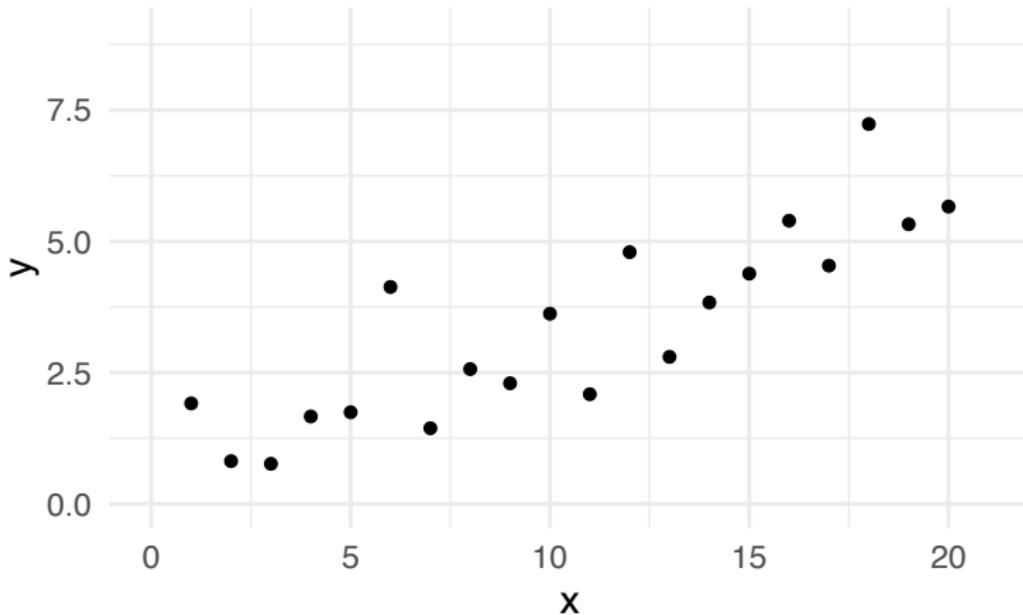


Chapter 3

- 3.1 Marginalization
- 3.2 Normal distribution with a noninformative prior (important)
- 3.3 Normal distribution with a conjugate prior (important)
- 3.4 Multinomial model (can be skipped)
- 3.5 Multivariate normal with known variance (useful for chapter 4)
- 3.6 Multivariate normal with unknown variance (glance through)
- 3.7 Bioassay example (very important, related to one of the exercises)
- 3.8 Summary (summary)

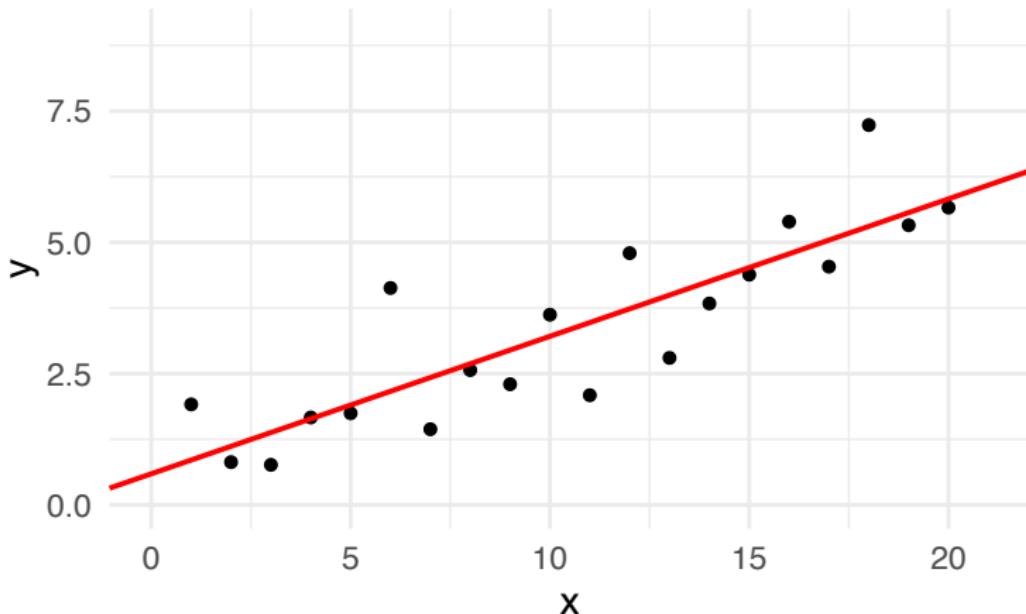
Example of uncertainty in modeling

Data



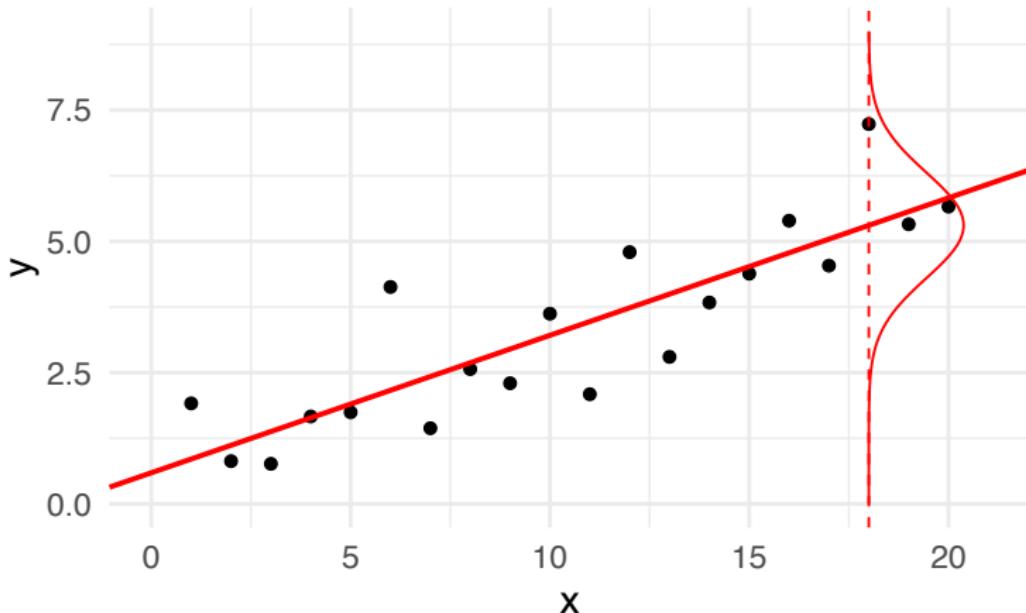
Example of uncertainty in modeling

Posterior mean



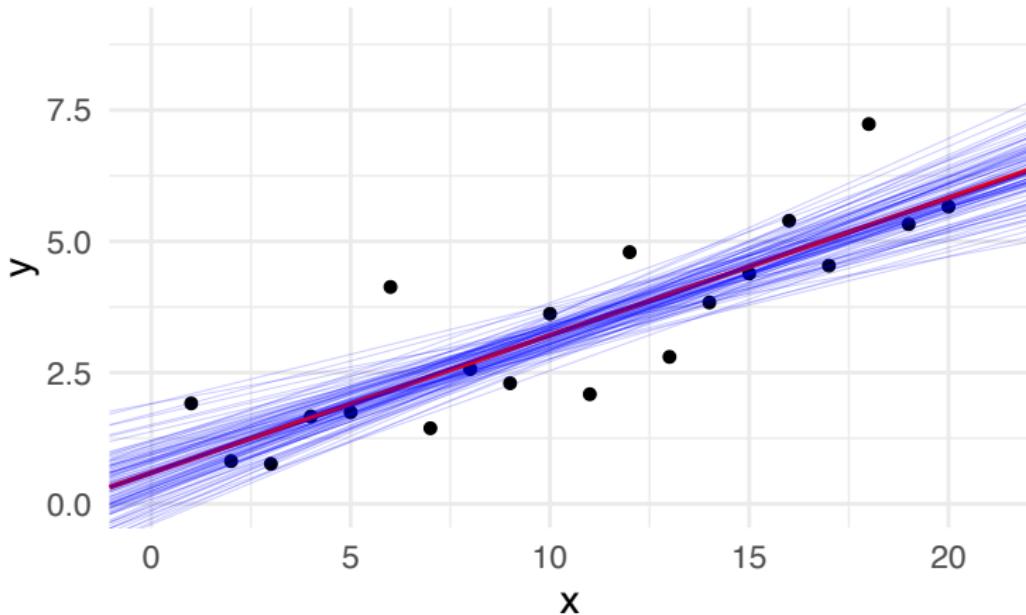
Example of uncertainty in modeling

Predictive distribution given posterior mean



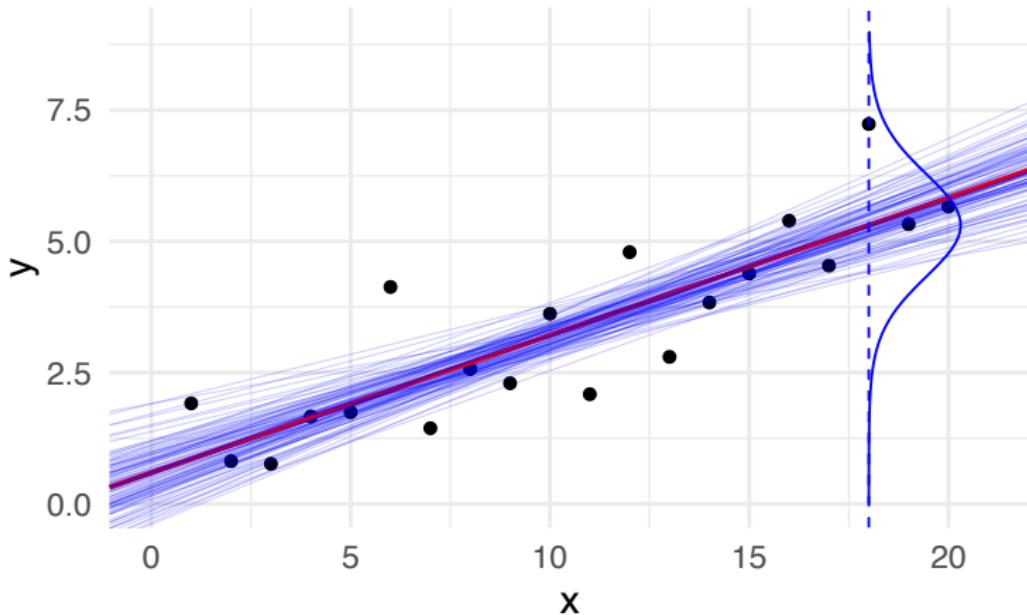
Example of uncertainty in modeling

Posterior draws



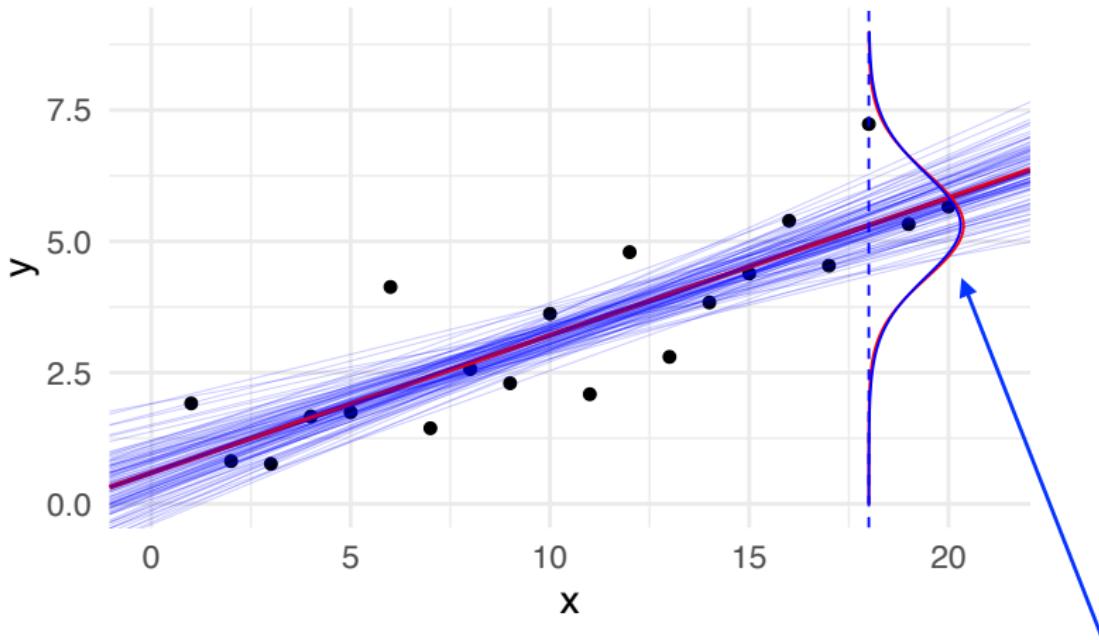
Example of uncertainty in modeling

Posterior draws and predictive distribution



Example of uncertainty in modeling

Posterior draws and predictive distribution



blue dist is from the samples and red is from the exact analytical solution

Monte Carlo and posterior draws

- $\theta^{(s)}$ draws from $p(\theta | y)$ can be used
 - for visualization
 - to approximate expectations (integrals)

$$E_{p(\theta|y)}[\theta] = \int \theta p(\theta | y) \approx \frac{1}{S} \sum_{s=1}^S \theta^{(s)}$$

Marginalization

- Joint distribution of parameters

$$p(\theta_1, \theta_2 | y) \propto p(y | \theta_1, \theta_2)p(\theta_1, \theta_2)$$

- Marginalization

$$p(\theta_1 | y) = \int p(\theta_1, \theta_2 | y) d\theta_2$$

$p(\theta_1 | y)$ is a marginal distribution

- Monte Carlo approximation

$$p(\theta_1 | y) \approx \frac{1}{S} \sum_{s=1}^S p(\theta_1, \theta_2^{(s)} | y),$$

where $\theta_2^{(s)}$ are draws from $p(\theta_2 | y)$

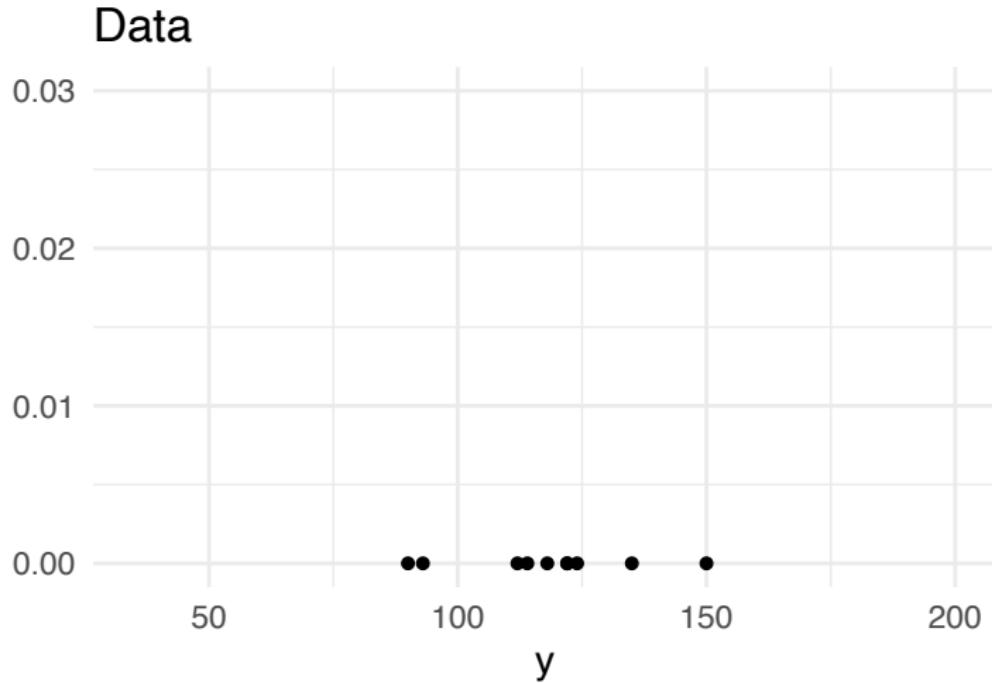
Marginalization - predictive distribution

- Marginalization over posterior distribution

$$\begin{aligned} p(\tilde{y} \mid y) &= \int p(\tilde{y} \mid \theta) p(\theta \mid y) d\theta \\ &= \int p(\tilde{y}, \theta \mid y) d\theta \end{aligned}$$

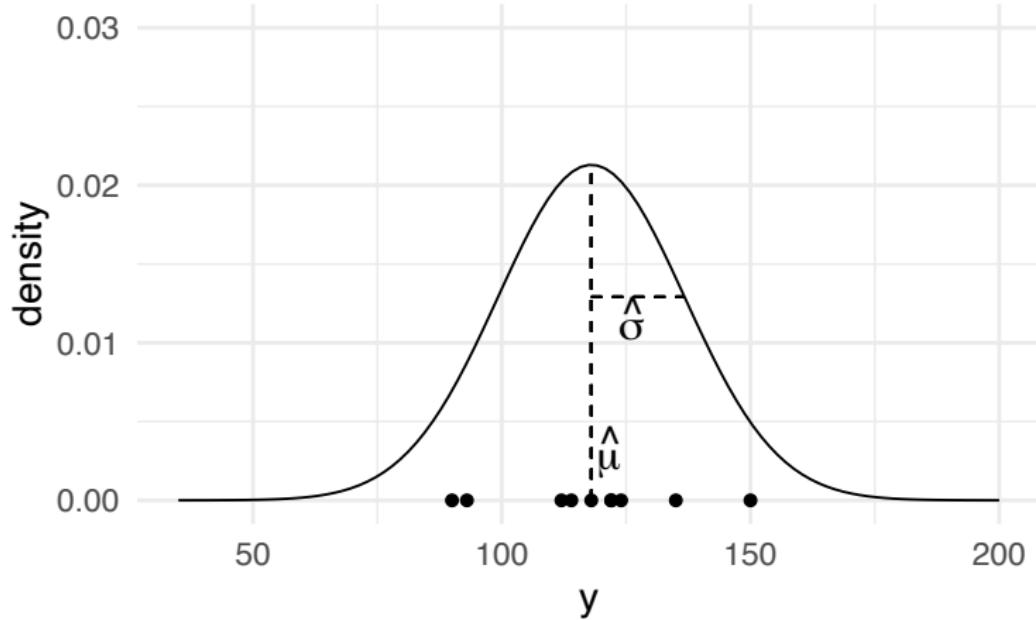
$p(\tilde{y} \mid y)$ is a predictive distribution

Gaussian example



Gaussian example

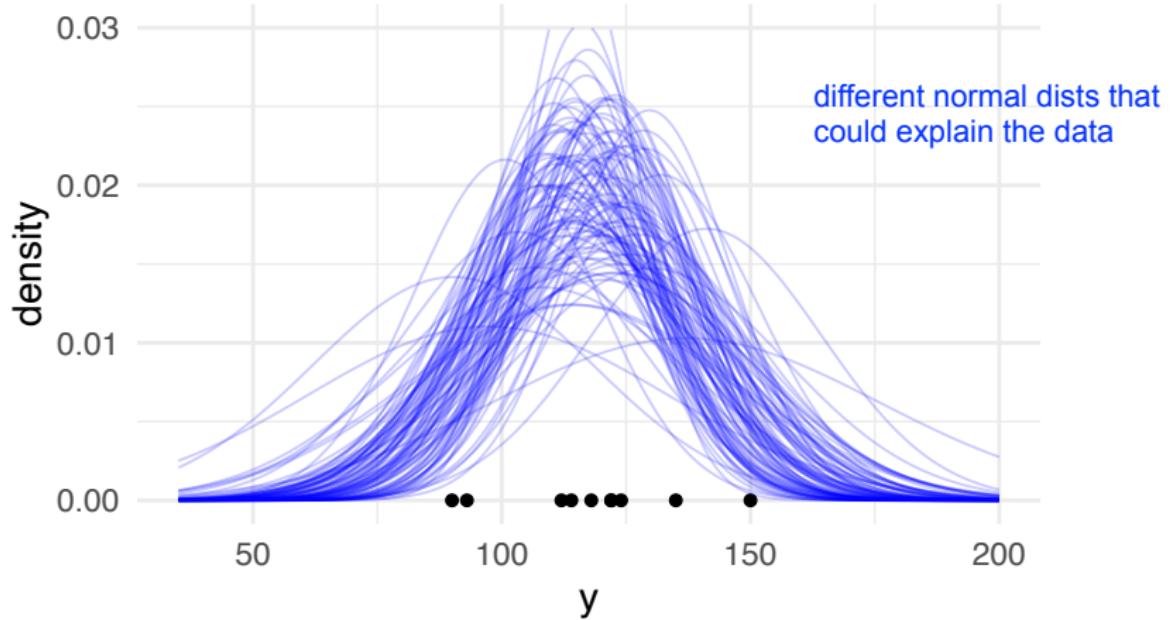
Gaussian fit with posterior mean



$$p(y | \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y - \mu)^2\right)$$

Gaussian example

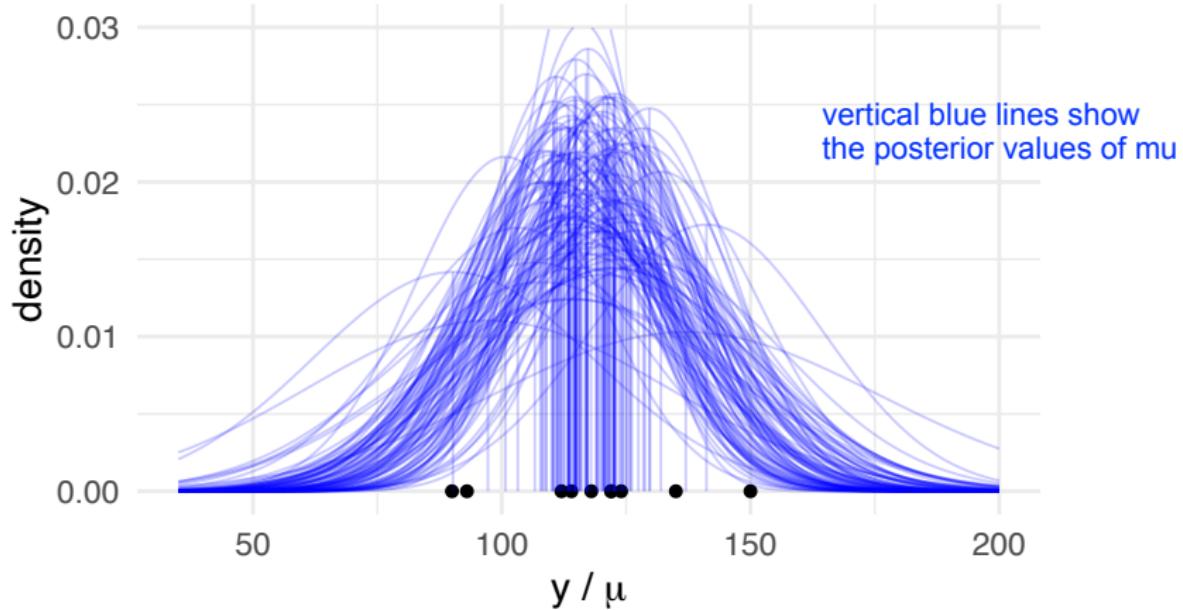
Gaussians with posterior draw parameters



$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

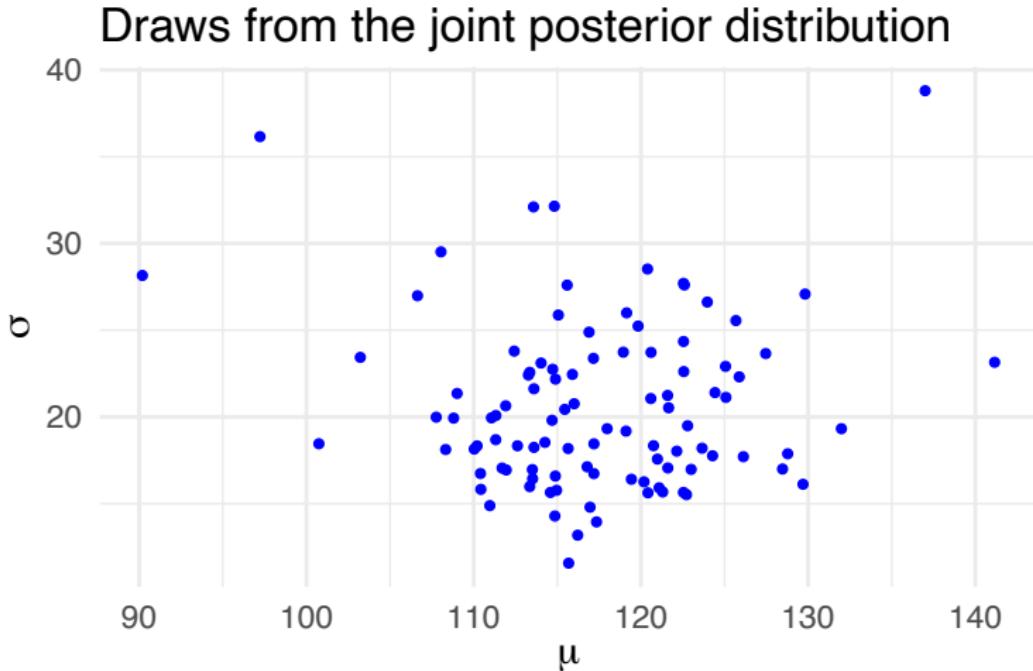
Gaussian example

Gaussians with posterior draw parameters



$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

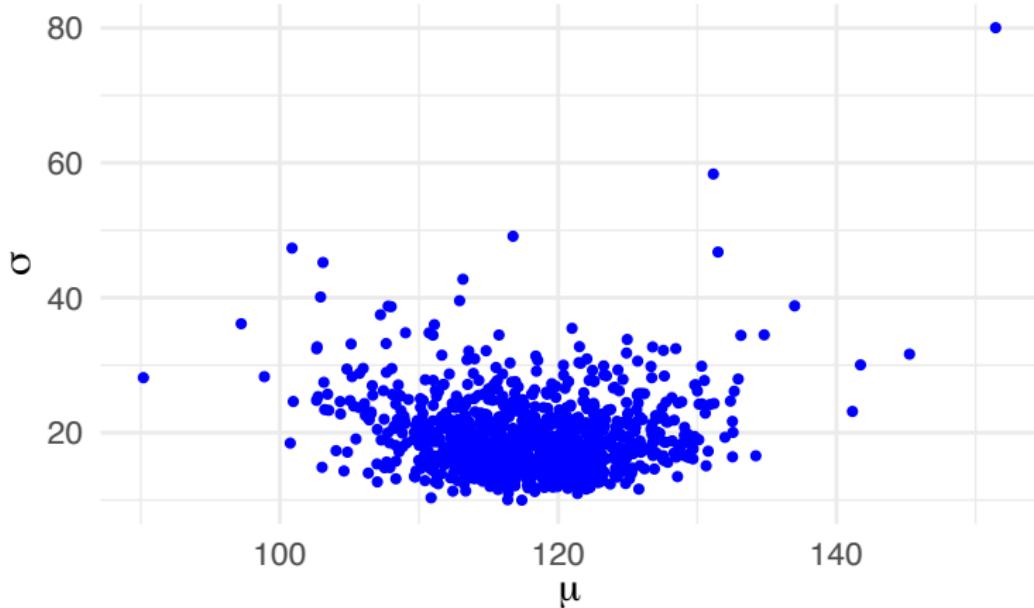
Gaussian example



$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

Gaussian example

Draws from the joint posterior distribution



$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

“equidensity contours” (analogous to a topo map showing elevations)

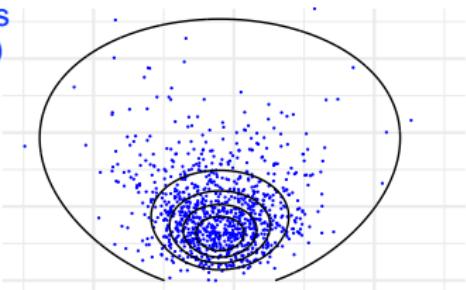
Joint posterior

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

$$\text{with } p(\mu, \sigma^2) \propto \sigma^{-2}$$

$$p(\mu, \sigma^2 | y) \propto \sigma^{-2} \prod_{i=1}^n \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y_i - \mu)^2\right)$$

this example uses an uniform prior that is improper,
but here, it results in a proper posterior



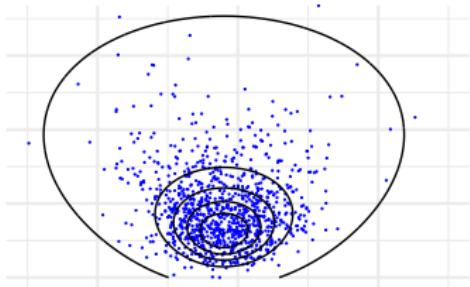
Joint posterior

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

with $p(\mu, \sigma^2) \propto \sigma^{-2}$

$$p(\mu, \sigma^2 | y) \propto \sigma^{-n-2} \exp \left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right)$$

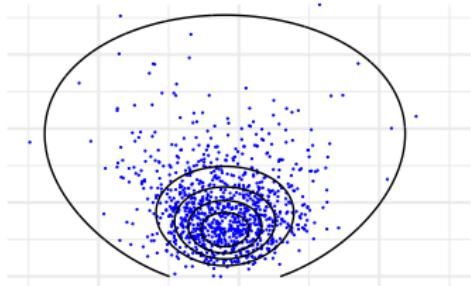
re-arrange to move product outside the exp to a sum inside the exp



Joint posterior

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

with $p(\mu, \sigma^2) \propto \sigma^{-2}$



$$p(\mu, \sigma^2 | y) \propto \sigma^{-n-2} \exp \left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2 \right)$$

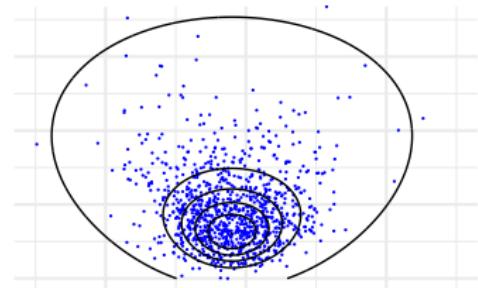
$$= \sigma^{-n-2} \exp \left(-\frac{1}{2\sigma^2} \left[\sum_{i=1}^n (y_i - \bar{y})^2 + n(\bar{y} - \mu)^2 \right] \right)$$

$$\text{where } \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$$

Joint posterior

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

with $p(\mu, \sigma^2) \propto \sigma^{-2}$



$$\begin{aligned} p(\mu, \sigma^2 | y) &\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n (y_i - \mu)^2\right) \\ &= \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[\sum_{i=1}^n (y_i - \bar{y})^2 + n(\bar{y} - \mu)^2 \right]\right) \end{aligned}$$

$$\text{where } \bar{y} = \frac{1}{n} \sum_{i=1}^n y_i$$

$$= \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2 \right]\right)$$

$$\text{where } s^2 = \frac{1}{n-1} \sum_{i=1}^n (y_i - \bar{y})^2$$

Gaussian - non-informative prior

$$\sum_{i=1}^n (y_i - \mu)^2$$

$$\sum_{i=1}^n (y_i^2 - 2y_i\mu + \mu^2)$$

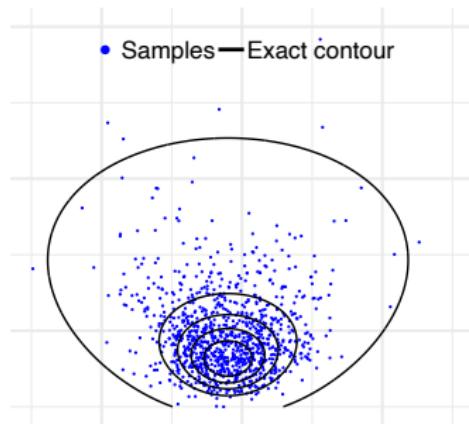
$$\sum_{i=1}^n (y_i^2 - 2y_i\mu + \mu^2 - \bar{y}^2 + \bar{y}^2 - 2y_i\bar{y} + 2y_i\bar{y})$$

$$\sum_{i=1}^n (y_i^2 - 2y_i\bar{y} + \bar{y}^2) + \sum_{i=1}^n (\mu^2 - 2y_i\mu - \bar{y}^2 + 2y_i\bar{y})$$

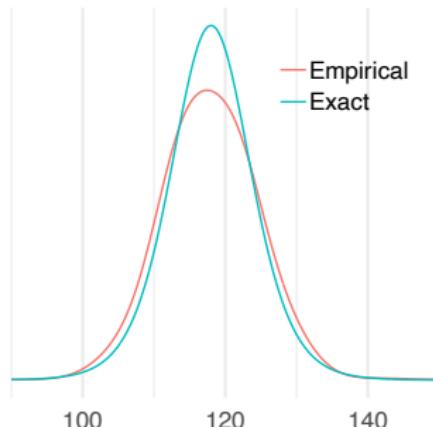
$$\sum_{i=1}^n (y_i - \bar{y})^2 + n(\mu^2 - 2\bar{y}\mu - \bar{y}^2 + 2\bar{y}\bar{y})$$

$$\sum_{i=1}^n (y_i - \bar{y})^2 + n(\bar{y} - \mu)^2$$

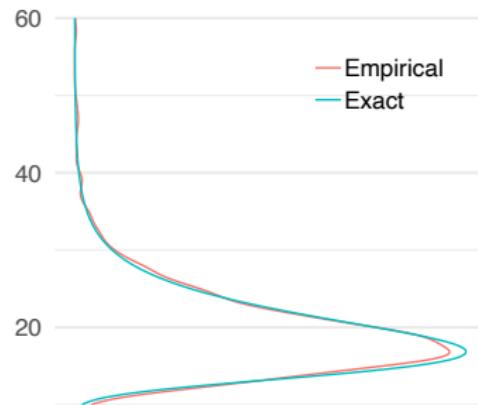
Joint posterior



Marginal of mu



Marginal of sigma



$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$
marginals

$$p(\mu | y) = \int p(\mu, \sigma | y) d\sigma$$

$$p(\sigma | y) = \int p(\mu, \sigma | y) d\mu$$

Marginal posterior $p(\sigma^2 | y)$ (easier for σ^2 than σ)

$$p(\sigma^2 | y) \propto \int p(\mu, \sigma^2 | y) d\mu$$

insert part derived in earlier slide

$$\propto \int \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} [(n-1)s^2 + n(\bar{y} - \mu)^2]\right) d\mu$$

$$\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right)$$

$$\int \exp\left(-\frac{n}{2\sigma^2}(\bar{y} - \mu)^2\right) d\mu$$

$$\int \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y - \theta)^2\right) d\theta = 1$$

$$\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \sqrt{2\pi\sigma^2/n}$$

$$\propto (\sigma^2)^{-(n+1)/2} \exp\left(-\frac{(n-1)s^2}{2\sigma^2}\right)$$

$$p(\sigma^2 | y) = \text{Inv-}\chi^2(\sigma^2 | n-1, s^2)$$

this simplification was the reason
for creating "s" in a previous slide

Gaussian - non-informative prior

Known mean

$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(n, v)$$

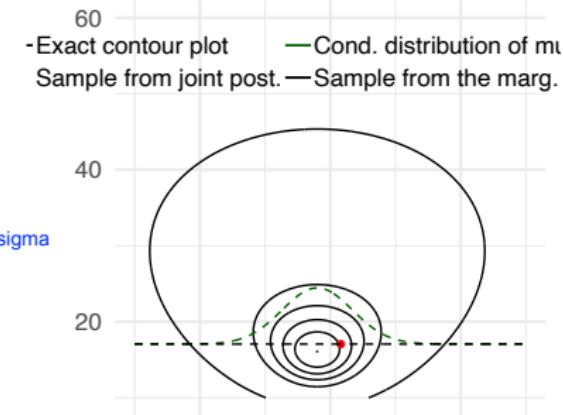
where $v = \frac{1}{n} \sum_{i=1}^n (y_i - \theta)^2$

Unknown mean

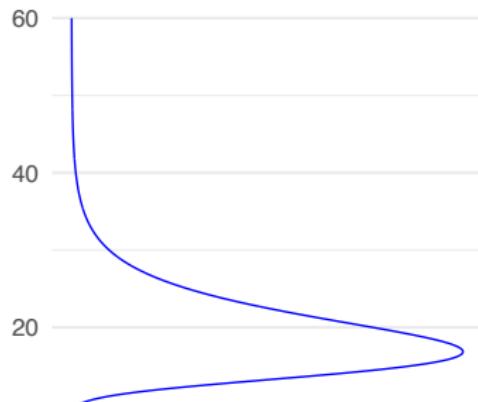
$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(n - 1, s^2)$$

where $s^2 = \frac{1}{n - 1} \sum_{i=1}^n (y_i - \bar{y})^2$

Joint posterior



Marginal of sigma



Factorization

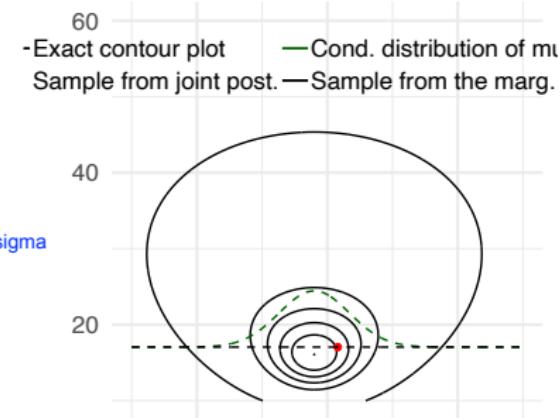
$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y) p(\sigma^2 | y)$$

$$p(\sigma^2 | y) = \text{Inv-}\chi^2(\sigma^2 | n - 1, s^2)$$

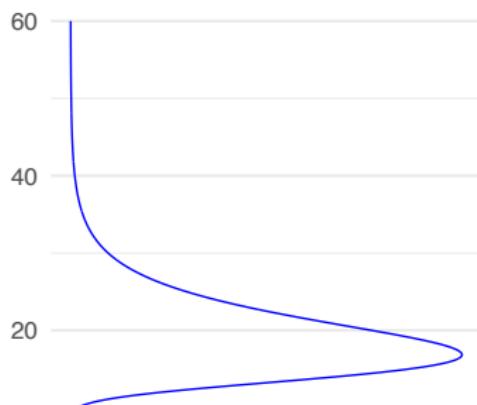
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

$$p(\mu | \sigma^2, y) = N(\mu | \bar{y}, \sigma^2/n)$$

Joint posterior



Marginal of sigma



Factorization

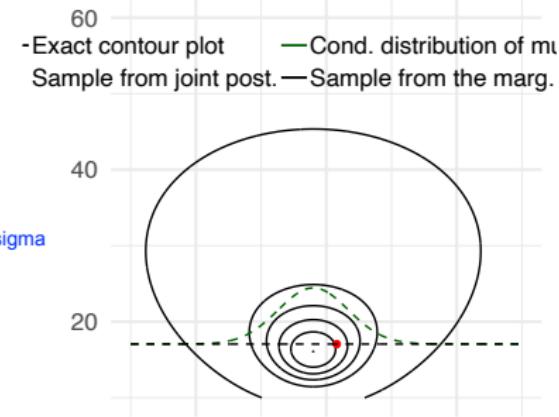
$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y) p(\sigma^2 | y)$$

$$p(\sigma^2 | y) = \text{Inv-}\chi^2(\sigma^2 | n - 1, s^2)$$

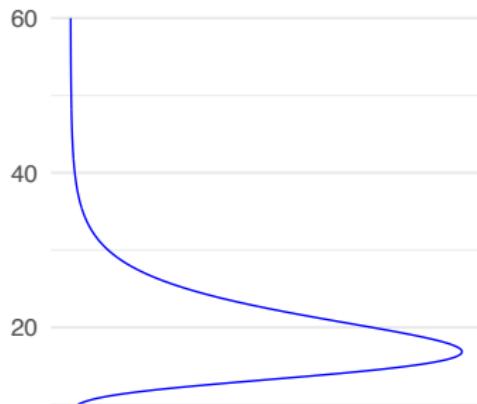
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

$$p(\mu | \sigma^2, y) = N(\mu | \bar{y}, \sigma^2/n) \propto \exp\left(-\frac{n}{2\sigma^2}(\bar{y} - \mu)^2\right)$$

Joint posterior



Marginal of sigma



Factorization

$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y) p(\sigma^2 | y)$$

$$p(\sigma^2 | y) = \text{Inv-}\chi^2(\sigma^2 | n - 1, s^2)$$

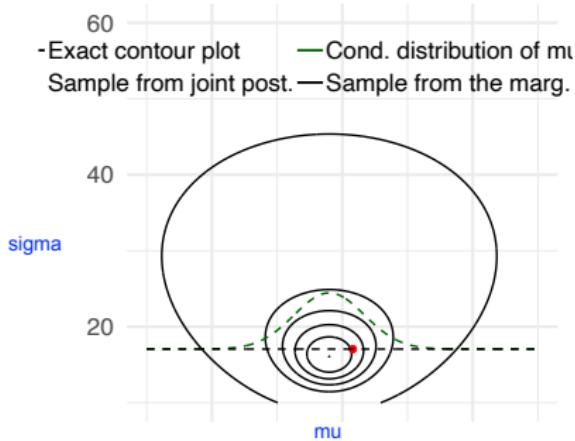
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

$$p(\mu | \sigma^2, y) = N(\mu | \bar{y}, \sigma^2/n)$$

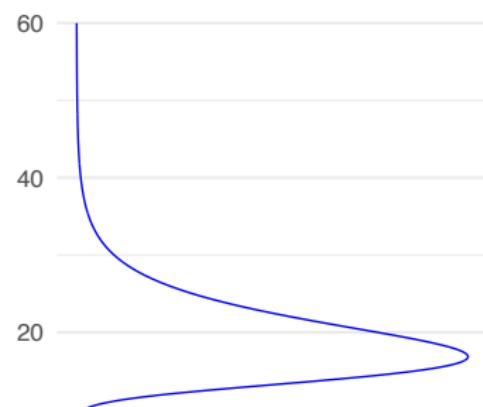
$$\mu^{(s)} \sim p(\mu | \sigma^2, y)$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

Joint posterior



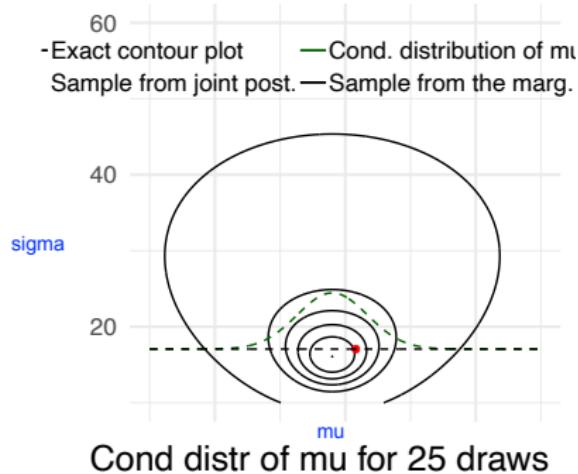
Marginal of sigma



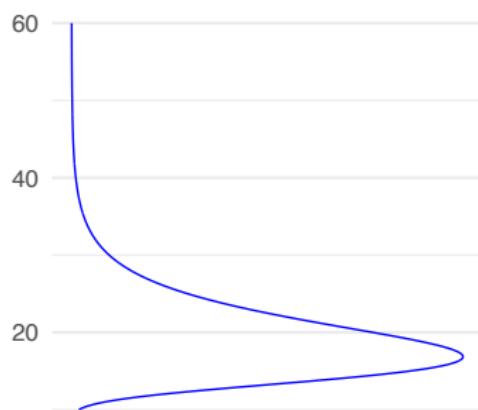
Factorization

$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y)p(\sigma^2 | y)$$
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

Joint posterior



Marginal of sigma

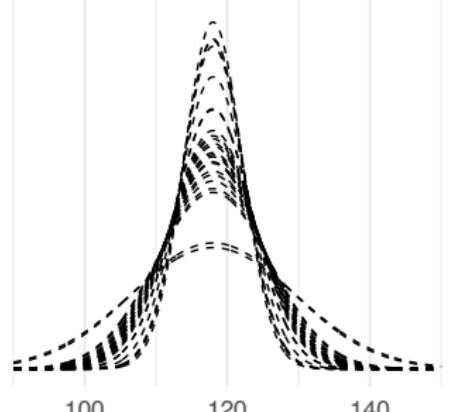


Factorization

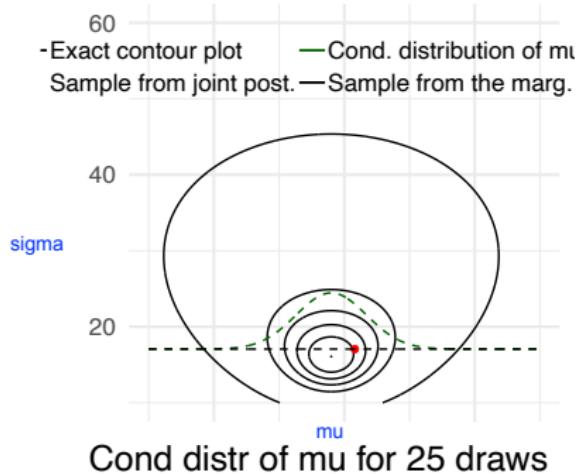
$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y)p(\sigma^2 | y)$$

$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

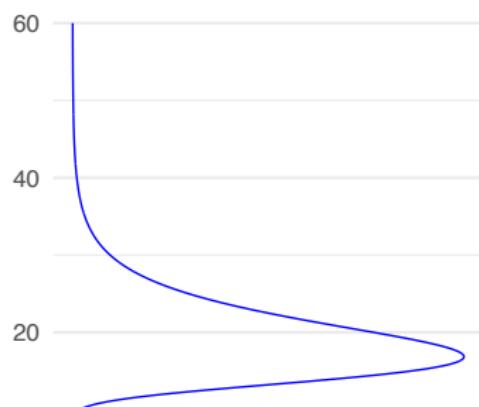
$$p(\mu | (\sigma^2)^{(s)}, y) = N(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$



Joint posterior



Marginal of sigma



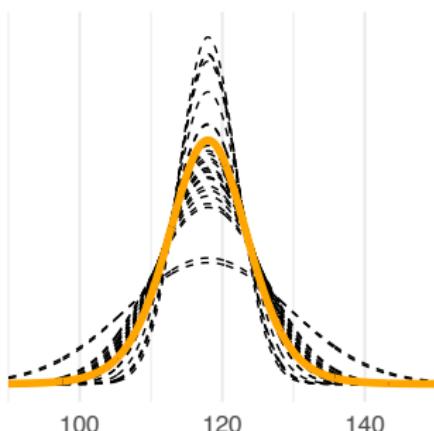
Factorization

$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y)p(\sigma^2 | y)$$

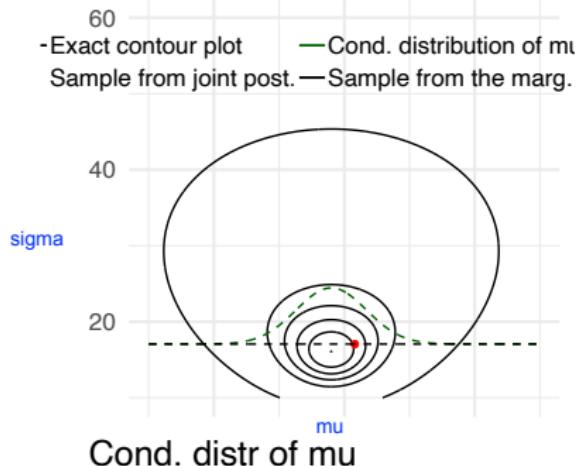
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

$$p(\mu | (\sigma^2)^{(s)}, y) = N(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$

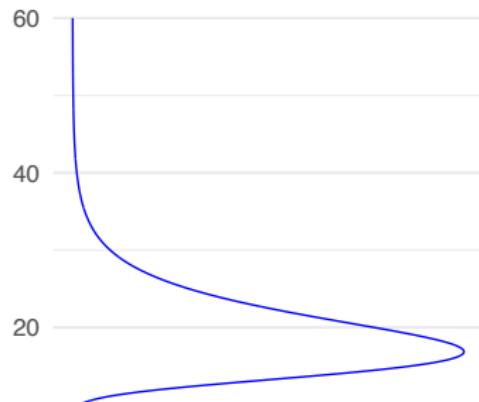
$$p(\mu | y) \approx \frac{1}{S} \sum_{s=1}^S N(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$



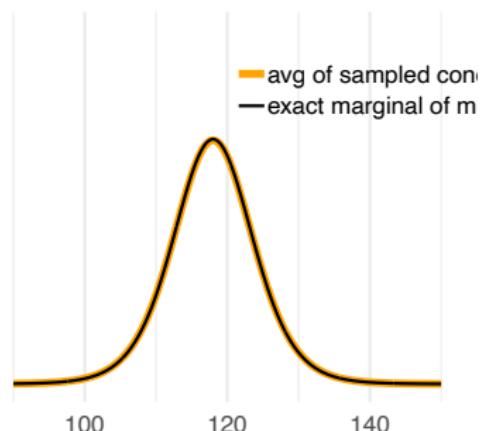
Joint posterior



Marginal of sigma



Factorization



$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y)p(\sigma^2 | y)$$

$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

$$p(\mu | (\sigma^2)^{(s)}, y) = N(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$

$$p(\mu | y) \approx \frac{1}{S} \sum_{s=1}^S N(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$

Marginal posterior $p(\mu | y)$

$$p(\mu | y) = \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2$$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

same joint distribution as before with the sufficient statistic

Marginal posterior $p(\mu | y)$

$$p(\mu | y) = \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2$$

$$\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(\textcolor{blue}{n}-1)s^2 + n(\bar{y} - \mu)^2 \right]\right) d\sigma^2$$

Transformation

$$A = (\textcolor{blue}{n}-1)s^2 + n(\mu - \bar{y})^2$$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

Transformation

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

Transformation

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

$$p(\mu | y) \propto A^{-n/2} \int_0^\infty z^{(n-2)/2} \exp(-z) dz$$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

Transformation

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

$$p(\mu | y) \propto A^{-n/2} \int_0^\infty z^{(n-2)/2} \exp(-z) dz$$

Recognize gamma integral $\Gamma(u) = \int_0^\infty x^{u-1} \exp(-x) dx$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

Transformation

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

$$p(\mu | y) \propto A^{-n/2} \int_0^\infty z^{(n-2)/2} \exp(-z) dz$$

Recognize gamma integral $\Gamma(u) = \int_0^\infty x^{u-1} \exp(-x) dx$

$$\propto [(n-1)s^2 + n(\mu - \bar{y})^2]^{-n/2}$$

Marginal posterior $p(\mu | y)$

$$\begin{aligned} p(\mu | y) &= \int_0^\infty p(\mu, \sigma^2 | y) d\sigma^2 \\ &\propto \int_0^\infty \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2} \left[(n-1)s^2 + n(\bar{y} - \mu)^2\right]\right) d\sigma^2 \end{aligned}$$

Transformation

$$A = (n-1)s^2 + n(\mu - \bar{y})^2 \quad \text{and} \quad z = \frac{A}{2\sigma^2}$$

$$p(\mu | y) \propto A^{-n/2} \int_0^\infty z^{(n-2)/2} \exp(-z) dz$$

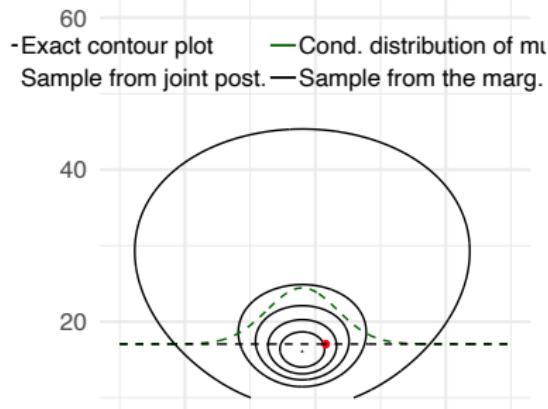
Recognize gamma integral $\Gamma(u) = \int_0^\infty x^{u-1} \exp(-x) dx$

$$\propto [(n-1)s^2 + n(\mu - \bar{y})^2]^{-n/2}$$

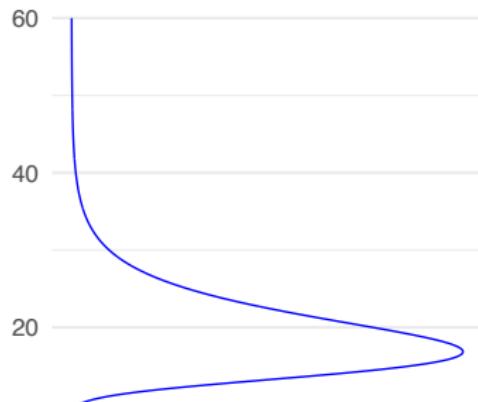
$$\propto \left[1 + \frac{n(\mu - \bar{y})^2}{(n-1)s^2}\right]^{-n/2}$$

$$p(\mu | y) = t_{n-1}(\mu | \bar{y}, s^2/n) \quad \text{Student's } t$$

Joint posterior



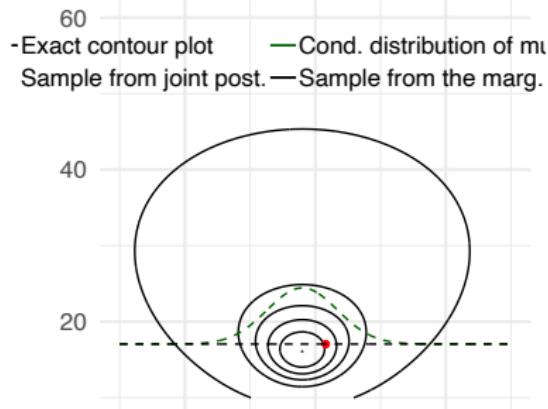
Marginal of sigma



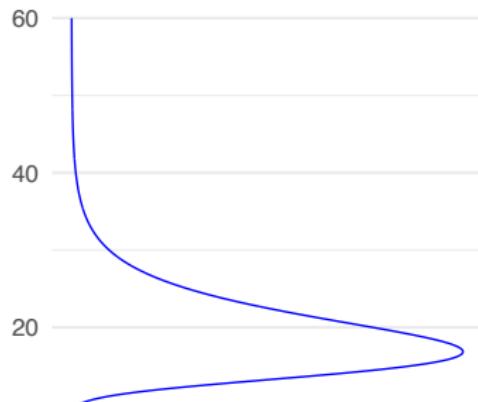
Predictive distribution for new \tilde{y}

$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

Joint posterior



Marginal of sigma



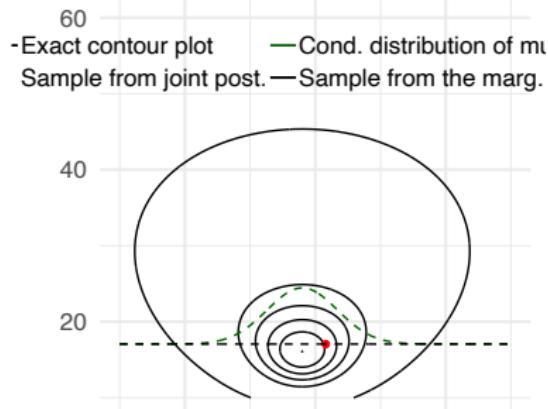
Predictive distribution for new \tilde{y}

$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

sample the parameters for a normal distribution from the joint prob.

Joint posterior



Predictive distribution for new \tilde{y}

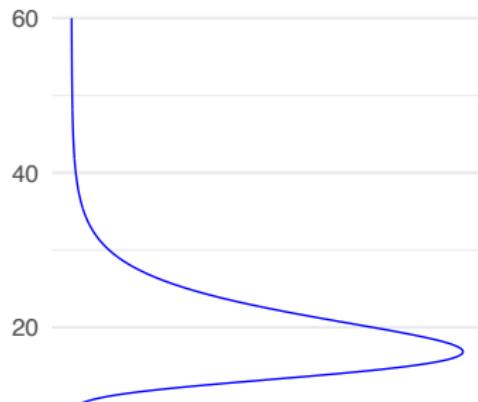
$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

$$\tilde{y}^{(s)} \sim p(\tilde{y} | \mu^{(s)}, \sigma^{(s)})$$

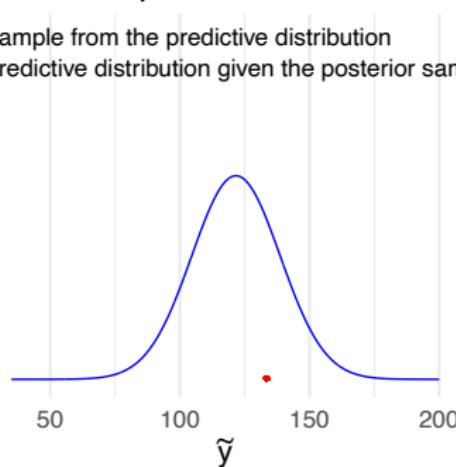
from the sampled mu and sigma, sample a posterior pred. data point

Marginal of sigma

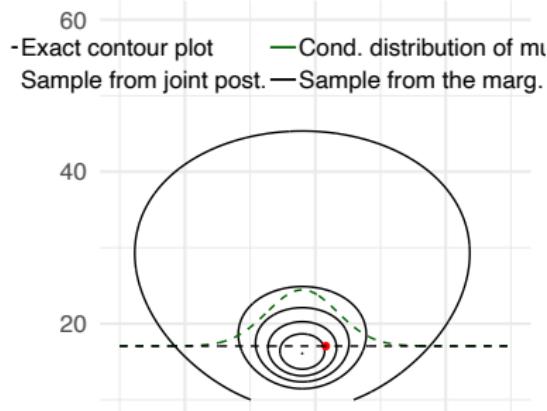


Posterior predictive distribution

Sample from the predictive distribution
Predictive distribution given the posterior samp



Joint posterior



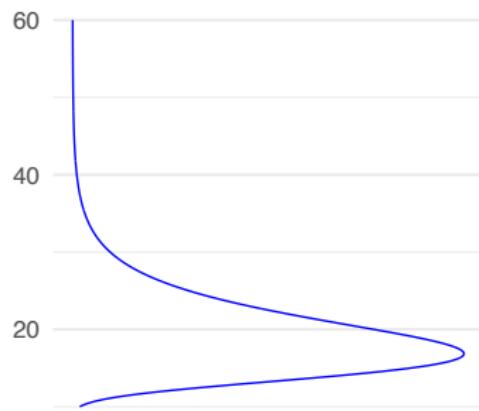
Predictive distribution for new \tilde{y}

$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

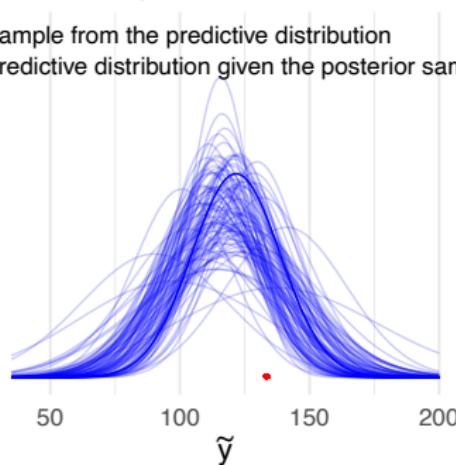
$$\tilde{y}^{(s)} \sim p(\tilde{y} | \mu^{(s)}, \sigma^{(s)})$$

Marginal of sigma

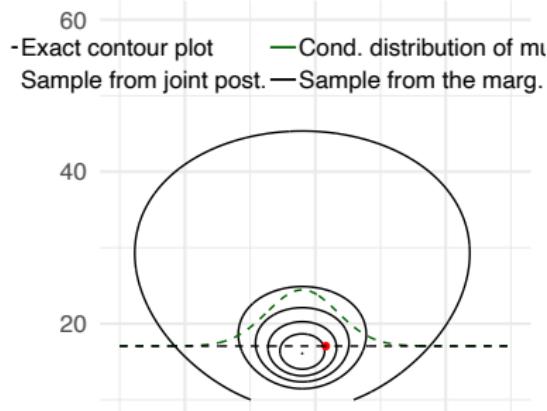


Posterior predictive distribution

Sample from the predictive distribution
Predictive distribution given the posterior sample



Joint posterior



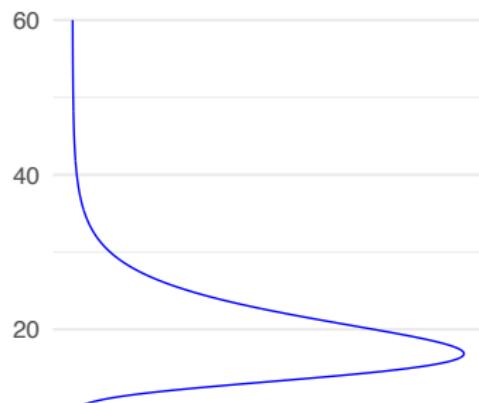
Predictive distribution for new \tilde{y}

$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

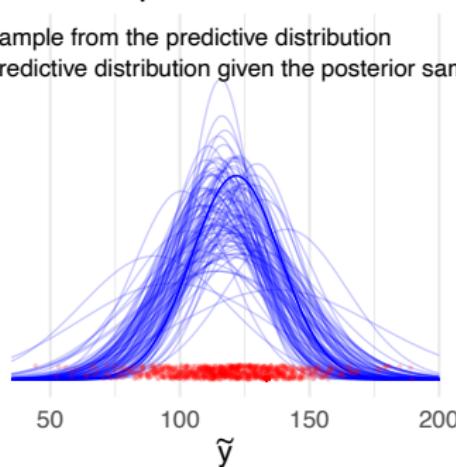
$$\tilde{y}^{(s)} \sim p(\tilde{y} | \mu^{(s)}, \sigma^{(s)})$$

Marginal of sigma

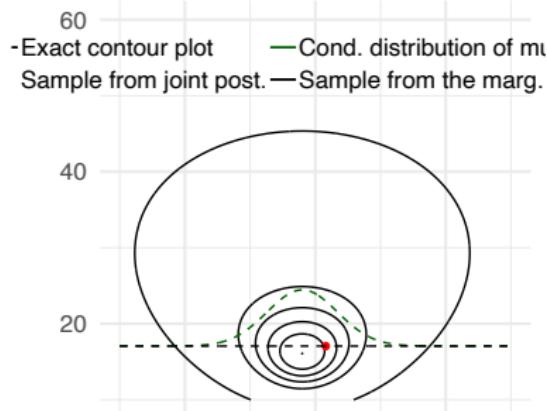


Posterior predictive distribution

Sample from the predictive distribution
Predictive distribution given the posterior samp



Joint posterior



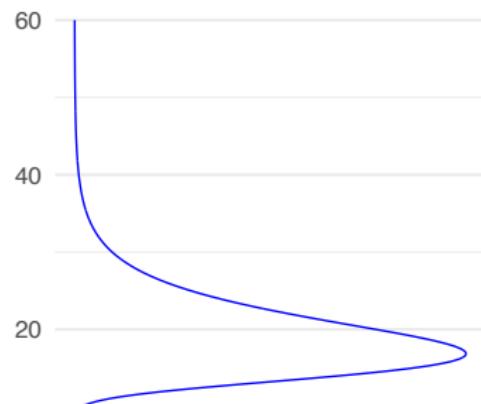
Predictive distribution for new \tilde{y}

$$p(\tilde{y} | y) = \int p(\tilde{y} | \mu, \sigma) p(\mu, \sigma | y) d\mu d\sigma$$

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$

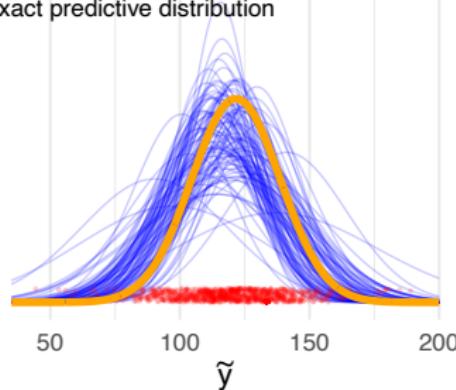
$$\tilde{y}^{(s)} \sim p(\tilde{y} | \mu^{(s)}, \sigma^{(s)})$$

Marginal of sigma



Posterior predictive distribution

- Sample from the predictive distribution
- Predictive distribution given the posterior sample
- Exact predictive distribution



Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

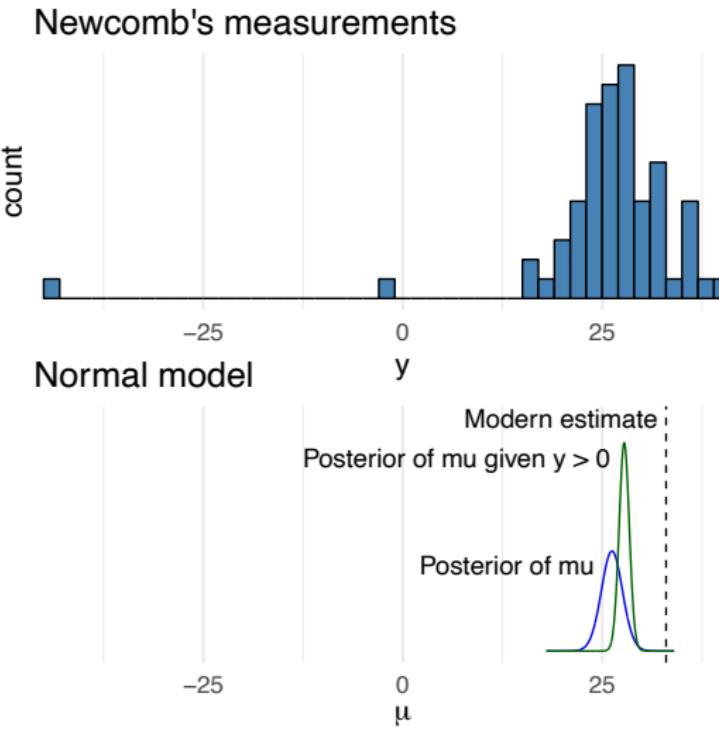
$$\begin{aligned} p(\tilde{y} \mid \sigma^2, y) &= \int p(\tilde{y} \mid \mu, \sigma^2) p(\mu \mid \sigma^2, y) d\mu \\ &= \int N(\tilde{y} \mid \mu, \sigma^2) N(\mu \mid \bar{y}, \sigma^2/n) d\mu \\ &= N(\tilde{y} \mid \bar{y}, (1 + \frac{1}{n})\sigma^2) \end{aligned}$$

this is up to scaling factor same as $p(\mu \mid \sigma^2, y)$

$$p(\tilde{y} \mid y) = t_{n-1}(\tilde{y} \mid \bar{y}, (1 + \frac{1}{n})s^2)$$

Simon Newcomb's light of speed experiment in 1882

Newcomb measured ($n = 66$) the time required for light to travel from his laboratory on the Potomac River to a mirror at the base of the Washington Monument and back, a total distance of 7422 meters.



Gaussian - conjugate prior

- Conjugate prior has to have a form $p(\sigma^2)p(\mu | \sigma^2)$ (see the chapter notes)
- Handy parameterization

$$\mu | \sigma^2 \sim N(\mu_0, \sigma^2 / \kappa_0)$$

$$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$$

which can be written as

$$p(\mu, \sigma^2) = N\text{-Inv-}\chi^2(\mu_0, \sigma_0^2 / \kappa_0; \nu_0, \sigma_0^2)$$

- μ and σ^2 are a priori dependent
 - if σ^2 is large, then μ has wide prior

Gaussian - conjugate prior

Joint posterior (exercise 3.9)

$$p(\mu, \sigma^2 | y) = \text{N-Inv-}\chi^2(\mu_n, \sigma_n^2 / \kappa_n; \nu_n, \sigma_n^2)$$

where

$$\mu_n = \frac{\kappa_0}{\kappa_0 + n} \mu_0 + \frac{n}{\kappa_0 + n} \bar{y}$$

$$\kappa_n = \kappa_0 + n$$

$$\nu_n = \nu_0 + n$$

$$\nu_n \sigma_n^2 = \nu_0 \sigma_0^2 + (n - 1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n} (\bar{y} - \mu_0)^2$$

Multinomial model for categorical data

- Extension of binomial
- Observation model

$$p(y \mid \theta) \propto \prod_{j=1}^k \theta_j^{y_j},$$

- BDA3 p. 69–

Multivariate Gaussian

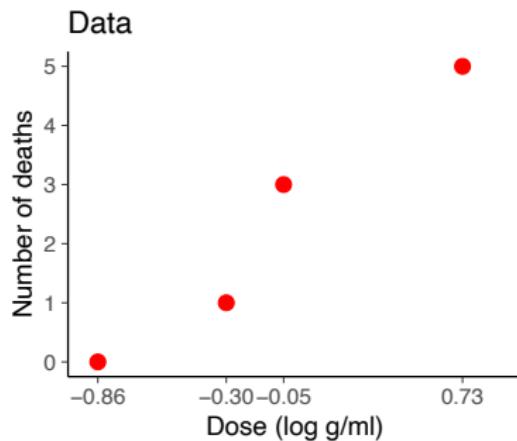
- Observation model

$$p(y | \mu, \Sigma) \propto |\Sigma|^{-1/2} \exp\left(-\frac{1}{2}(y - \mu)^T \Sigma^{-1} (y - \mu)\right),$$

- BDA3 p. 72–
- New recommended LKJ-prior mentioned in Appendix A, see more in Stan manual

Bioassay

Dose, x_i (log g/ml)	Number of animals, n_i	Number of deaths, y_i
-0.86	5	0
-0.30	5	1
-0.05	5	3
0.73	5	5



Find out lethal dose 50% (LD50)

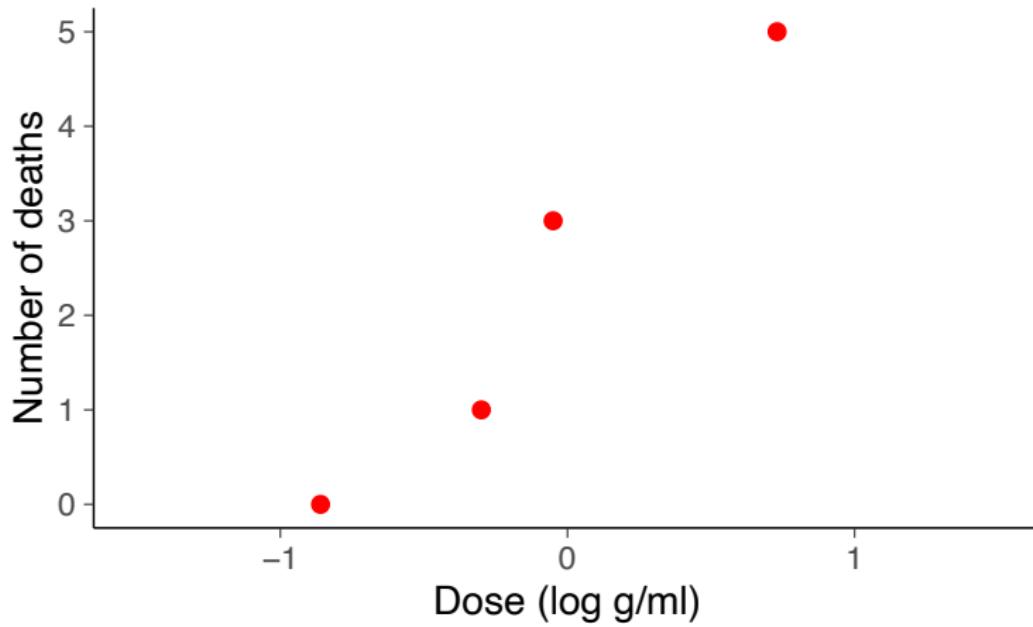
- used to classify how hazardous chemical is
- 1984 EEC directive has 4 levels (see the chapter notes)

Bayesian methods help to

- reduce the number of animals needed
- easy to make sequential experiment and stop as soon as desired accuracy is obtained

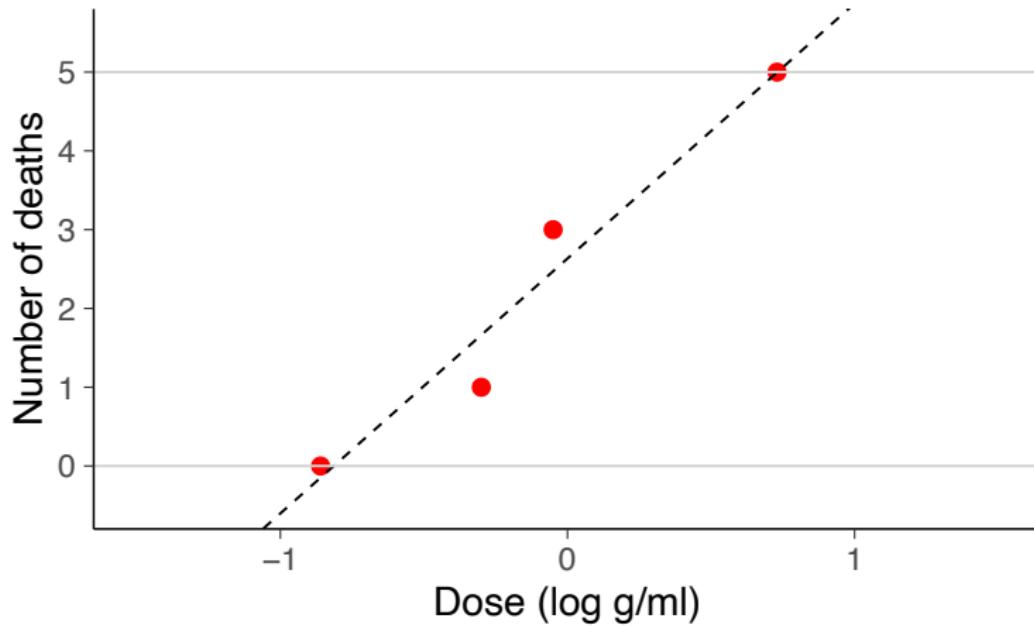
Bioassay

Data

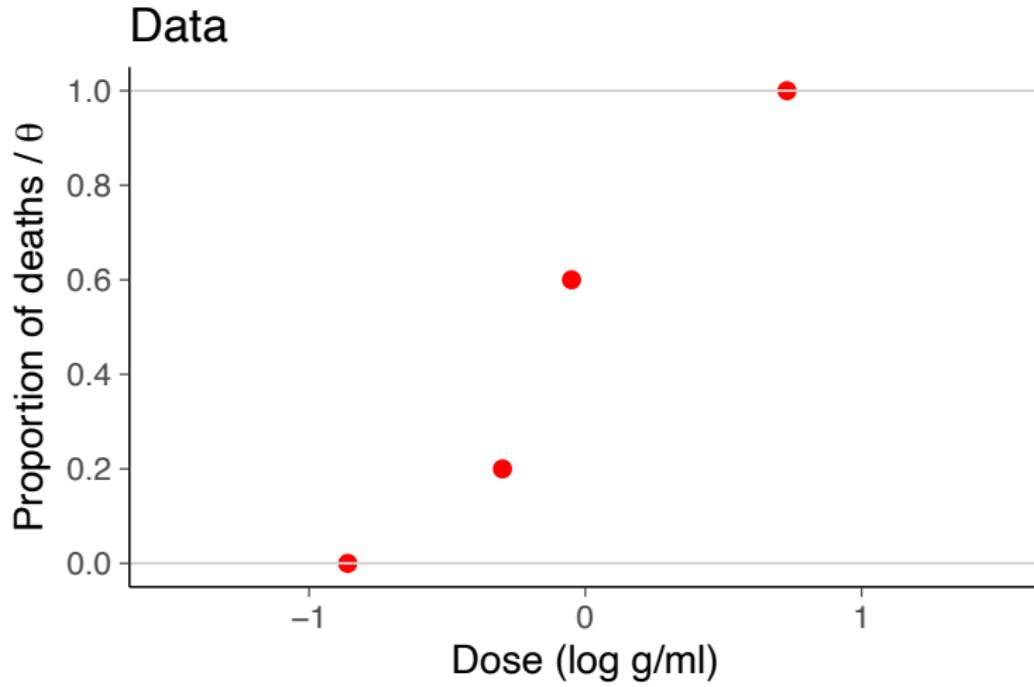


Bioassay

Linear fit



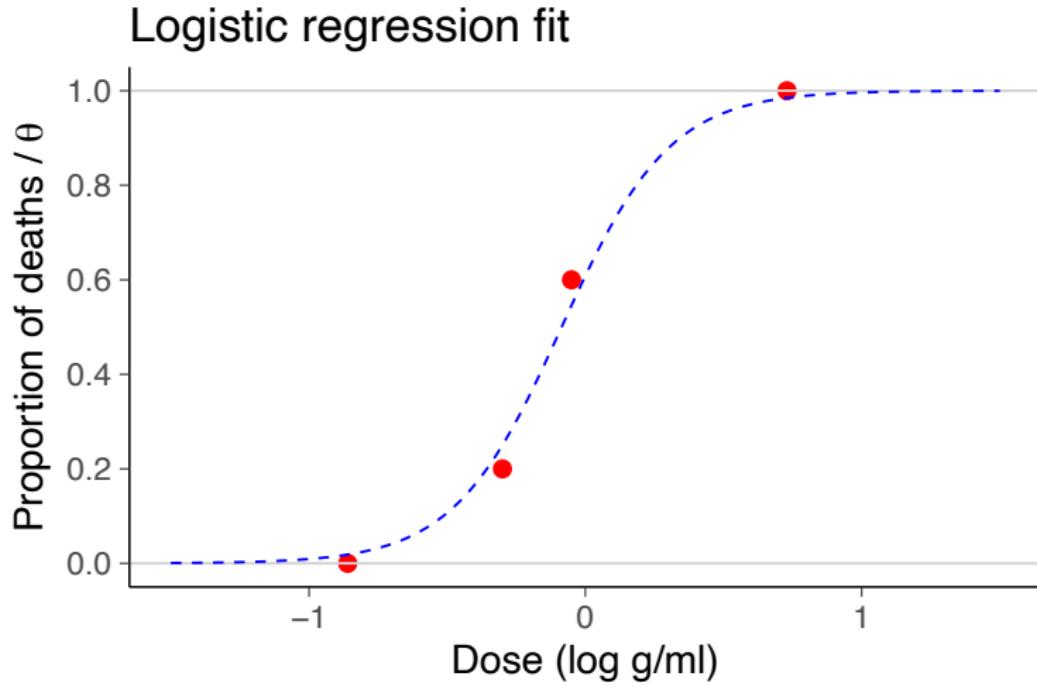
Bioassay



Binomial model

$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

Bioassay



Binomial model

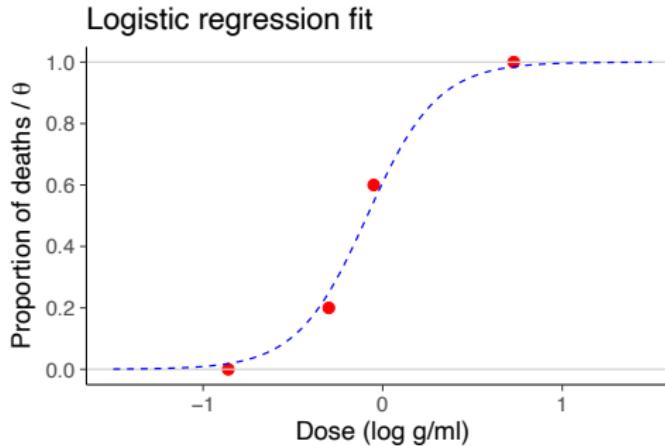
$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i), \quad \text{logit}(\theta_i) = \log \left(\frac{\theta_i}{1 - \theta_i} \right) = \alpha + \beta x_i$$

Bioassay

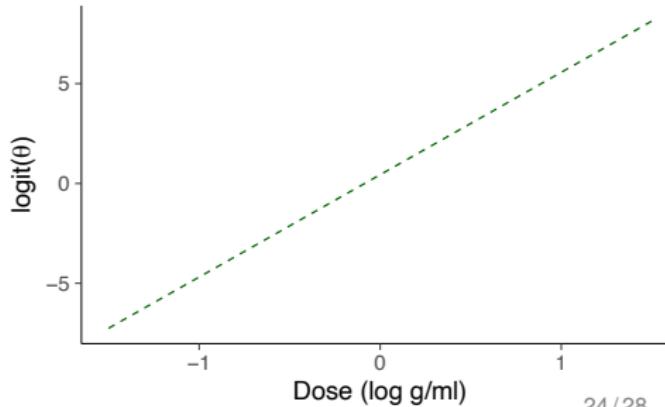
$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

$$\begin{aligned}\text{logit}(\theta_i) &= \log \left(\frac{\theta_i}{1 - \theta_i} \right) \\ &= \alpha + \beta x_i\end{aligned}$$

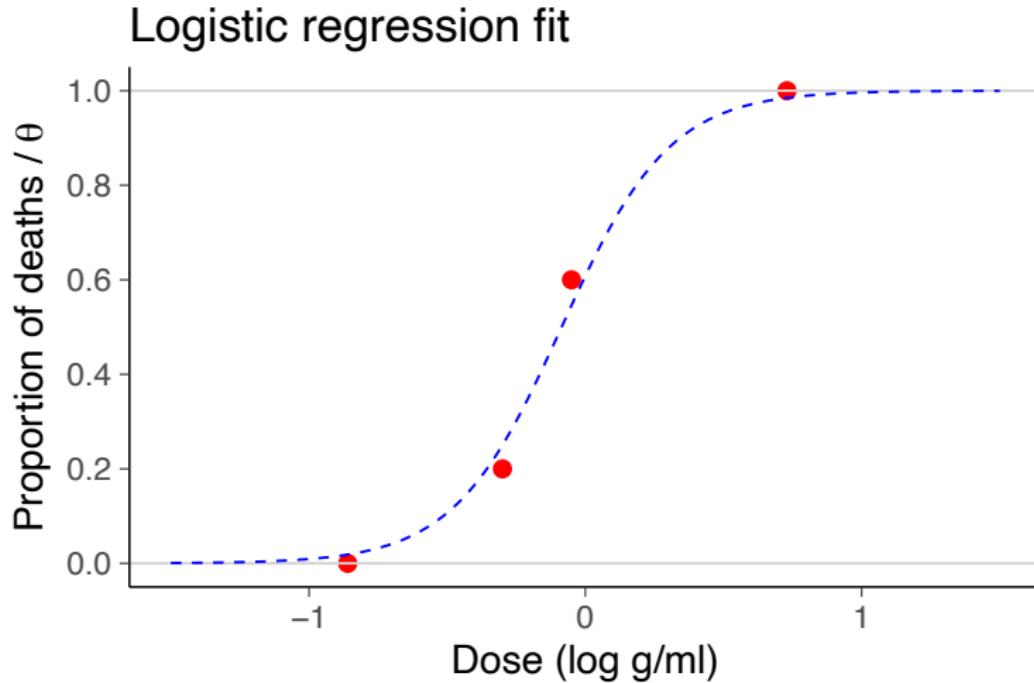
$$\theta_i = \frac{1}{1 + \exp(-(\alpha + \beta x_i))}$$



Logistic regression in latent space

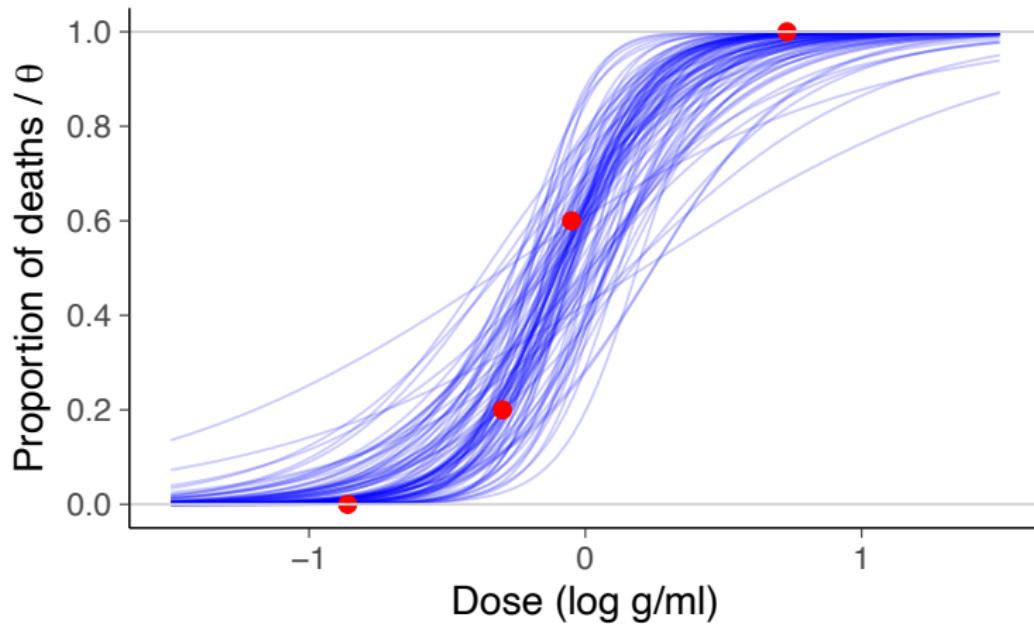


Bioassay

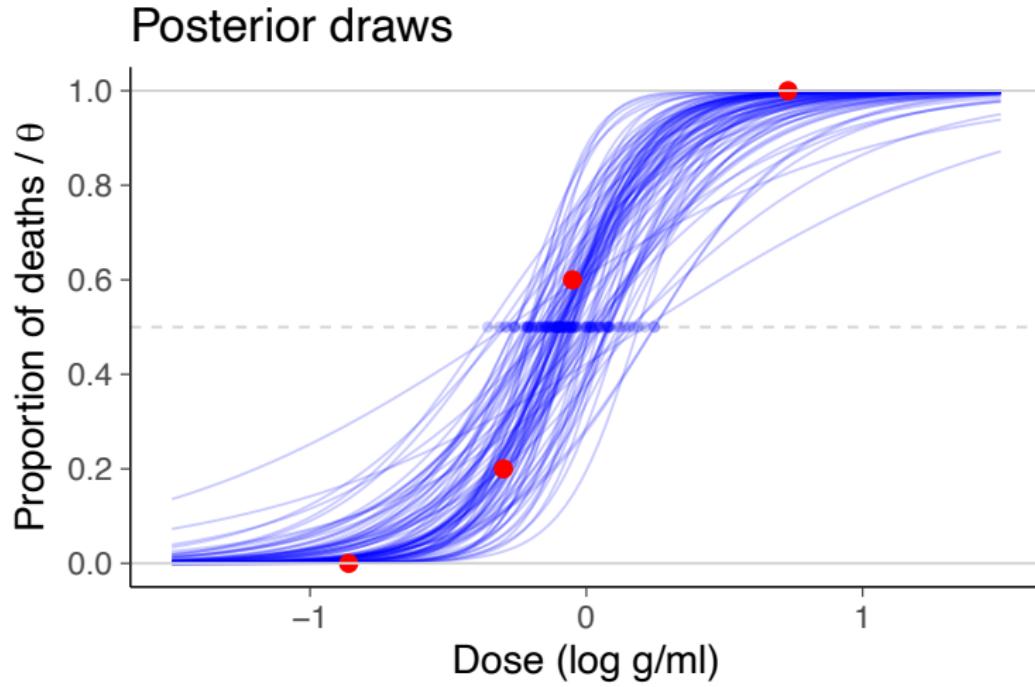


Bioassay

Posterior draws

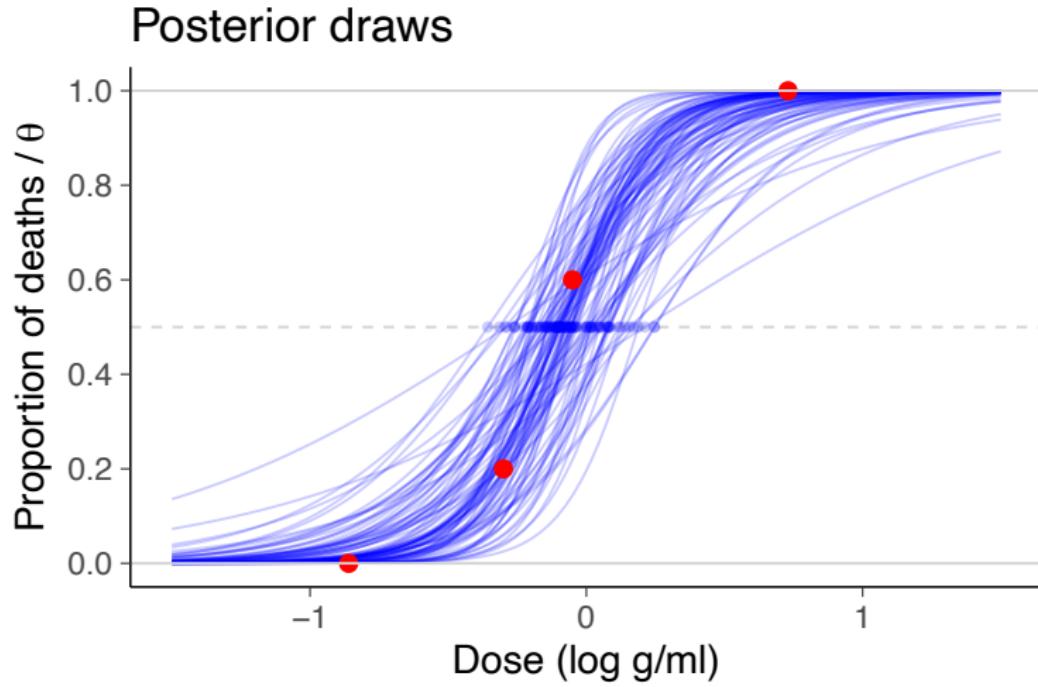


Bioassay



$$\text{LD50: } E\left(\frac{y}{n}\right) = \text{logit}^{-1}(\alpha + \beta x) = 0.5$$

Bioassay

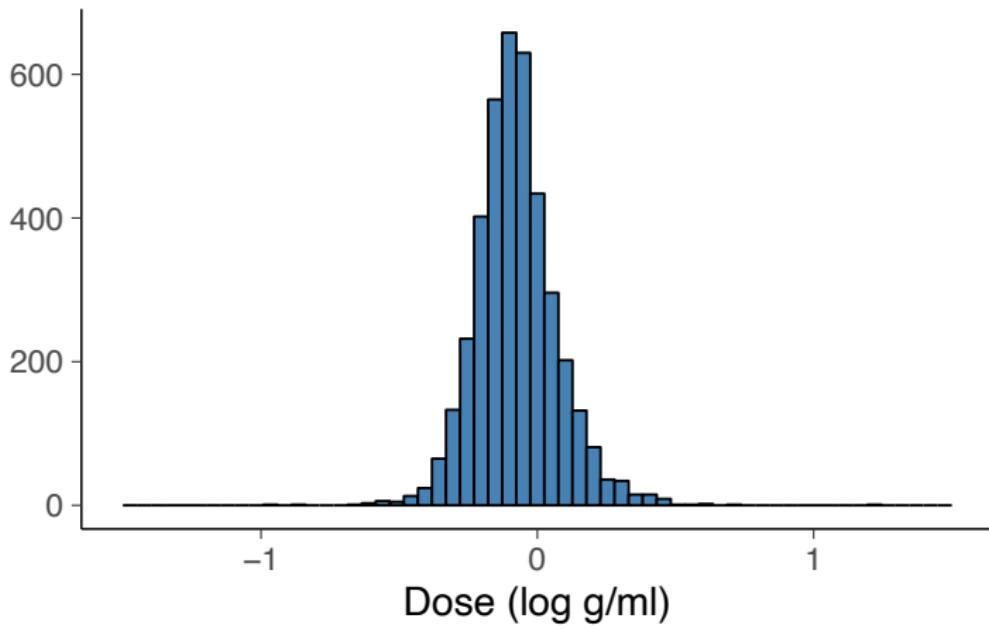


$$\text{LD50: } E\left(\frac{y}{n}\right) = \text{logit}^{-1}(\alpha + \beta x) = 0.5 \Rightarrow x_{\text{LD50}} = -\alpha/\beta$$

$$x_{\text{LD50}}^{(s)} = -\alpha^{(s)}/\beta^{(s)}$$

Bioassay

Bioassay LD50



Bioassay posterior

Binomial model

$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

Link function

$$\text{logit}(\theta_i) = \alpha + \beta x_i$$

Bioassay posterior

Binomial model

$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

Link function

$$\text{logit}(\theta_i) = \alpha + \beta x_i$$

Likelihood

$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto \theta_i^{y_i} [1 - \theta_i]^{n_i - y_i}$$

$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto [\text{logit}^{-1}(\alpha + \beta x_i)]^{y_i} [1 - \text{logit}^{-1}(\alpha + \beta x_i)]^{n_i - y_i}$$

Bioassay posterior

Binomial model

$$y_i \mid \theta_i \sim \text{Bin}(\theta_i, n_i)$$

Link function

$$\text{logit}(\theta_i) = \alpha + \beta x_i$$

Likelihood

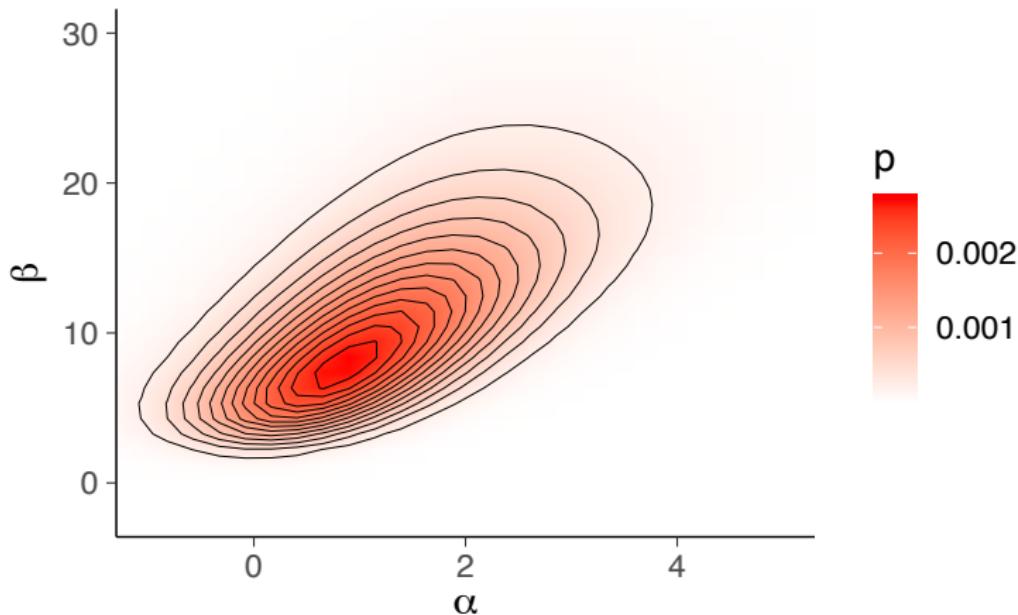
$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto \theta_i^{y_i} [1 - \theta_i]^{n_i - y_i}$$

$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto [\text{logit}^{-1}(\alpha + \beta x_i)]^{y_i} [1 - \text{logit}^{-1}(\alpha + \beta x_i)]^{n_i - y_i}$$

Posterior (with uniform prior on α, β)

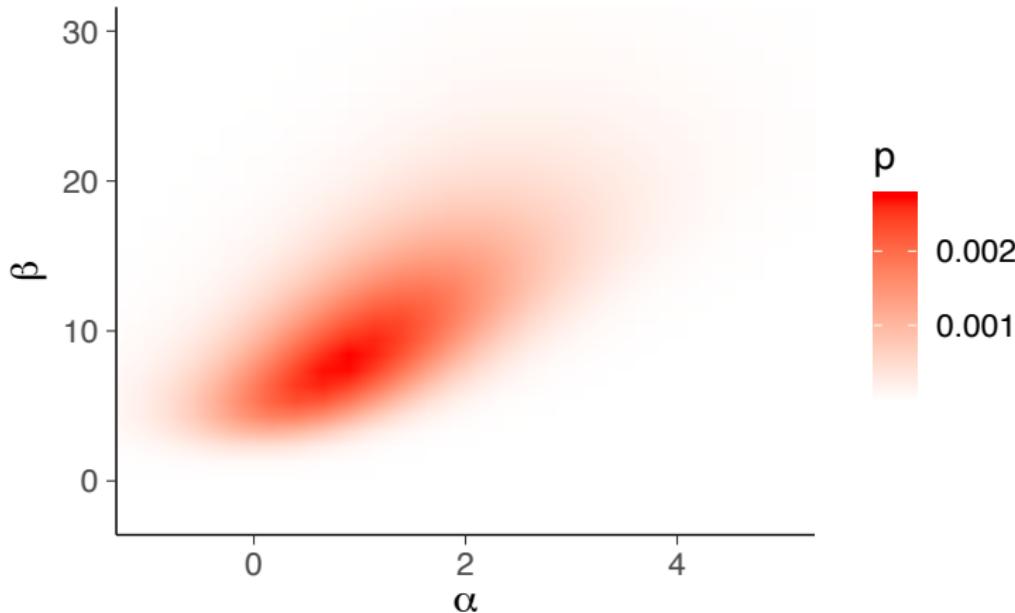
$$p(\alpha, \beta \mid y, n, x) \propto p(\alpha, \beta) \prod_{i=1}^n p(y_i \mid \alpha, \beta, n_i, x_i)$$

Posterior density evaluated in a grid



Bioassay

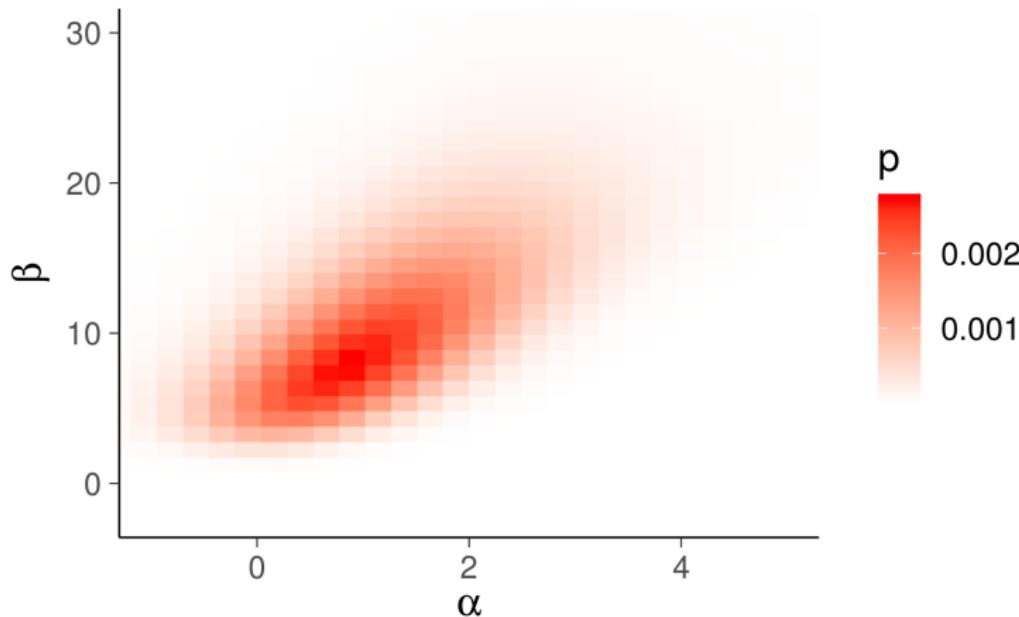
Posterior density evaluated in a grid



Density evaluated in grid, but plotted using interpolation

Bioassay

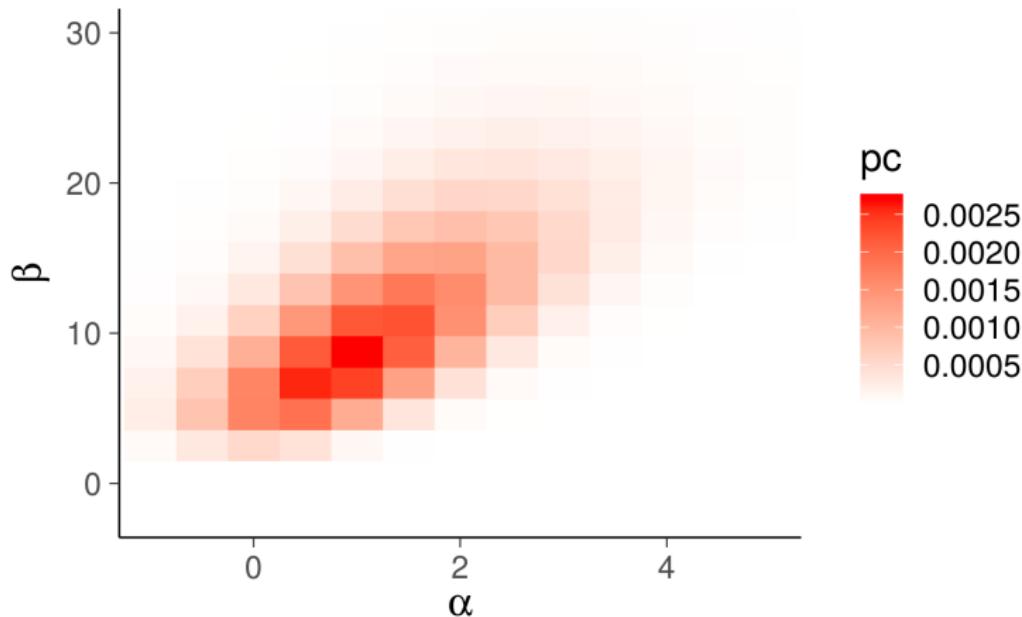
Posterior density evaluated in a grid



Density evaluated in grid, and plotted without interpolation

Bioassay

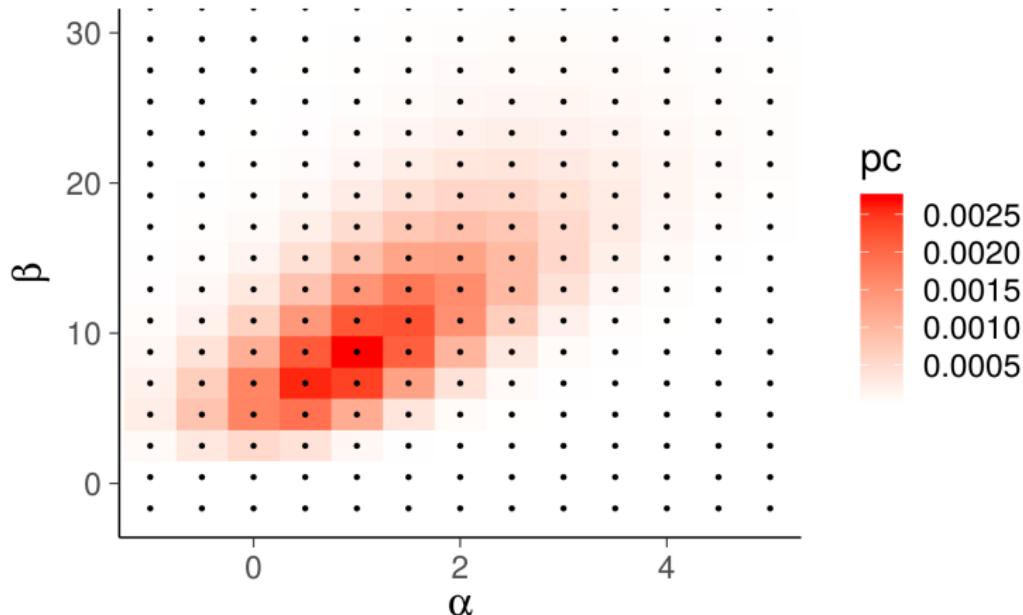
Posterior density evaluated in a grid



Density evaluated in a coarser grid

Bioassay

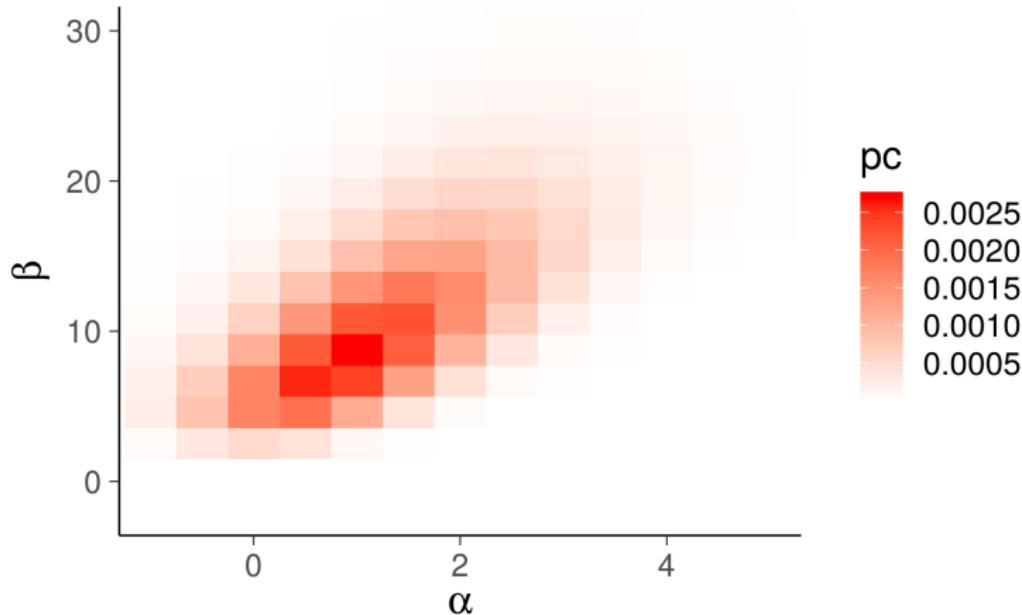
Posterior density evaluated in a grid



- Approximate the density as piecewise constant function
- Evaluate density in a grid over some finite region
- Density times cell area gives probability mass in each cell

Bioassay

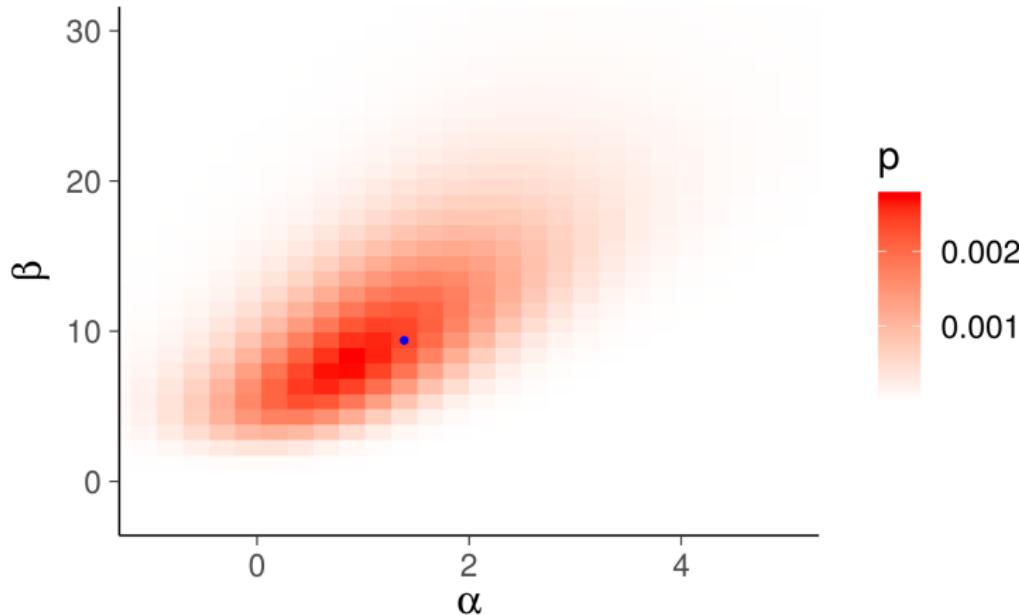
Posterior density evaluated in a grid



- Densities at 1, 2, and 3: 0.0027 0.0010 0.0001
- Probabilities of cells 1, 2, and 3: 0.0431 0.0166 0.0010
- Probabilities of cells sum to 1

Bioassay

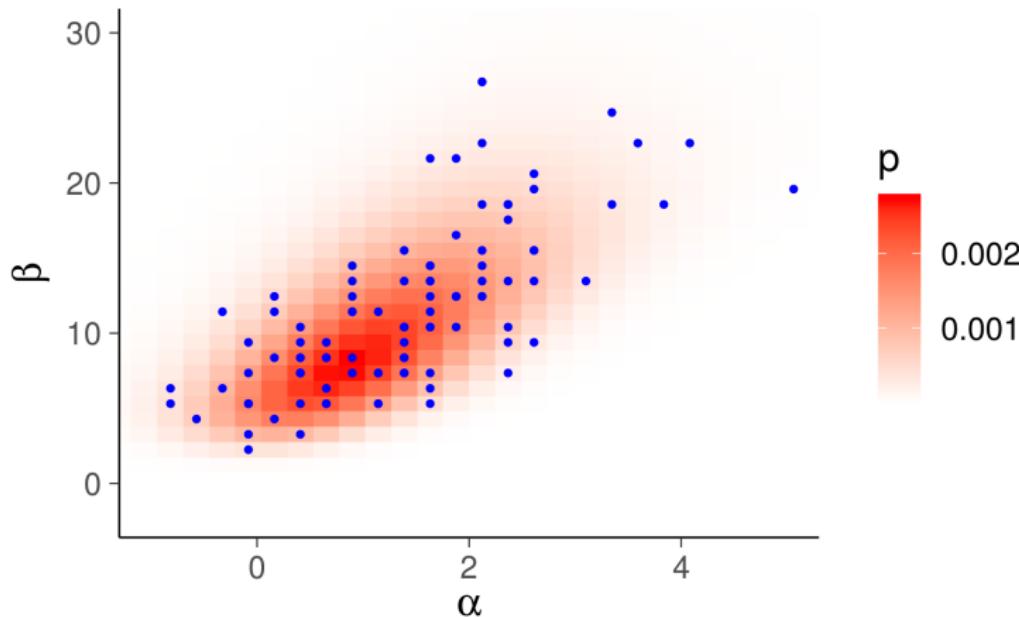
Posterior density and draws in a grid



- Sample according to grid cell probabilities

Bioassay

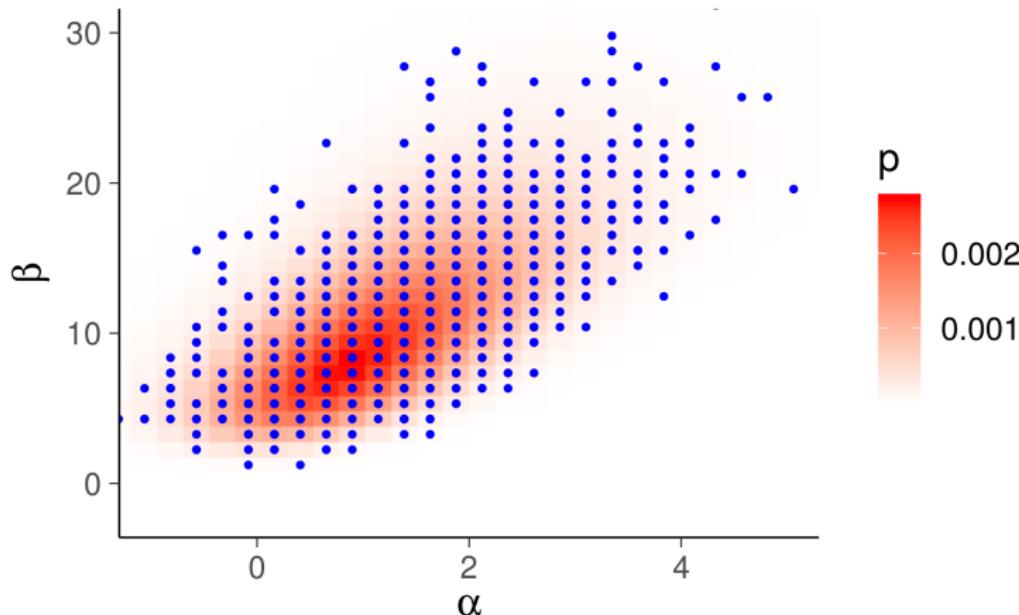
Posterior density and draws in a grid



- Sample according to grid cell probabilities

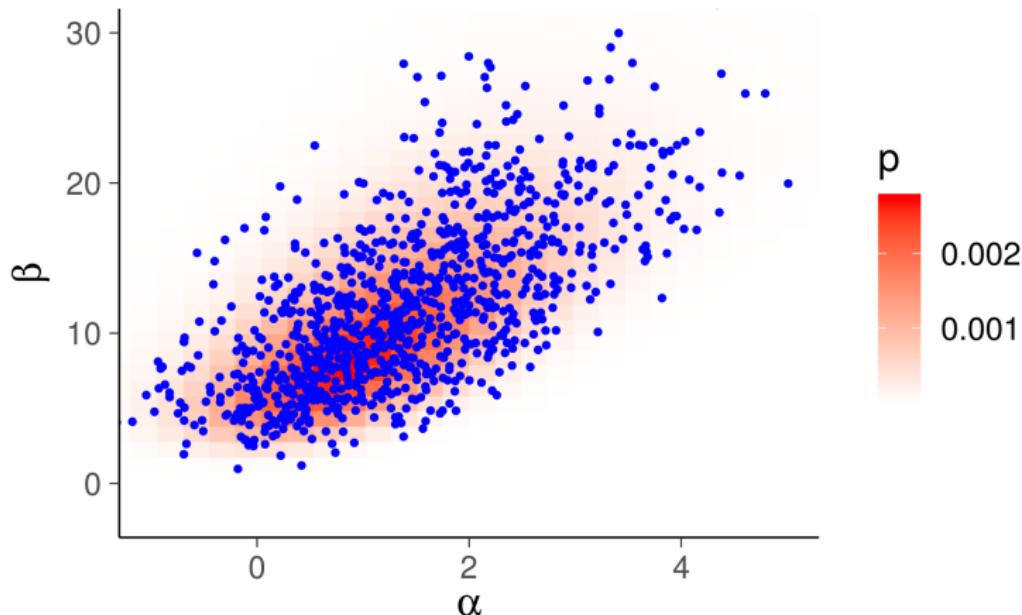
Bioassay

Posterior density and draws in a grid



- Sample according to grid cell probabilities
- Several draws can be from the same grid cell

Posterior density in a grid and jittered draws



- Jitter can be added to improve visualization

Grid sampling

- Draws can be used to estimate expectations, for example

$$E[x_{\text{LD50}}] = E[-\alpha/\beta] \approx \frac{1}{S} \sum_{s=1}^S \frac{\alpha^{(s)}}{\beta^{(s)}}$$

- Instead of sampling, grid could be used to evaluate functions directly, for example

$$E[-\alpha/\beta] \approx \sum_{t=1}^T w_{\text{cell}}^{(t)} \frac{\alpha^{(t)}}{\beta^{(t)}},$$

where $w_{\text{cell}}^{(t)}$ is the normalized probability of a grid cell t , and $\alpha^{(t)}$ and $\beta^{(t)}$ are center locations of grid cells

- Grid sampling gets computationally too expensive in high dimensions