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Bayesian Statistics and Data Analysis
Lecture 3

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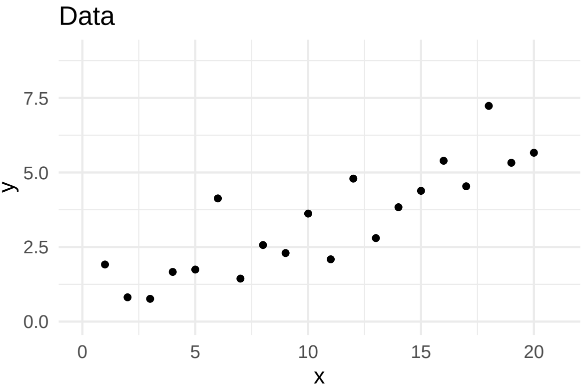
Department of Statistics, Uppsala University
Thanks to Aki Vehtari, Aalto University

Example of uncertainty in modeling



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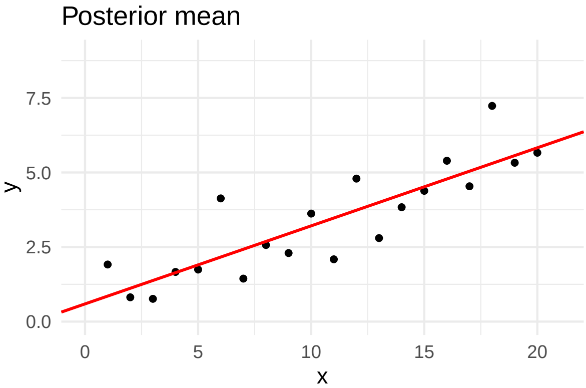

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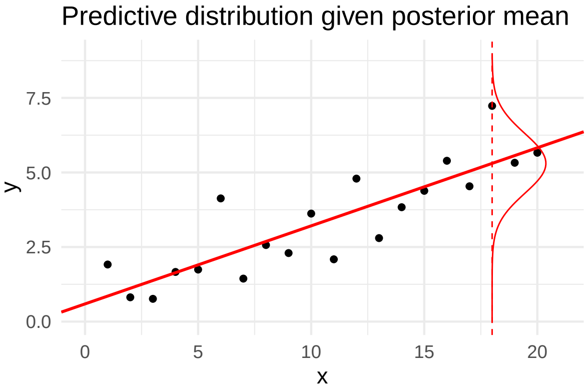

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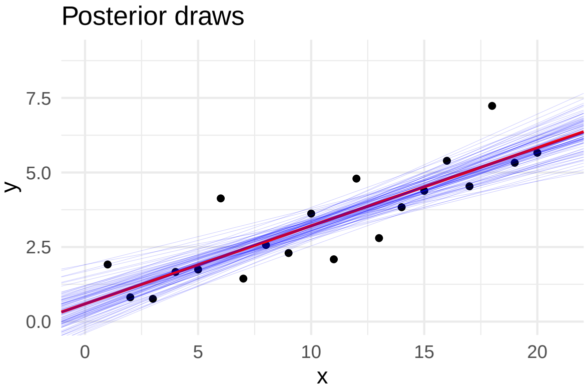
  - Multivariate Gaussian
- Bioassay example

Example of uncertainty in modeling



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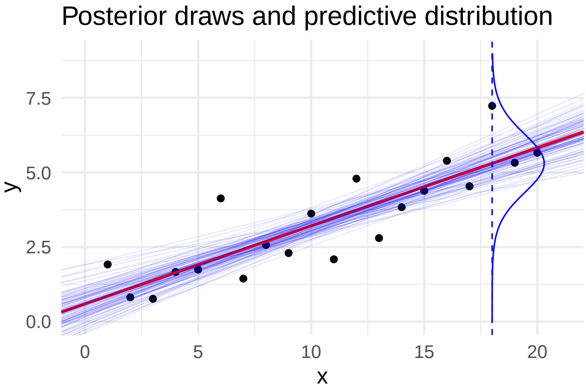

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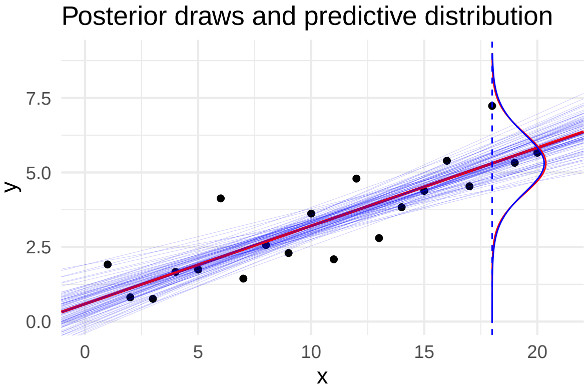

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Monte Carlo and Posterior Draws

- Assume we can get draws from $p(\theta \mid y)$

Monte Carlo and Posterior Draws

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

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

Monte Carlo and Posterior Draws

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

- to approximate uncertainty intervals for θ

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Marginalization

- Joint posterior distribution of multiple parameters

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

Marginalization

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- Marginalization

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

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

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Marginalization

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- Marginalization

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

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

- Goal is often to find marginal posterior of an interesting quantity
  - a parameter $p(\theta|y)$
  - a potential observation $p(\tilde{y}|y)$

Marginalization - predictive distribution

- Joint distribution of unknown future observation and parameters

$$
\begin{aligned}
p(\tilde{y}, \theta \mid y) &= p(\tilde{y} \mid \theta, y) p(\theta \mid y) \\
&= p(\tilde{y} \mid \theta) p(\theta \mid y) \qquad \text{(often)}
\end{aligned}
$$

Marginalization - predictive distribution

- Joint distribution of unknown future observation and parameters

$$\begin{aligned} p(\tilde{y}, \theta \mid y) &= p(\tilde{y} \mid \theta, y) p(\theta \mid y) \\ &= p(\tilde{y} \mid \theta) p(\theta \mid y) \qquad \text{(often)} \end{aligned}$$

- 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 with unknown μ and σ^2

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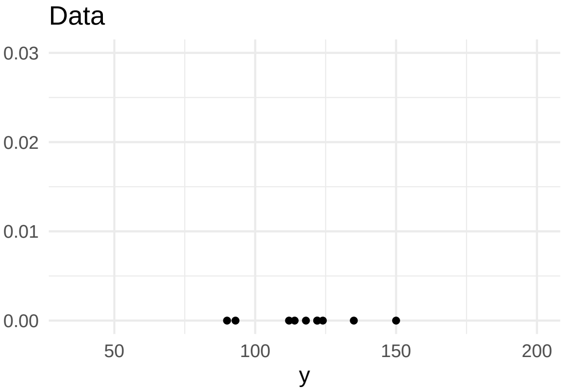
- Observation model

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

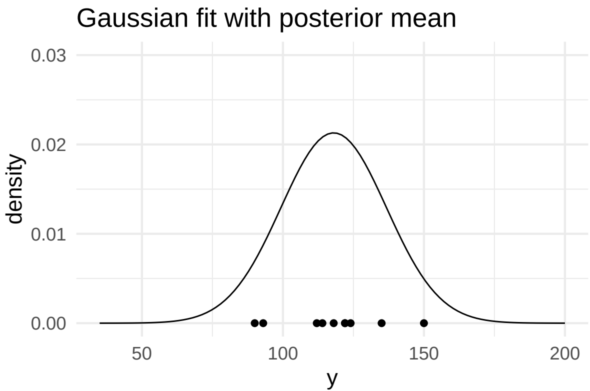
- Uninformative prior

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

Gaussian example



Gaussian example



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

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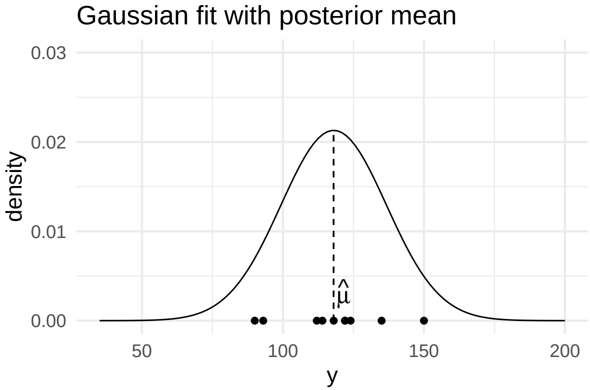
Gaussian example



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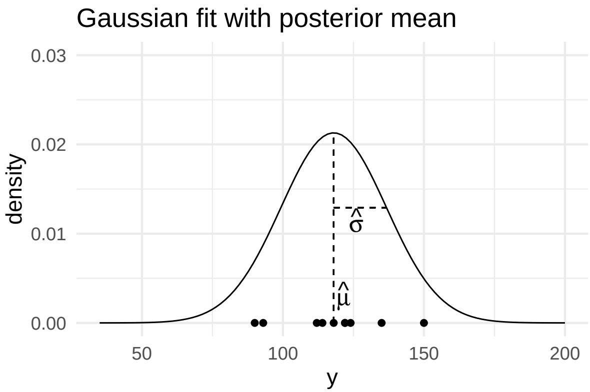

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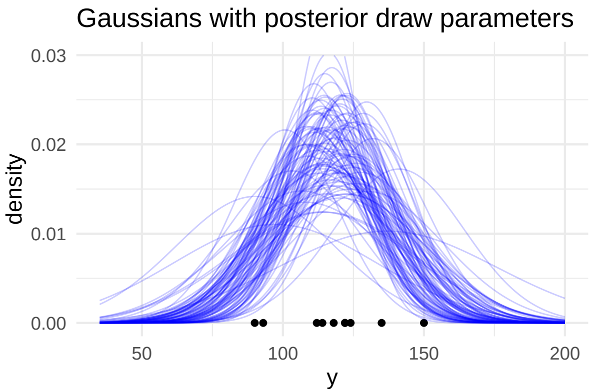

$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma \mid y)$$

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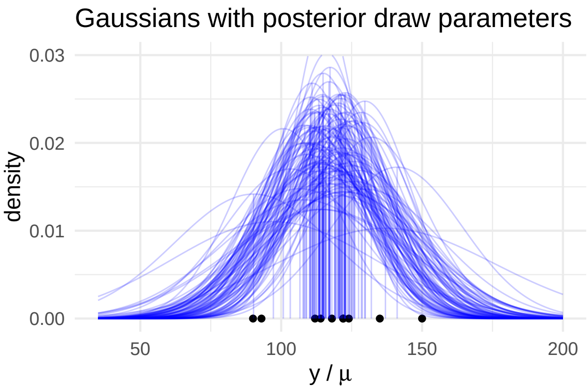
Gaussian example



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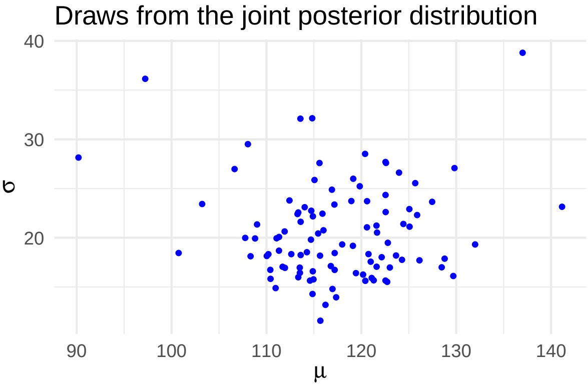

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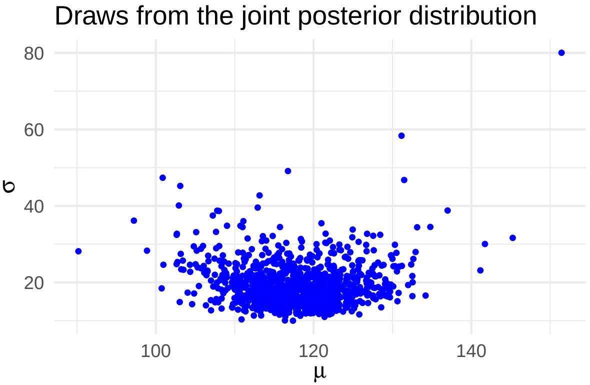

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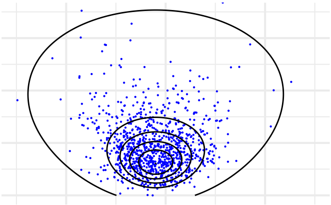
Joint posterior



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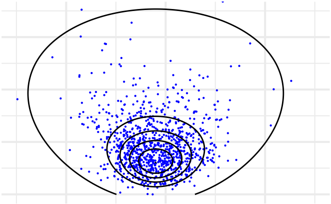
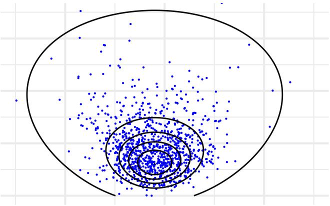
Joint posterior

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

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





Joint posterior

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

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

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

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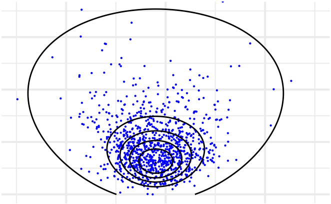
Joint posterior



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

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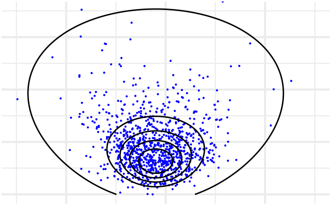
$$p(\mu, \sigma^2 \mid y) \propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^{n}(y_i - \mu)^2\right)$$

Joint posterior



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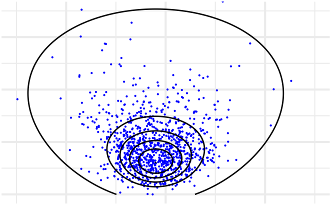
$$= \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[\sum_{i=1}^{n}(y_i - \bar{y})^2 + n(\bar{y} - \mu)^2\right]\right)$$

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

Joint posterior



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

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

Gaussian: Completing the square

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

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Gaussian: Completing the square

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

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

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

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Gaussian: Completing the square

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

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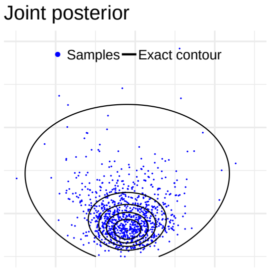
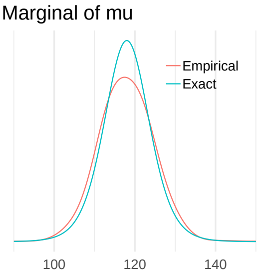
Marginal $p(\mu)$ and $p(\sigma^2)$





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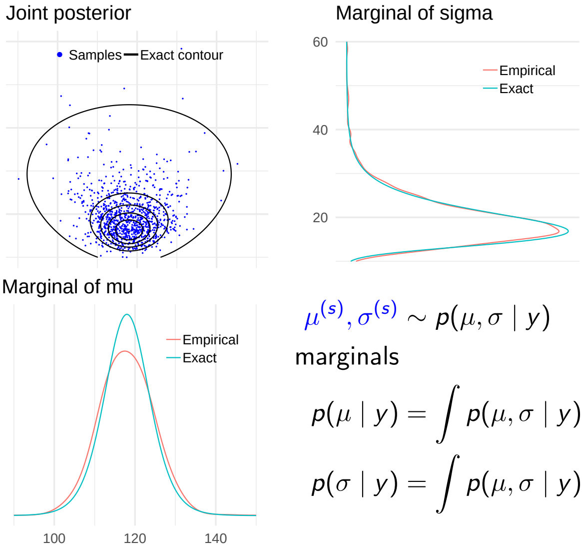
Marginal $p(\mu)$ and $p(\sigma^2)$



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

marginals

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

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

Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

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

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

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Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

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

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

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&\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \cdot \\
&\quad \int \exp\left(-\frac{n}{2\sigma^2}(\bar{y}-\mu)^2\right) d\mu
\end{aligned}
$$

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\end{aligned}
$$

$$
\textit{Note!} \quad \int \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y-\mu)^2\right) d\mu = 1
$$

Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

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

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Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

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&\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)
\end{aligned}
$$

Marginal $p(\mu|y)$ and $p(\sigma^2|y)$

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&\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 \mid y) &= \text{Inv-}\chi^2(\sigma^2 \mid n-1, s^2)
\end{aligned}
$$

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Gaussian - non-informative prior

Known mean

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

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

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

Unknown mean

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

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

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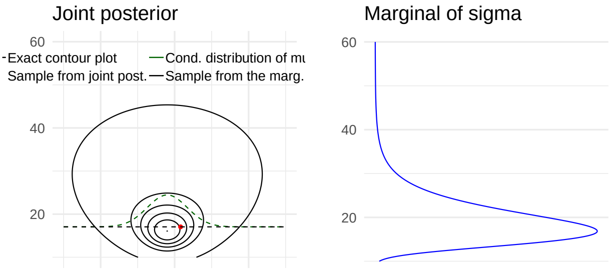
Gaussian - non-informative prior

- Marginal posterior $p(\mu \mid y)$

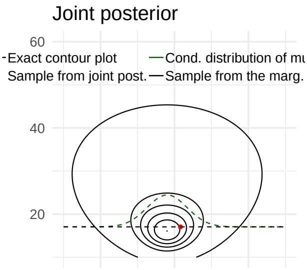
$$p(\mu \mid y) = \int_0^{\infty} p(\mu \mid \sigma^2, y) p(\sigma^2 \mid y) d\sigma^2$$

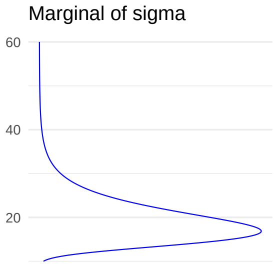
- Marginal posterior of μ, a mixture of normal distributions where mixing density is the marginal posterior of σ^2



Factorization

$$p(\mu, \sigma^2 \mid y) = {\color{darkred} p(\mu \mid \sigma^2, y)}{\color{blue} p(\sigma^2 \mid y)}$$

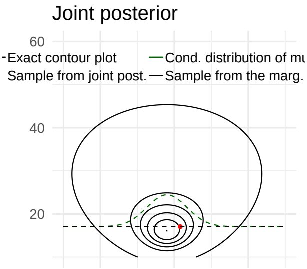


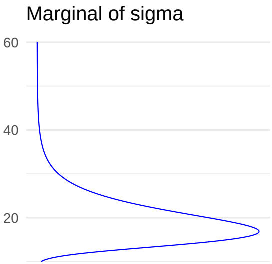


Factorization

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

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





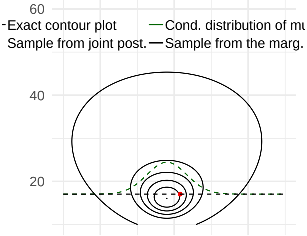
Factorization

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

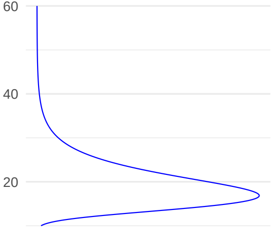
$$(\sigma^2)^{(s)} \sim p(\sigma^2 \mid y)$$

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

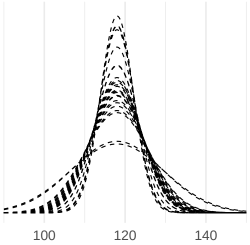
Joint posterior



Marginal of sigma



Cond distr of mu for 25 draws



Factorization

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

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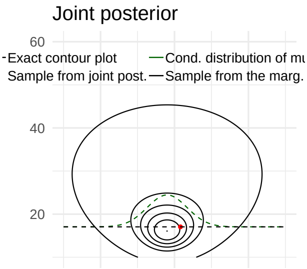
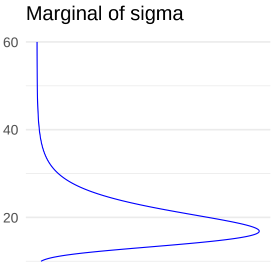
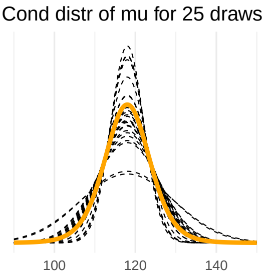






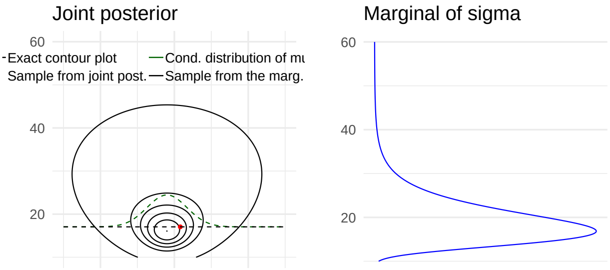
Factorization

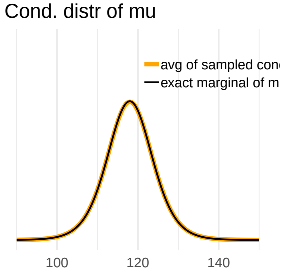
$$p(\mu, \sigma^2 \mid y) = p(\mu \mid \sigma^2, y) p(\sigma^2 \mid y)$$

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

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

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





Factorization

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

Marginal posterior $p(\mu \mid y)$

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

Marginal posterior $p(\mu \mid y)$

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

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Marginal posterior $p(\mu \mid y)$

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Transformation (integration by substitution)

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

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Transformation (integration by substitution)

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

$$dz = \left(-\frac{A}{2(\sigma^2)^2}\right) d\sigma^2$$

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- Introduction
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Marginal posterior $p(\mu \mid y)$

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

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$$
\begin{aligned}
p(\mu \mid y) &= \int_0^\infty p(\mu, \sigma^2 \mid y) d\sigma^2 \\
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\end{aligned}
$$

Transformation (integration by substitution)

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

$$
dz = \left(-\frac{A}{2(\sigma^2)^2}\right) d\sigma^2
$$

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

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

Marginal posterior $p(\mu \mid y)$

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

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

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

Marginal posterior $p(\mu \mid y)$

$$
\begin{aligned}
p(\mu|y) &\propto [(n-1)s^2 + n(\mu - \bar{y})^2]^{-n/2} \\
&\propto \left[1 + \frac{n(\mu - \bar{y})^2}{(n-1)s^2}\right]^{-n/2}
\end{aligned}
$$

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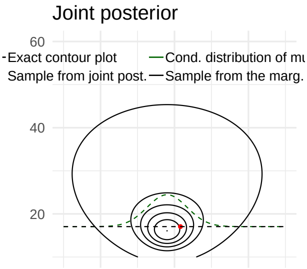
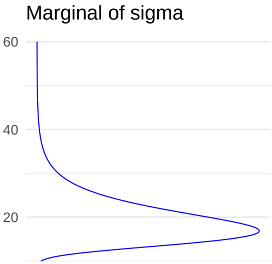
Marginal posterior $p(\mu \mid y)$

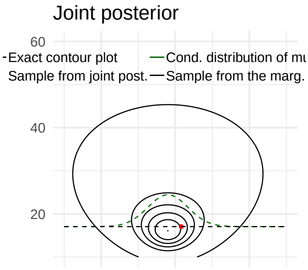
$$
\begin{aligned}
p(\mu|y) &\propto [(n-1)s^2 + n(\mu - \bar{y})^2]^{-n/2} \\
&\propto \left[1 + \frac{n(\mu - \bar{y})^2}{(n-1)s^2}\right]^{-n/2} \\
p(\mu \mid y) &= t_{n-1}(\mu \mid \bar{y}, s^2/n) \quad \text{Student's } t
\end{aligned}
$$

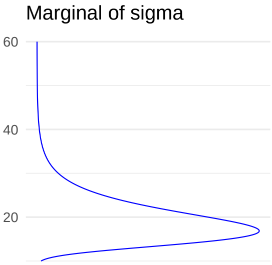




Predictive distribution for new $\tilde{y}$

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

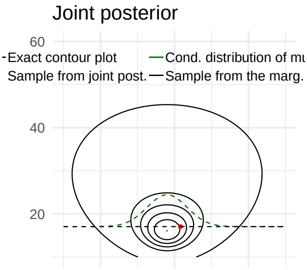


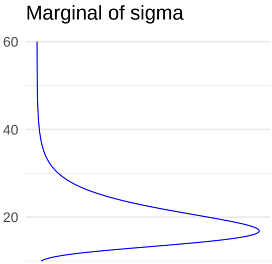


Predictive distribution for new $\tilde{y}$

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

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





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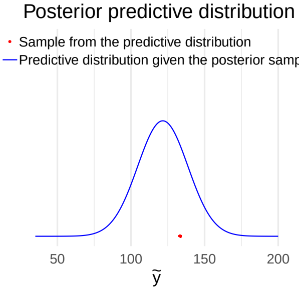
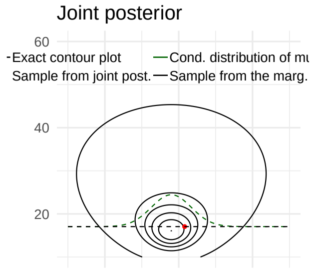
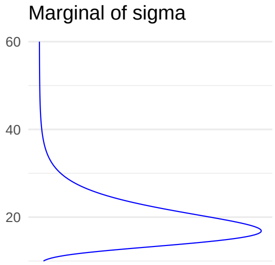
$$\tilde{y}^{(s)} \sim p(\tilde{y}|\mu^{(s)},\sigma^{(s)})$$





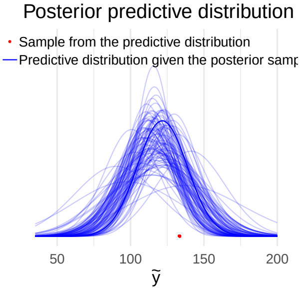


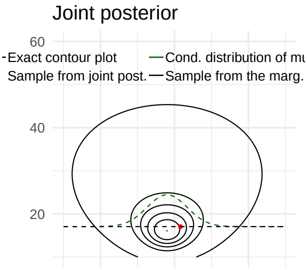
Predictive distribution for new $\tilde{y}$

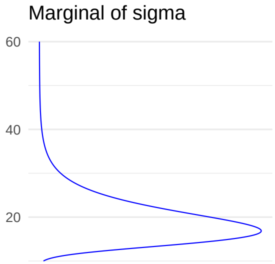
$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu,\sigma)p(\mu,\sigma|y)d\mu\sigma$$

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

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







Predictive distribution for new $\tilde{y}$

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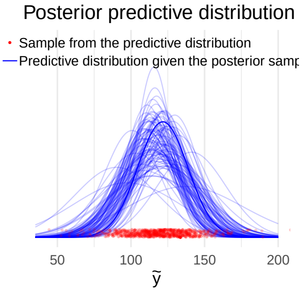

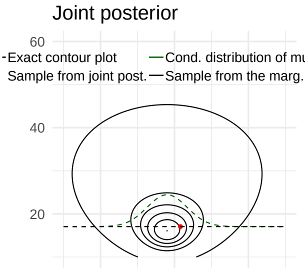

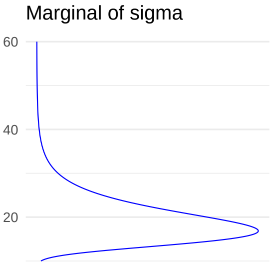

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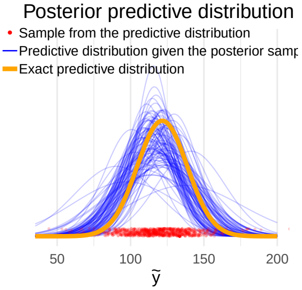

Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

$$p(\tilde{y} \mid \sigma^2, y) = \int p(\tilde{y} \mid \mu, \sigma^2) p(\mu \mid \sigma^2, y) d\mu$$

Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

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

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Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

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

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Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

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

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

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Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

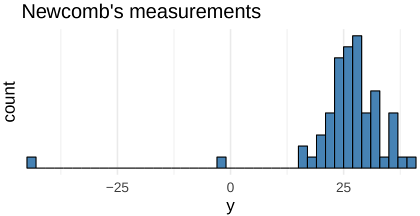
$$\begin{aligned} p(\tilde{y} \mid \sigma^2, y) &= \int p(\tilde{y} \mid \mu, \sigma^2) p(\mu \mid \sigma^2, y) d\mu \\ &= \int \mathcal{N}(\tilde{y} \mid \mu, \sigma^2) \mathcal{N}(\mu \mid \bar{y}, \sigma^2/n) d\mu \\ &= \mathcal{N}(\tilde{y} \mid \bar{y}, (1 + \tfrac{1}{n})\sigma^2) \end{aligned}$$

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

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

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.



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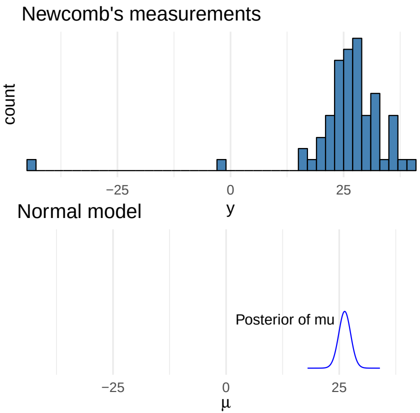

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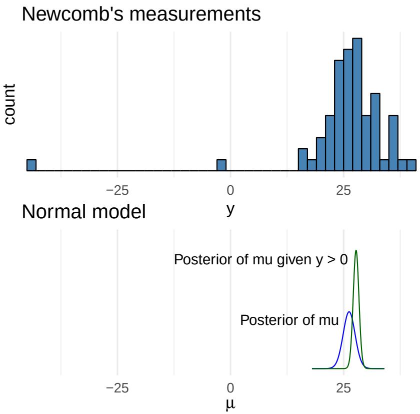

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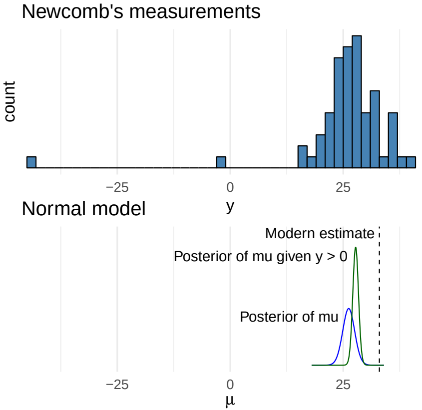

Gaussian - conjugate prior

- Conjugate prior has to have a form $p(\sigma^2)p(\mu \mid \sigma^2)$

Gaussian - conjugate prior

- Conjugate prior has to have a form $p(\sigma^2)p(\mu \mid \sigma^2)$
- Handy parameterization

$$\mu \mid \sigma^2 \sim \mathrm{N}(\mu_0, \sigma^2/\kappa_0)$$
$$\sigma^2 \sim \text{Inv-}\chi^2(\nu_0, \sigma_0^2)$$

which can be written as

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

Gaussian - conjugate prior

- Conjugate prior has to have a form $p(\sigma^2)p(\mu \mid \sigma^2)$
- Handy parameterization

$$\begin{aligned} \mu \mid \sigma^2 &\sim \mathrm{N}(\mu_0, \sigma^2/\kappa_0) \\ \sigma^2 &\sim \mathsf{Inv}\text{-}\chi^2(\nu_0, \sigma_0^2) \end{aligned}$$

which can be written as

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

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

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Gaussian - conjugate prior

Joint posterior (exercise 3.9)

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

where

$$\begin{aligned}
\mu_n &= \frac{\kappa_0}{\kappa_0 + n}\mu_0 + \frac{n}{\kappa_0 + n}\bar{y} \\
\kappa_n &= \kappa_0 + n \\
\nu_n &= \nu_0 + n \\
\nu_n\sigma_n^2 &= \nu_0\sigma_0^2 + (n-1)s^2 + \frac{\kappa_0 n}{\kappa_0 + n}(\bar{y} - \mu_0)^2
\end{aligned}$$

Gaussian - conjugate prior

- Conditional $p(\mu \mid \sigma^2, y)$

$$\begin{aligned}\mu \mid \sigma^2, y &\sim \mathrm{N}(\mu_n, \sigma^2/\kappa_n) \\ &= \mathrm{N}\left(\frac{\frac{\kappa_0}{\sigma^2}\mu_0 + \frac{n}{\sigma^2}\bar{y}}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}}, \frac{1}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}}\right)\end{aligned}$$

Gaussian - conjugate prior

- Conditional $p(\mu \mid \sigma^2, y)$

$$
\begin{aligned}
\mu \mid \sigma^2, y &\sim \mathrm{N}(\mu_n, \sigma^2/\kappa_n) \\
&= \mathrm{N}\left(\frac{\frac{\kappa_0}{\sigma^2}\mu_0 + \frac{n}{\sigma^2}\bar{y}}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}}, \frac{1}{\frac{\kappa_0}{\sigma^2} + \frac{n}{\sigma^2}} \right)
\end{aligned}
$$

- Marginal $p(\sigma^2 \mid y)$

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

Gaussian - conjugate prior

- Conditional $p(\mu \mid \sigma^2, y)$

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- Marginal $p(\sigma^2 \mid y)$

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

- Marginal $p(\mu \mid y)$

$$\mu \mid y \sim t_{\nu_n}(\mu \mid \mu_n, \sigma_n^2/\kappa_n)$$

Multinomial model for categorical data

- Extension of binomial to K categories
- Observation model (Categorical distribution, $n = 1$)
  $y_i = (0, 1, 0, 0, 0)$ - what is K here?

Multinomial model for categorical data

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

$$\text{where } \sum_{k}^{K} \theta_k = 1\,, \text{ and } \forall \theta_k > 0$$

- What is important when choosing the prior for θ?

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Multinomial model for categorical data

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- What is important when choosing the prior for θ?
- Conjugate prior: The Dirichlet distribution

$$p(\theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1},$$

$$\text{where } \forall \alpha_k > 0$$

Multinomial model for categorical data: The posterior

- The posterior $p(\theta|y)$

$$p(\theta \mid y) \propto p(y \mid \theta)p(\theta)$$

Multinomial model for categorical data: The posterior

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p(\theta \mid y) &\propto p(y \mid \theta)p(\theta) \\
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\end{aligned}
$$

Multinomial model for categorical data: The posterior

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\end{aligned}
$$

- The posterior is $p(\theta|y) = \mathrm{Dir}(\alpha + \sum y)$

Multivariate Gaussian

- Observation model

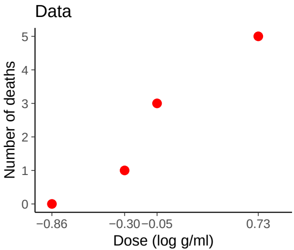
$$p(y \mid \mu, \Sigma) \propto \mid \Sigma \mid^{-1/2} \exp\left(-\frac{1}{2}(y-\mu)^T \Sigma^{-1}(y-\mu)\right),$$

where $y \in \mathcal{R}^D$

- See 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



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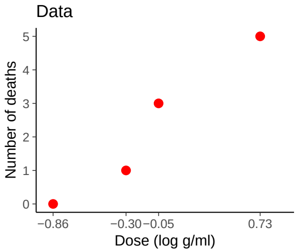

Find out lethal dose 50% (LD50)

- used to classify how hazardous chemical is
- 1984 EEC directive has 4 levels

Bioassay

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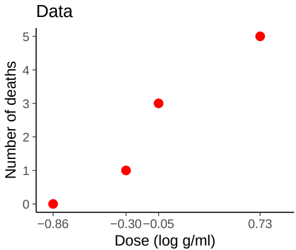


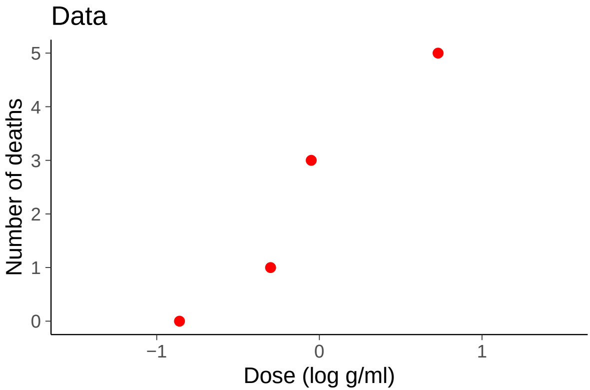
Find out lethal dose 50% (LD50)

- used to classify how hazardous chemical is
- 1984 EEC directive has 4 levels

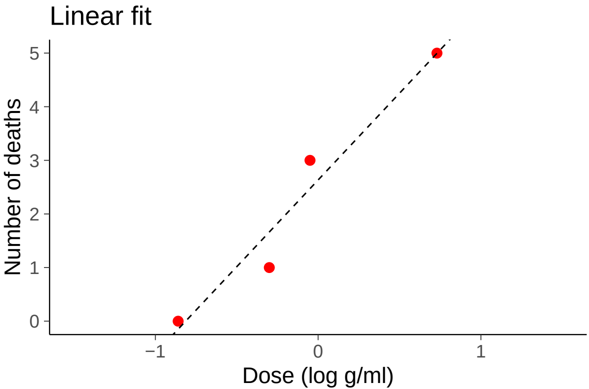
Bayesian methods help to

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

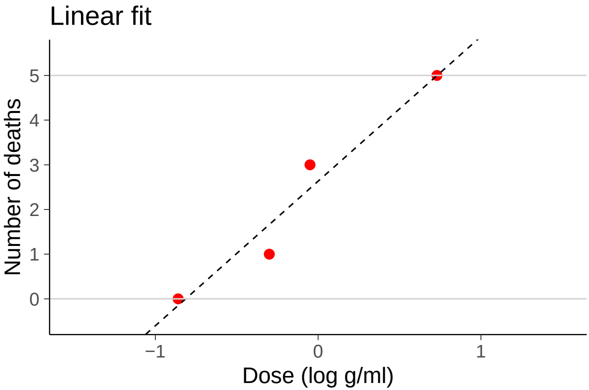
Bioassay



Bioassay



Bioassay



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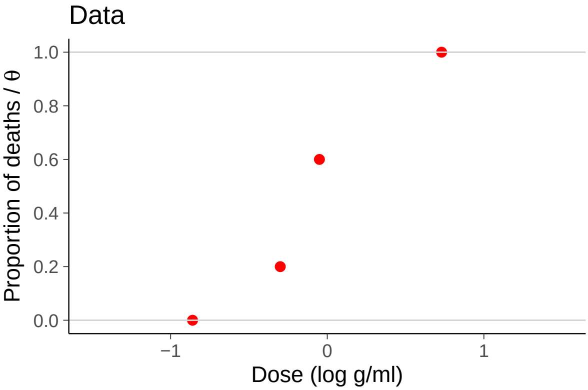
Bioassay



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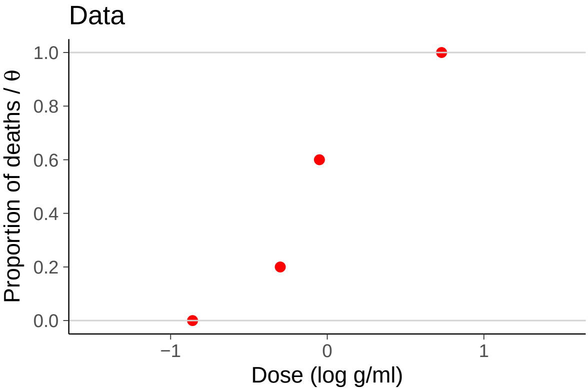
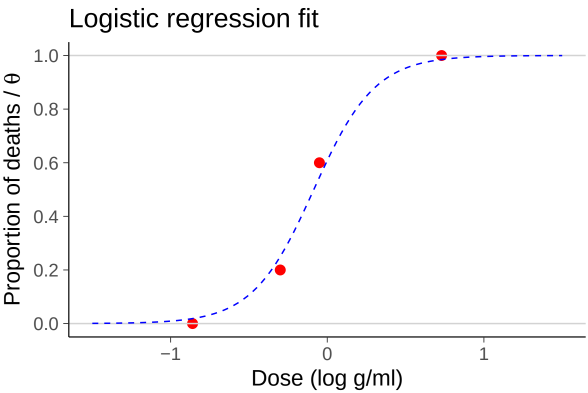
Bioassay



Binomial model

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

Bioassay



Binomial model

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

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Bioassay

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

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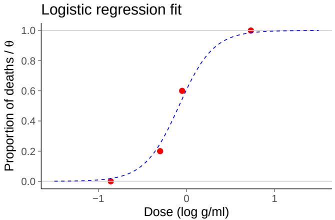
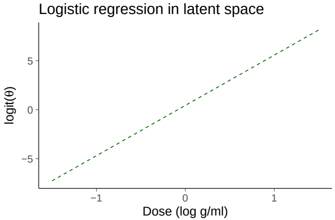
$$= \alpha + \beta x_i$$



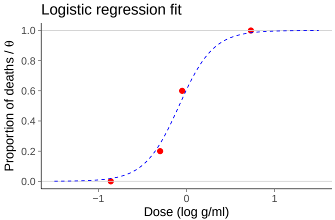


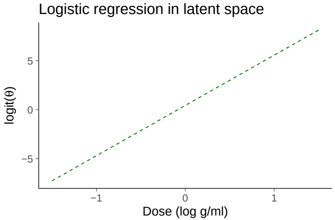
Bioassay

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

$$\mathrm{logit}(\theta_i) = \log\left(\frac{\theta_i}{1-\theta_i}\right) = \alpha + \beta x_i$$

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





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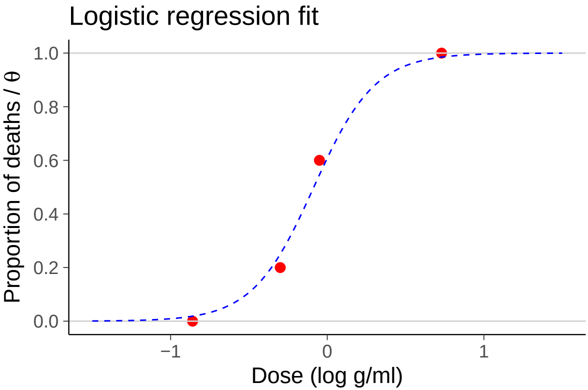
Bioassay: Lethal Dose 50%



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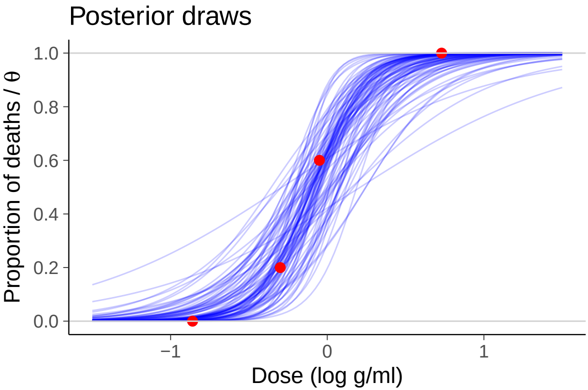

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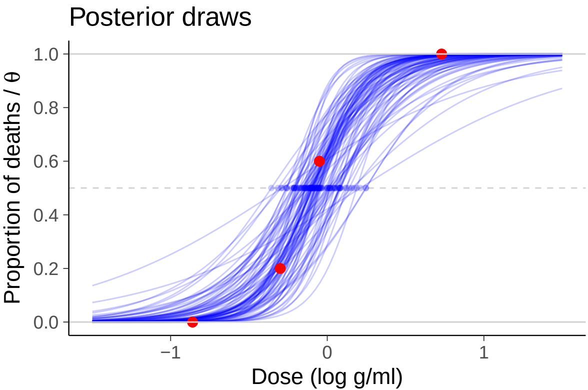
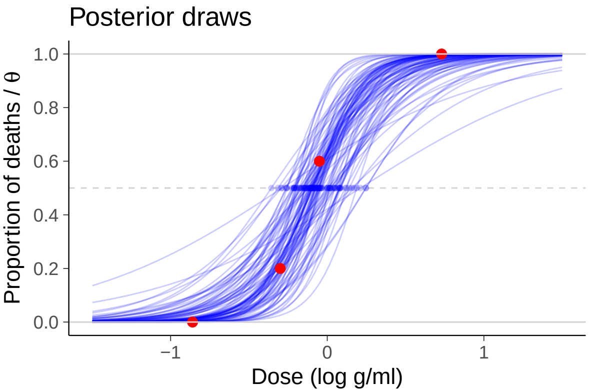


$$\mathrm{E}\left(\frac{y}{n}\right) = \text{logit}^{-1}(\alpha + \beta x) = 0.5$$

Bioassay: Lethal Dose 50%



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

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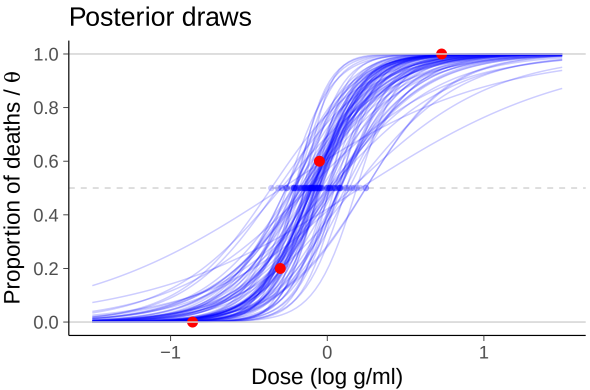
Bioassay: Lethal Dose 50%



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$$x^{(s)}_{\mathrm{LD50}} = -\alpha^{(s)}/\beta^{(s)}$$

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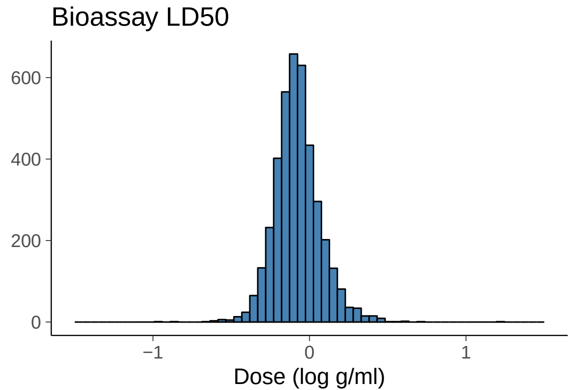

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Bioassay posterior

Binomial model

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

Link function

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

Bioassay posterior

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

Likelihood

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

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

Bioassay posterior

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Posterior

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

No analytic posterior distribution? What can we do?

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Grid evaluation

1. Setup an area (can be hard) for α and β that capture most mass (here $\alpha = [-1, 5]$ and $\beta = [0, 30]$)

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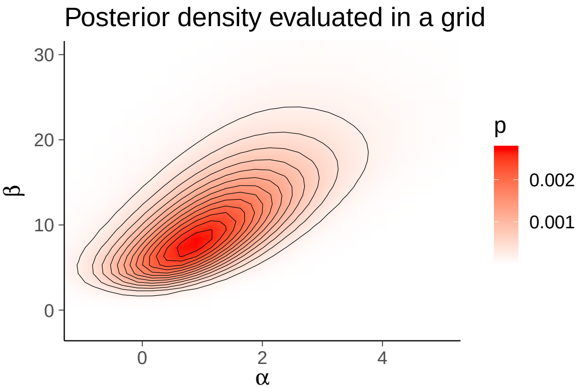
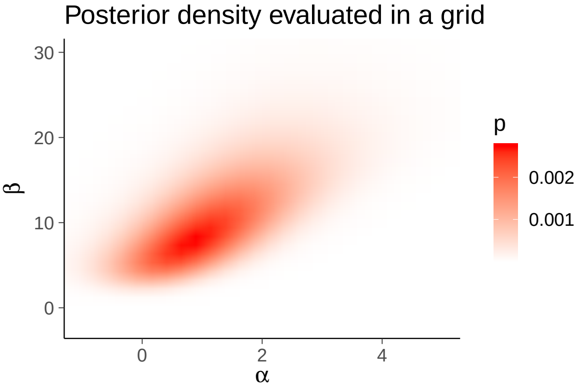
3. Sum up $\tilde{p}$ over the whole grid (for all $g \in \{1, ..., G\}$)
4. Compute (normalize) the pmf approximation of the posterior $\hat{p}$

g	$(\alpha,\ \beta)$	$\tilde{p}$	$\hat{p}$
1	(0, -1)	0.02	0.0002
2	(0, -0.8)	0.03	0.0003
...	...	...	...
G	(30, 5)	0.001	0.00001
$\sum_g^G$	-	100	1

Bioassay (with uniform prior on α, β)

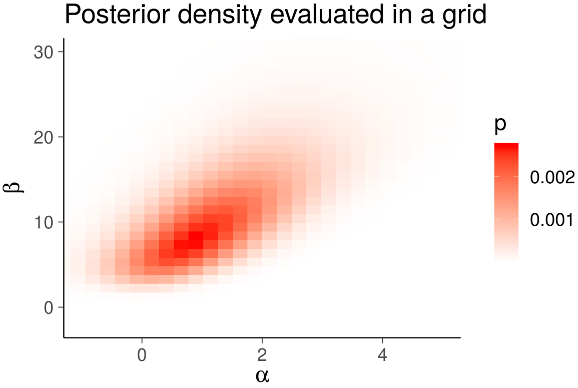


Bioassay (with uniform prior on α, β)



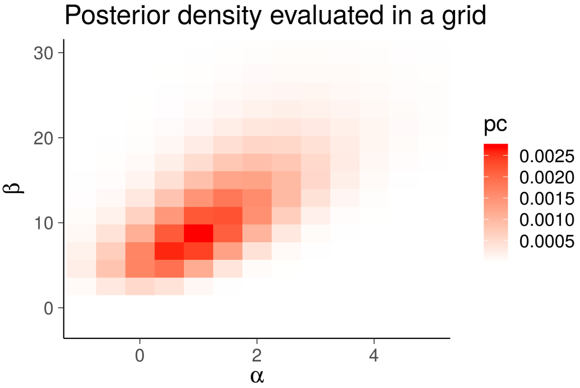
Density evaluated in grid, but plotted using interpolation

Bioassay (with uniform prior on α, β)



Density evaluated in grid, and plotted without interpolation

Bioassay (with uniform prior on α, β)



Density evaluated in a coarser grid

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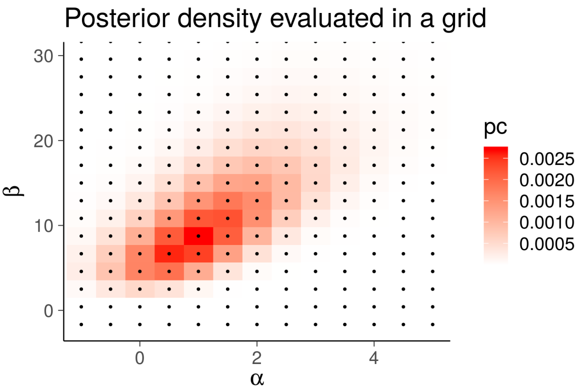
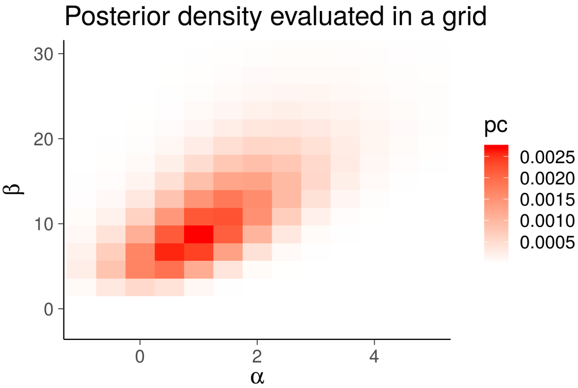
Bioassay (with uniform prior on α, β)



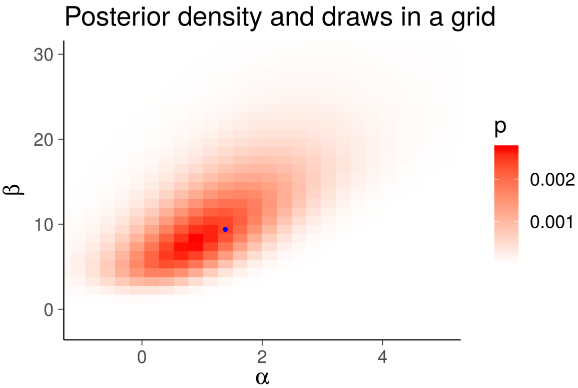
- Approximate the density as piecewise constant function
- Evaluate density in a grid over some finite region
- Density times cell area gives probability mass in each cell

Bioassay (with uniform prior on α, β)



- 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 (with uniform prior on α, β)



- Sample according to grid cell probabilities

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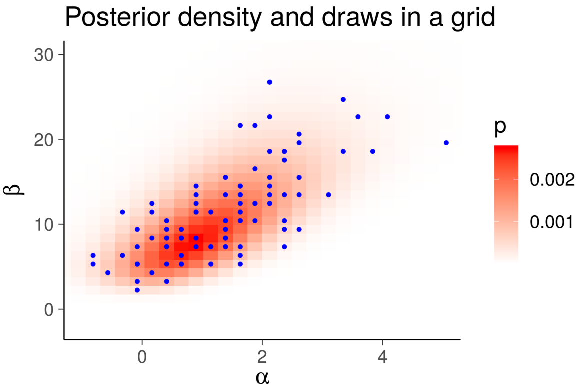

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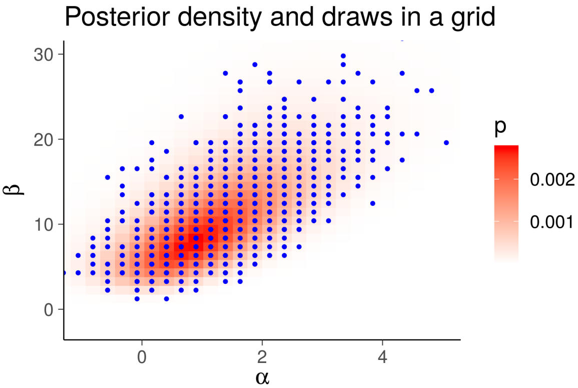
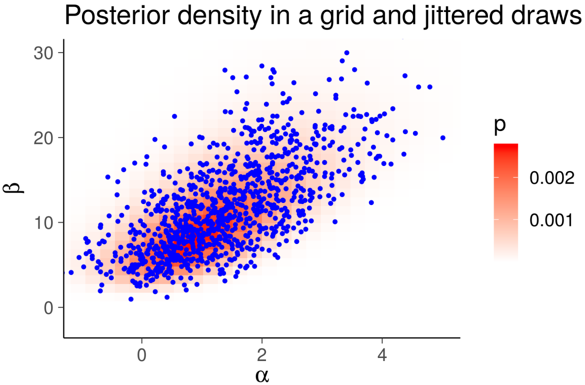


- Sample according to grid cell probabilities
- Several draws can be from the same grid cell

Bioassay (with uniform prior on α, β)



- Jitter can be added to improve visualization

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Grid sampling

- Draws can be used to estimate expectations, for example

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

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

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

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

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

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Grid sampling

- Draws can be used to estimate expectations, for example

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

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

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

where $w_{\mathrm{cell}}^{(t)}$ 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