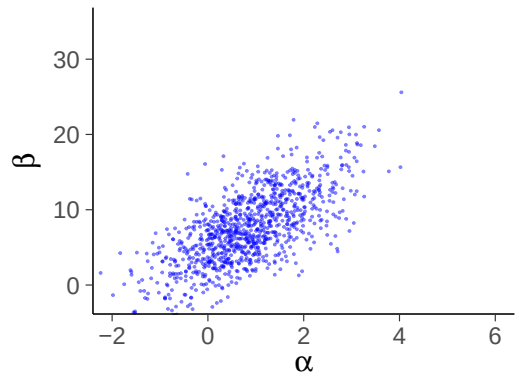


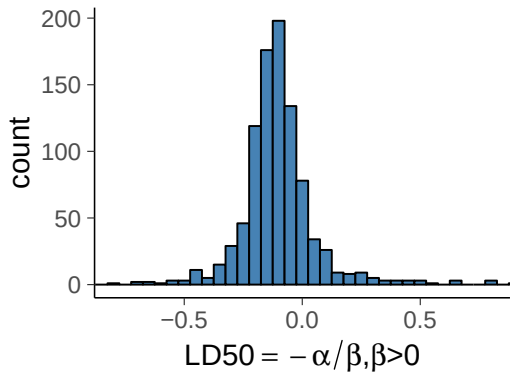


But the normal approximation is not that good here:
Grid sd(LD50) $\approx$ 0.1, Normal sd(LD50) $\approx$ .75!

# Example: Importance sampling in Bioassay

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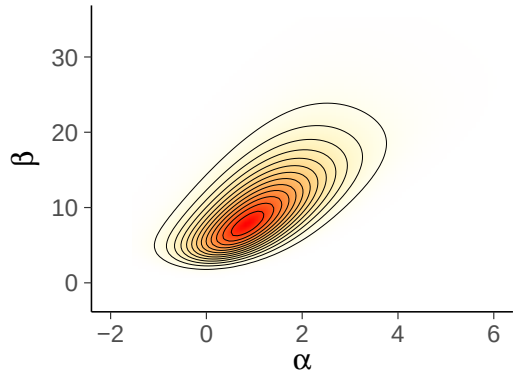


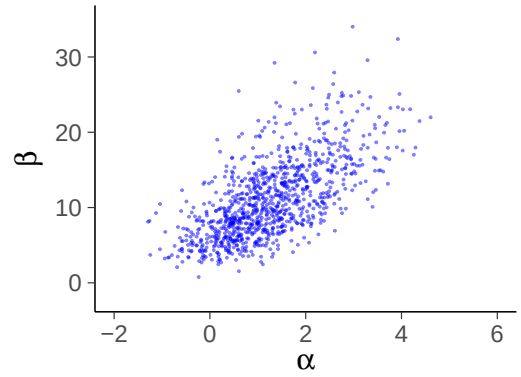


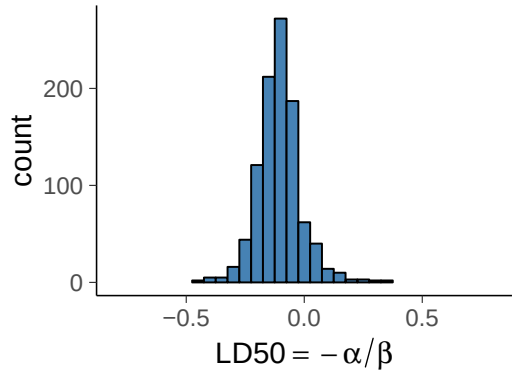


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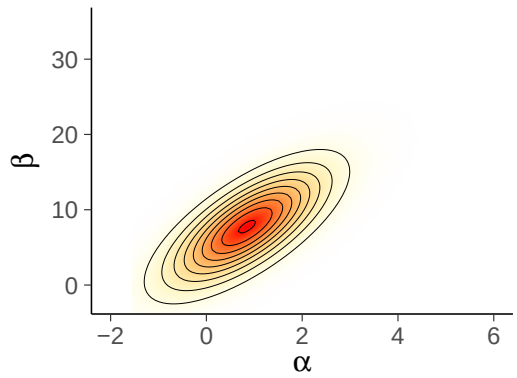
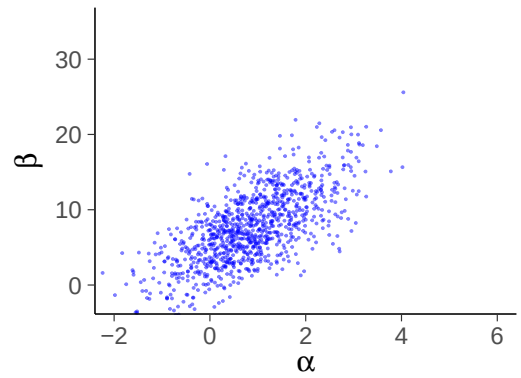
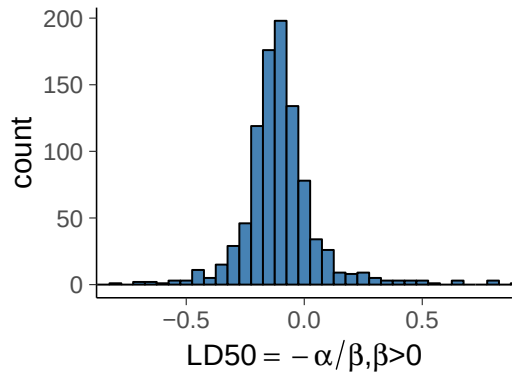
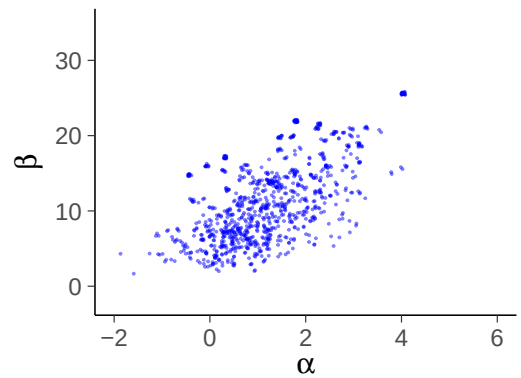
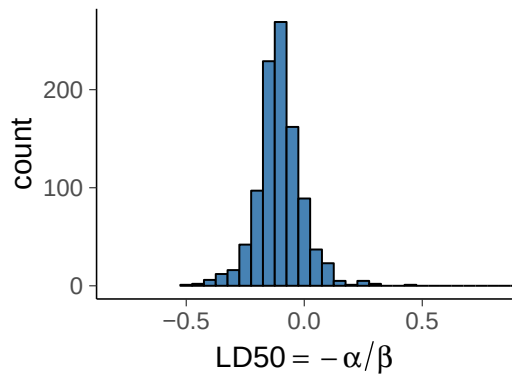



IS



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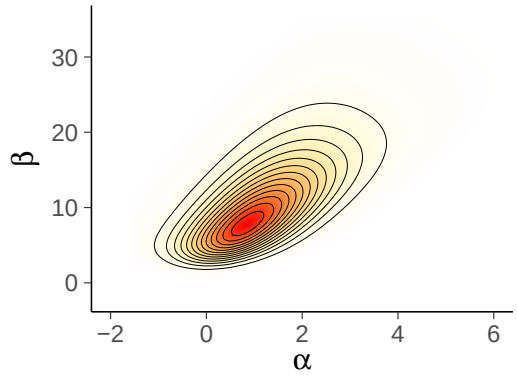


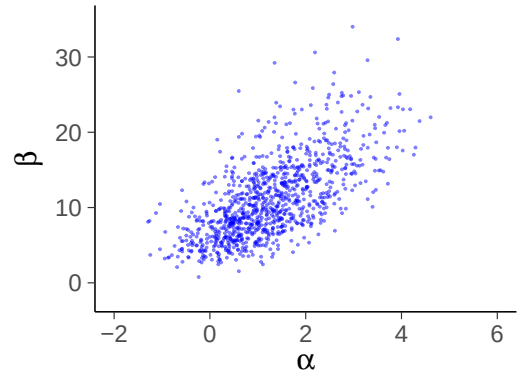


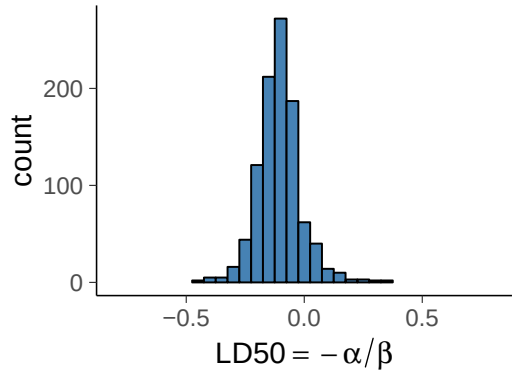


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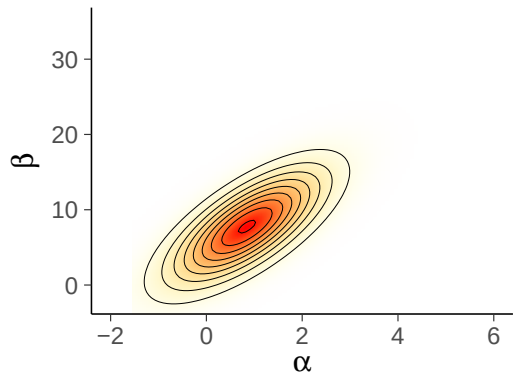


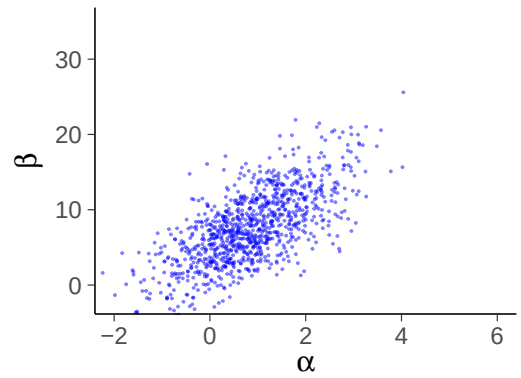


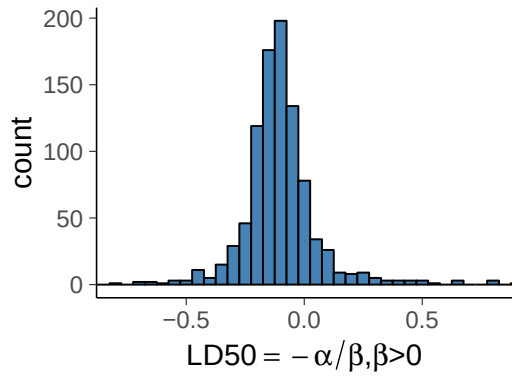


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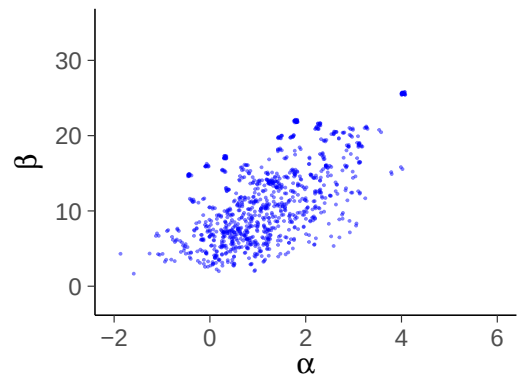


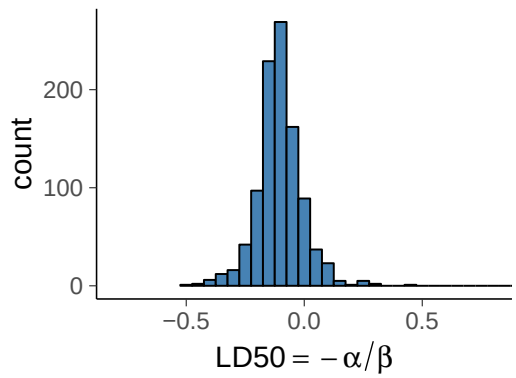


Grid sd(LD50) $\approx$ 0.1, IS sd(LD50) $\approx$ 0.1

# Normal approximation

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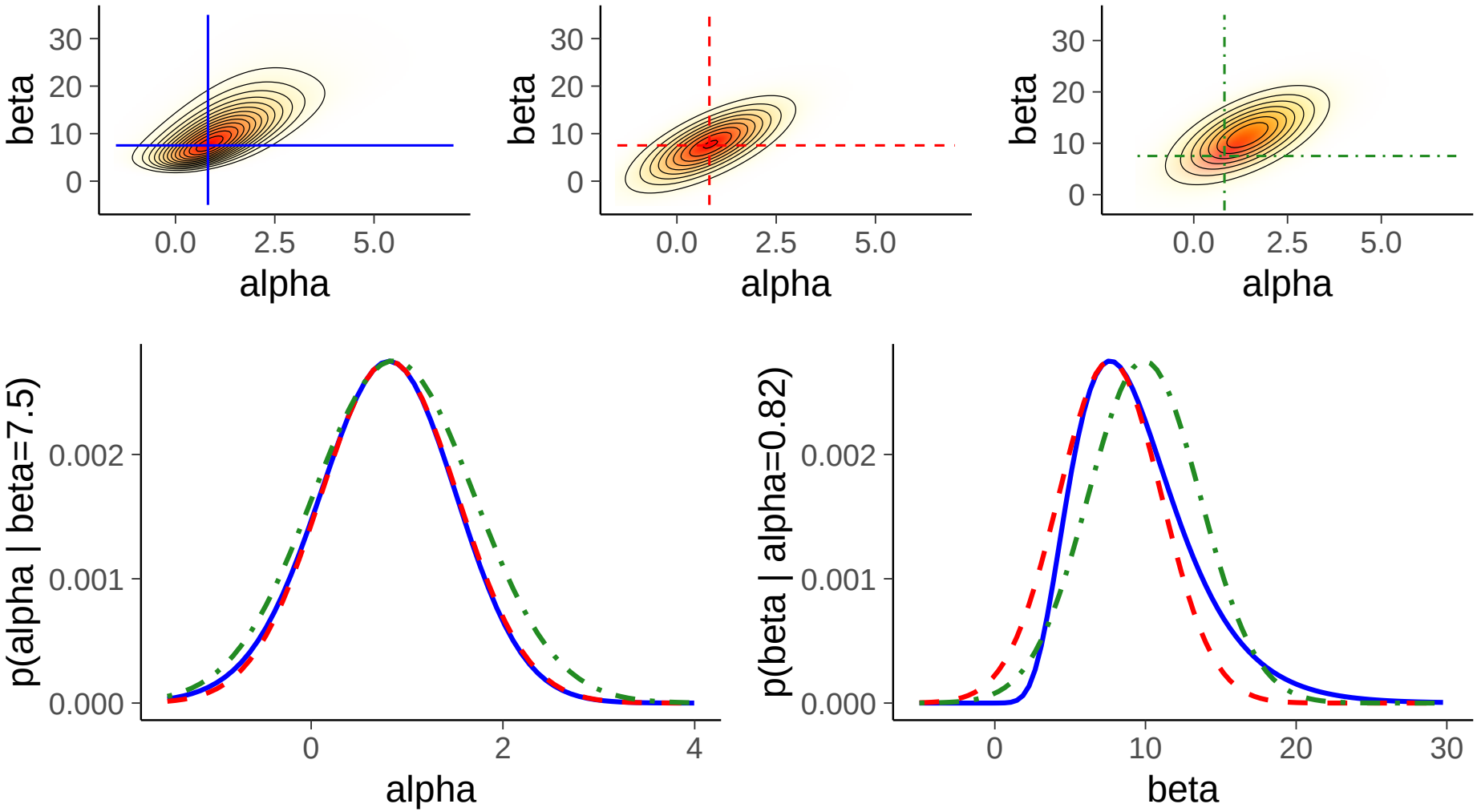
- Other distributions can be used (e.g. $t$-distribution)
- Instead of mode and Hessian at mode, e.g.
  - variational inference (Ch 13)
    - CS-E4820 - Machine Learning: Advanced Probabilistic Methods
    - Stan has an experimental ADVI algorithm
  - expectation propagation (Ch 13)
  - speed of these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

# Distributional approximations

Exact, Normal at mode, Normal with variational inference



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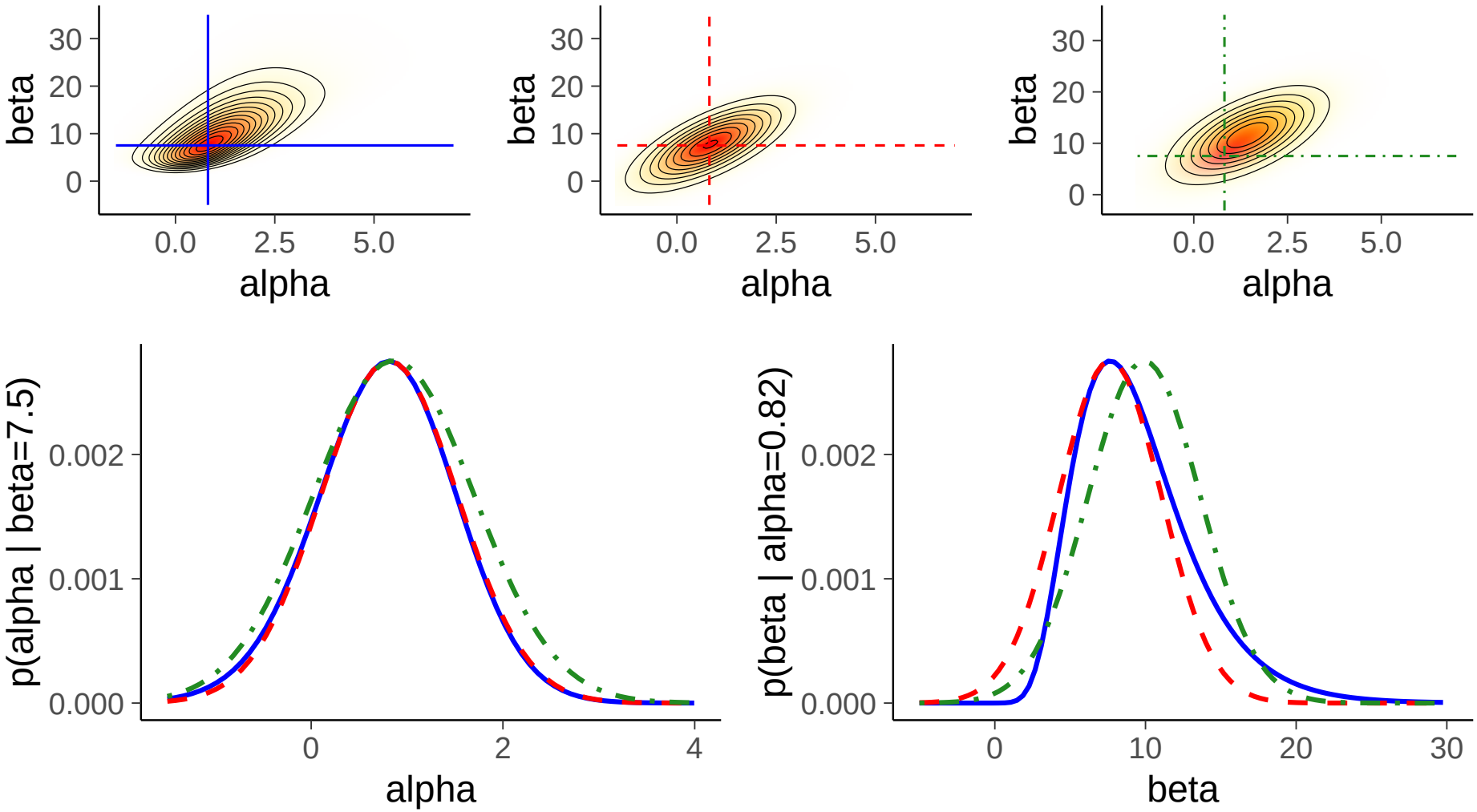


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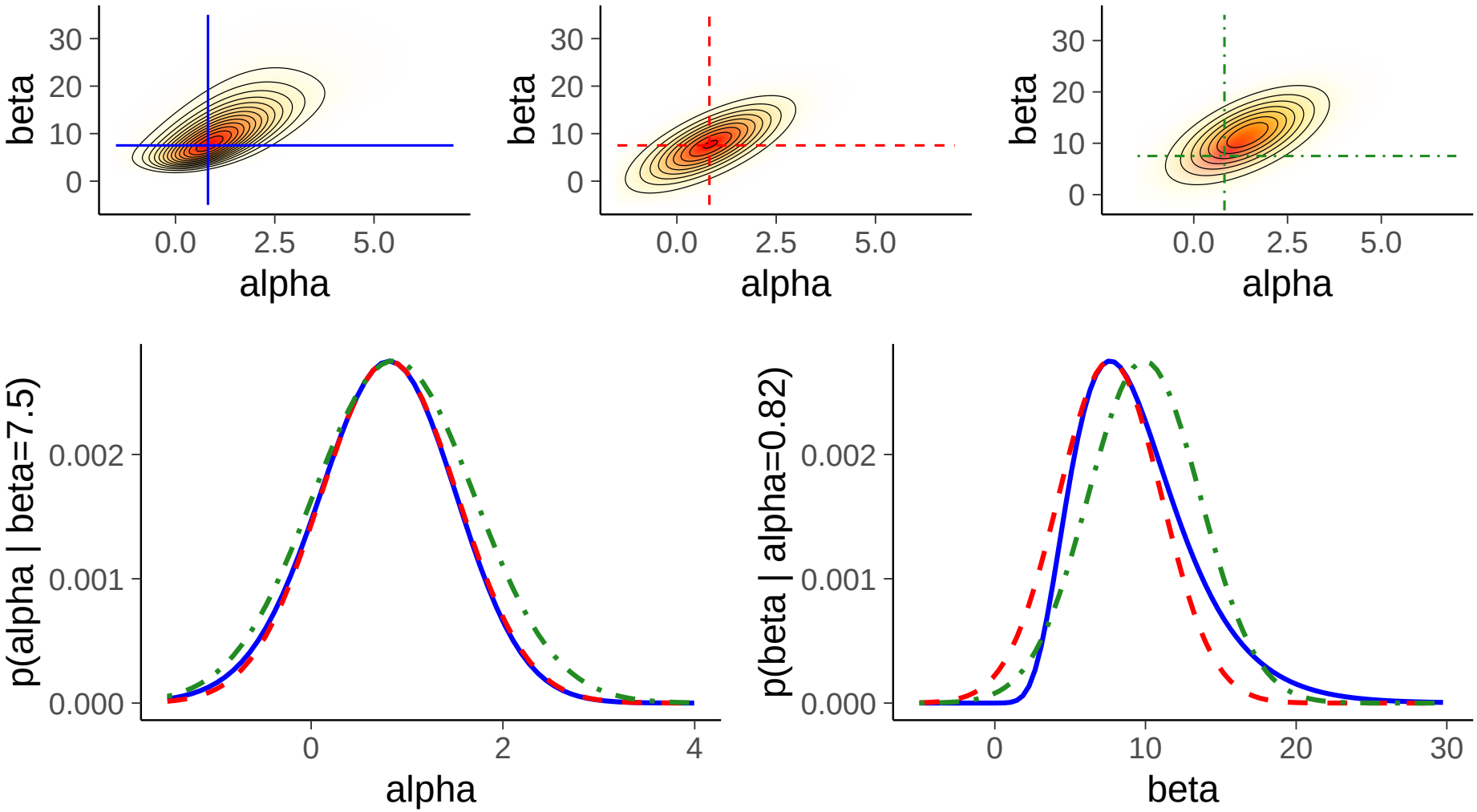


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  - see counter examples

# 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

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

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# Large sample theory – counter examples

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  - e.g. if we never observe $u$ and $v$ at the same time and the model is

$$\begin{pmatrix} u \\ v \end{pmatrix} \sim \mathrm{N}\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right)$$

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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 $\theta_i$ has prior in time
  - posterior of $\theta_i$ 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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- Problem for any inference method including MCMC
  - can be avoided with good priors

# Large sample theory – counter examples

- Unbounded (FI: rajoittamaton) likelihood
  - if likelihood is unbounded it is possible that there is no mode in the posterior
  - e.g. previous normal mixture model; assume $\lambda$ to be known (and not 0 or 1); if we set $\mu_1 = y_i$ for any $i$ and $\sigma_1^2 \to 0$, then likelihood $\to \infty$
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  - note that a prior close to a prior allowing unbounded posterior may produce almost unbounded posterior

# Large sample theory – counter examples

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

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  - e.g. $y_i \sim \text{N}(\theta, 1)$ with a restriction $\theta \geq 0$ and assume that $\theta_0 = 0$
    - posterior of $\theta$ 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

# Frequency evaluations

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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.

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  - unbiased estimate for strictly positive parameter can be negative
- Confidence interval is defined to have true value inside the interval in $\alpha\%$ cases of repeated data generation from the data generating mechanism
  - doesn't say how likely the true value is inside the interval given the observed data
  - doesn't need be useful to have perfect calibration

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- Bayesian inference
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- Lot of machine learning is not pure frequentist or Bayesian

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  - reporting just the null hypothesis testing result throws away lot of useful information
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- Frequentist null hypothesis testing
  - asks what if data is generated from the smaller model
  - doesn't tell whether the more complex model is good enough

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  - assumes that there is non-zero probability that the treatment effect can be exactly zero
- Predictive performance
  - is there difference in predictive performance with, e.g., treatment effect fixed to zero or unknown treatment effect

# Common statistical tests as Bayesian models

| | |
|---|---|
| *t*-test | `stan_glm(y ~ 1)` |
| paired *t*-test | `stan_glm((y_1 - y_2) ~ 1)` |
| pearson correlation | `stan_glm(y ~ 1 + x)` |
| two-sample *t*-test | `stan_glm(y ~ 1 + gid)` |
| ... | |

See longer list and illustrations (with `lm`) at
https://lindeloev.github.io/tests-as-linear/