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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bayesian Statistics and Data Analysis

## Lecture 3

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

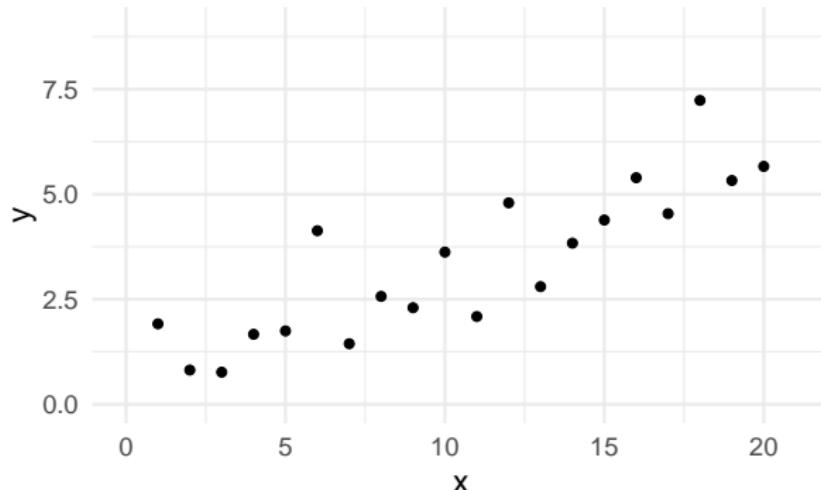


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Example of uncertainty in modeling

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Data

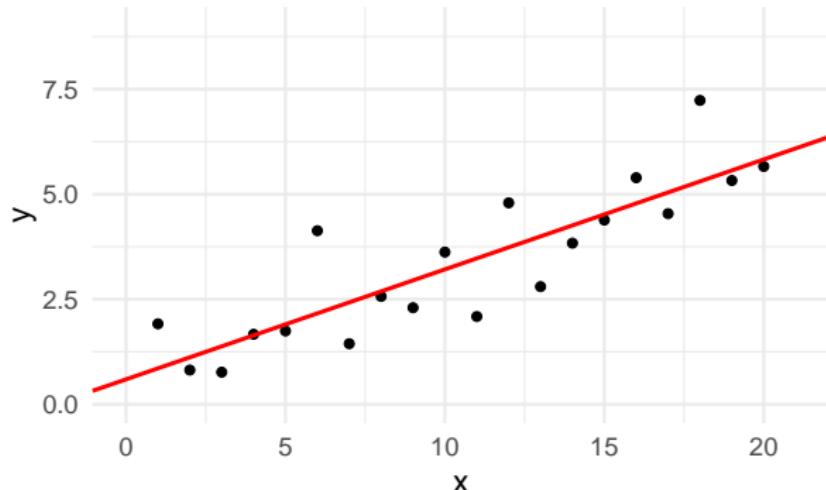




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Example of uncertainty in modeling

Posterior mean

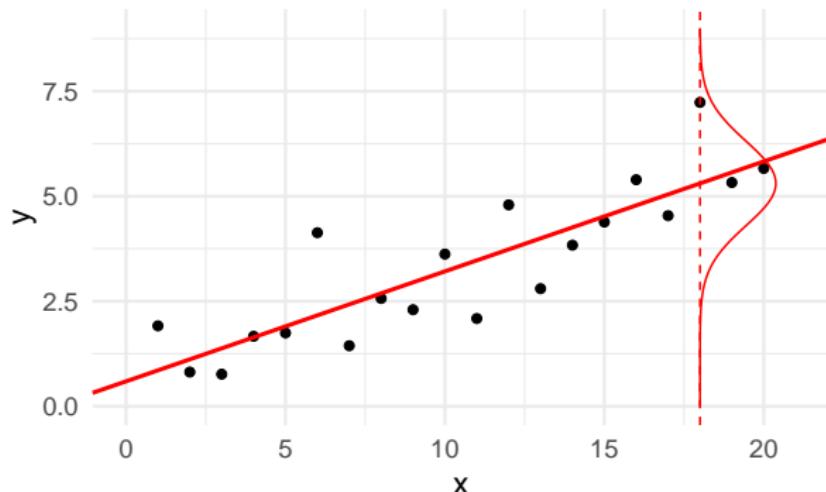




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Example of uncertainty in modeling

Predictive distribution given posterior mean



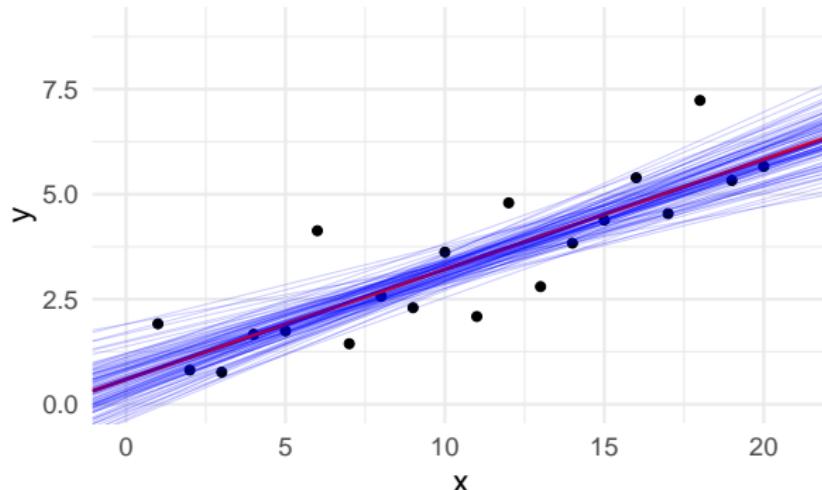


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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Example of uncertainty in modeling

Posterior draws

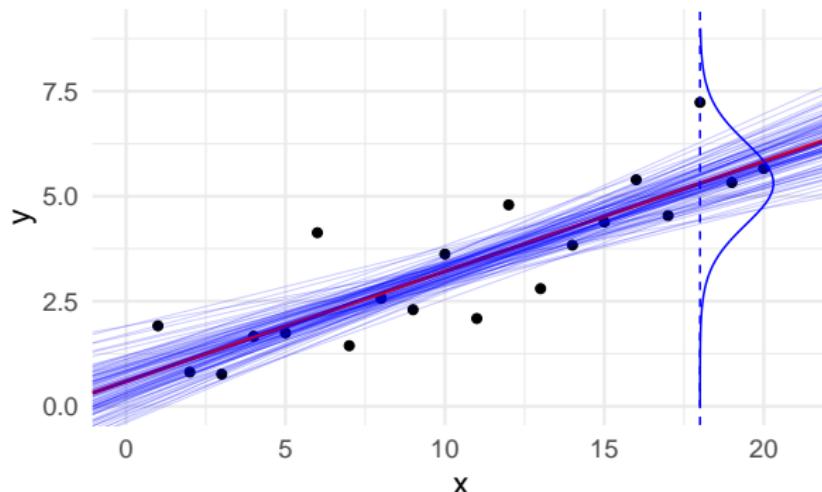




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Example of uncertainty in modeling

Posterior draws and predictive distribution

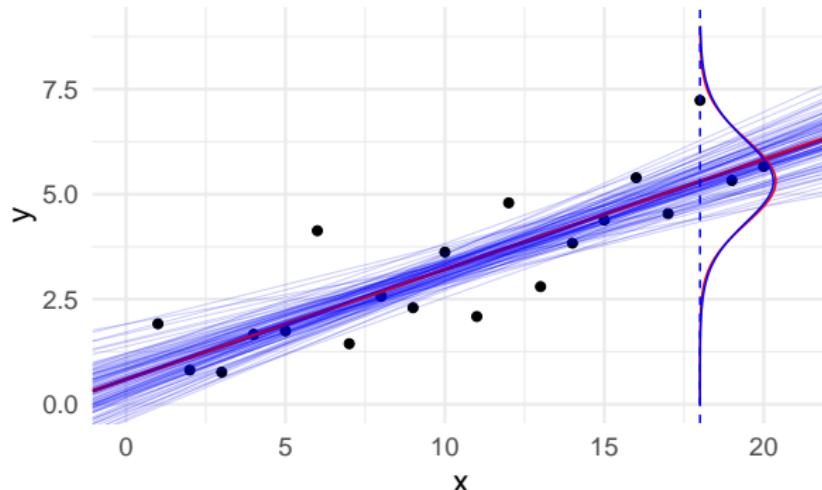




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Example of uncertainty in modeling

Posterior draws and predictive distribution





# Monte Carlo and Posterior Draws

---

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



# Monte Carlo and Posterior Draws

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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



# Monte Carlo and Posterior Draws

---

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

- to approximate uncertainty intervals for  $\theta$



# Marginalization

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

- Joint posterior distribution of multiple parameters

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Marginalization

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- Joint posterior distribution of multiple 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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Marginalization

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- Joint posterior distribution of multiple 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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Marginalization - predictive distribution

---

- Joint distribution of unknown future observation and parameters

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Marginalization - predictive distribution

---

- Joint distribution of unknown future observation and parameters

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

- 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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian with unknown $\mu$ and $\sigma^2$

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- Observation model

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

- Uninformative prior

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

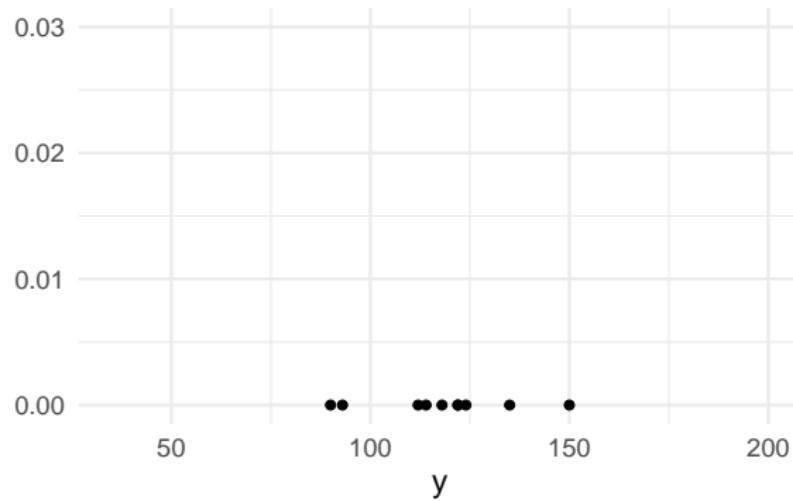


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian example

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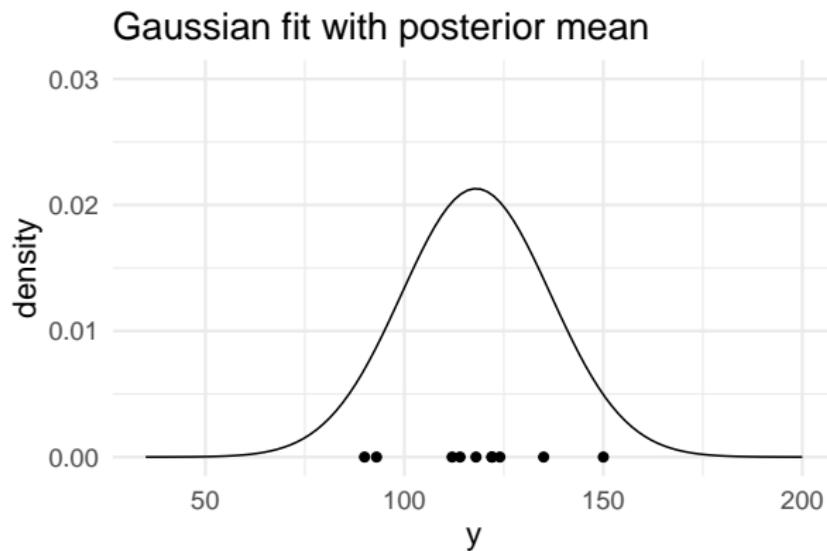
Data





- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example

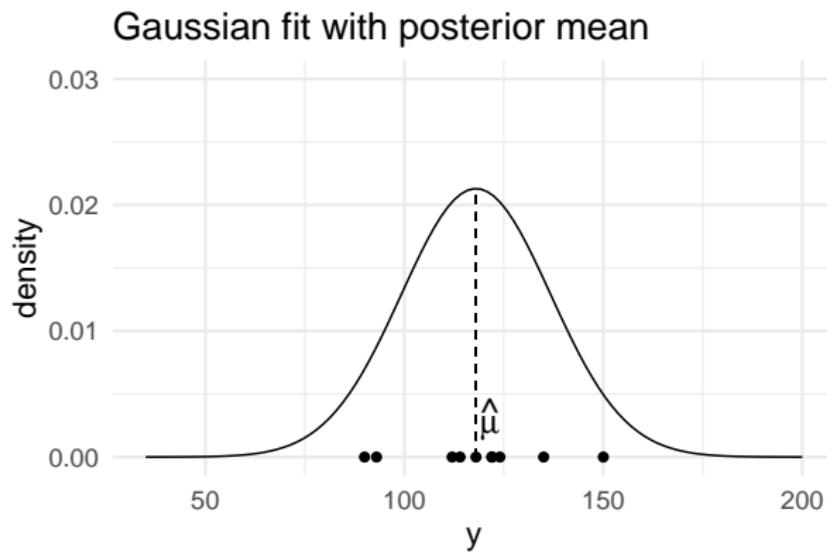


$$p(\textcolor{red}{y} \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(\textcolor{red}{y} - \mu)^2\right)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example



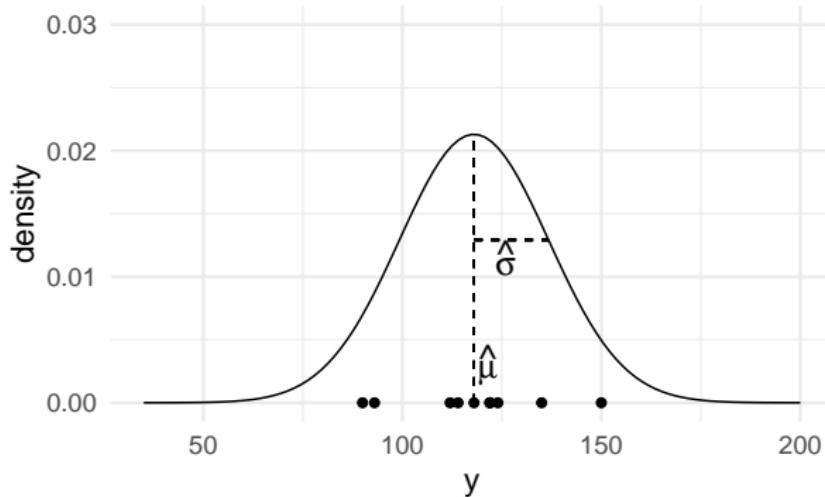
$$p(y | \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y - \mu)^2\right)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example

Gaussian fit with posterior mean



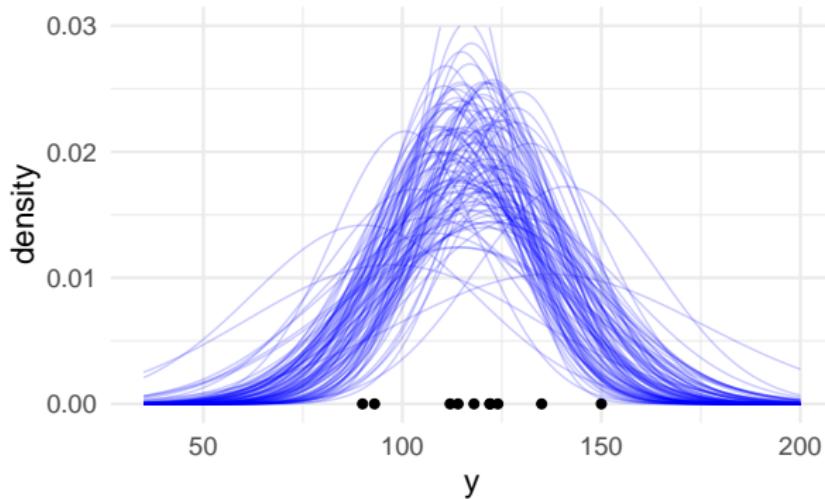
$$p(y | \mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y - \mu)^2\right)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example

Gaussians with posterior draw parameters



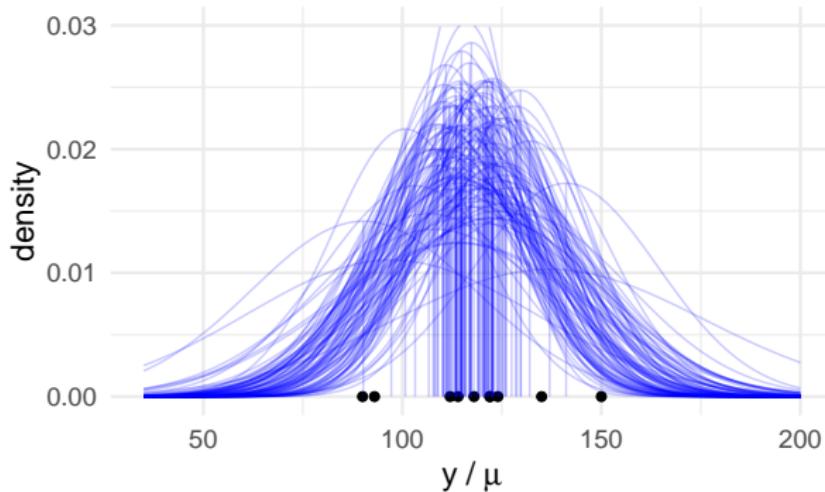
$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example

Gaussians with posterior draw parameters

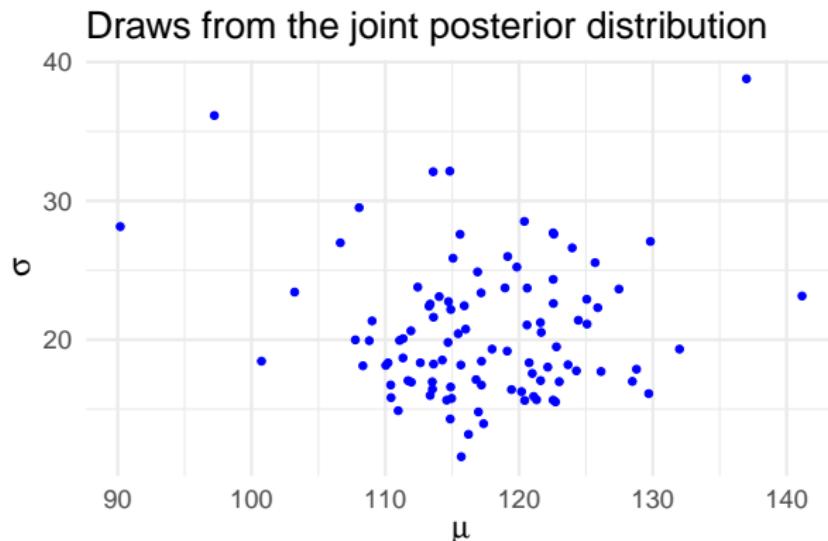


$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example



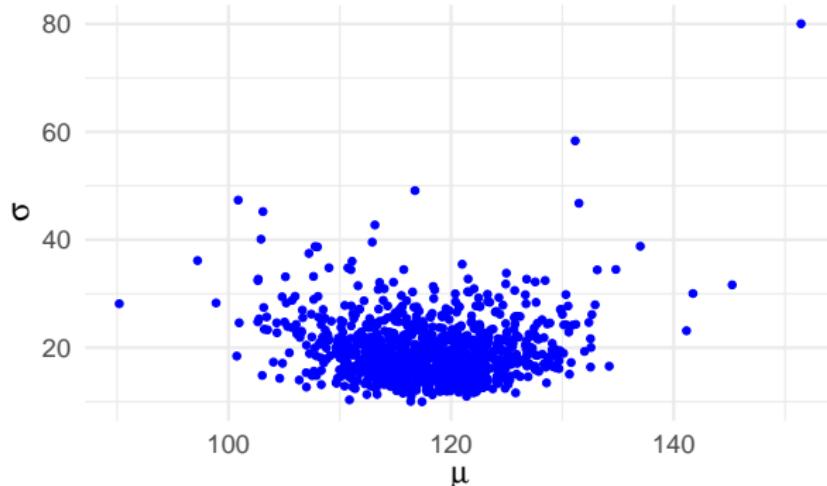
$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian example

Draws from the joint posterior distribution



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

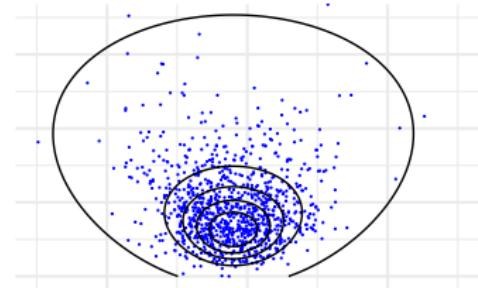


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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

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



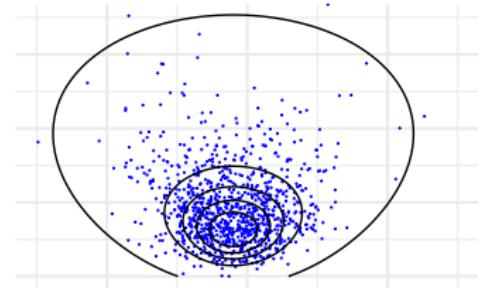


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

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

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





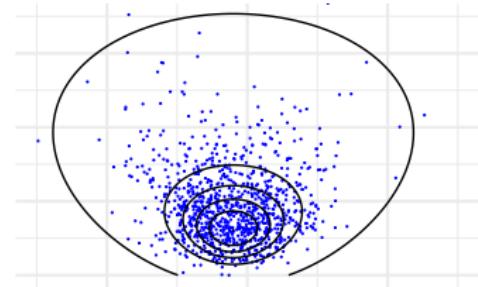
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

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

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

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





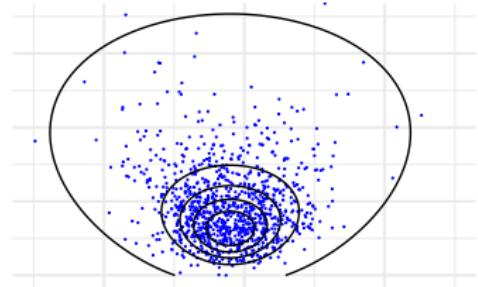
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

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

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

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



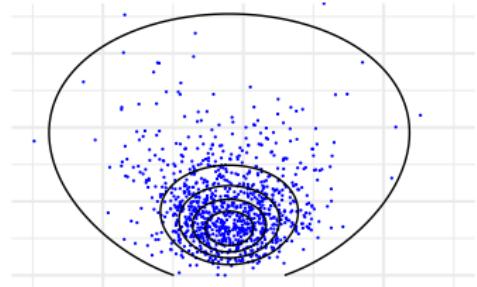


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

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

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



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

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

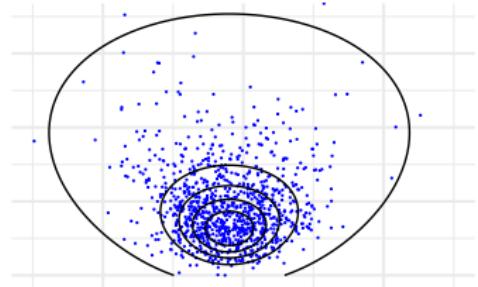


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

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



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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian: Completing the square

---

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



UPPSALA  
UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian: Completing the square

---

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

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



UPPSALA  
UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian: Completing the square

---

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

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

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



UPPSALA  
UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian: Completing the square

---

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

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

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

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



UPPSALA  
UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian: Completing the square

---

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

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

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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian: Completing the square

---

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

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

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

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

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

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

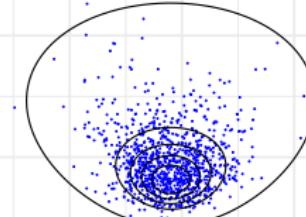


- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

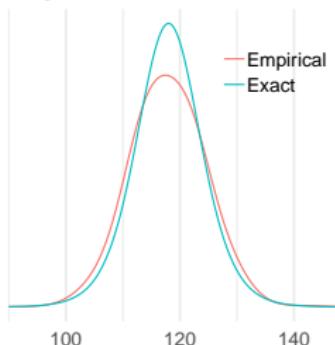
# Marginal $p(\mu)$ and $p(\sigma^2)$

## Joint posterior

- Samples — Exact contour



## Marginal of $\mu$



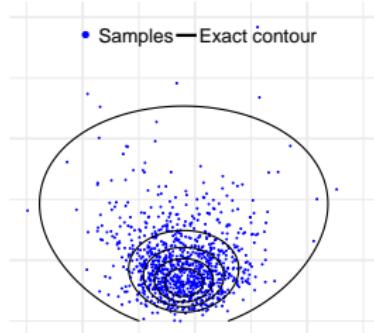
$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma | y)$$



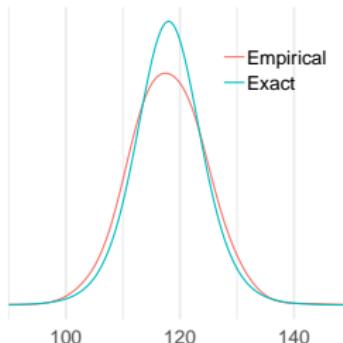
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

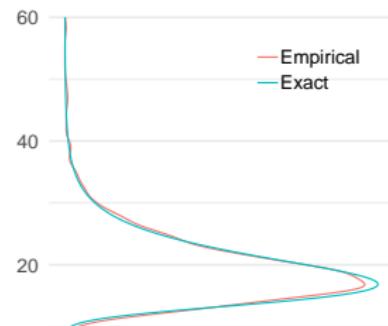
Joint posterior



Marginal of mu



Marginal of sigma



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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

---

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

---

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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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Note!

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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Note!

$$\begin{aligned} &\int \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{1}{2\sigma^2}(y - \theta)^2\right) d\theta = 1 \\ &\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \sqrt{2\pi\sigma^2/n} \\ &\propto (\sigma^2)^{-(n+1)/2} \exp\left(-\frac{(n-1)s^2}{2\sigma^2}\right) \end{aligned}$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Known mean

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

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



# Gaussian - non-informative prior

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Known mean

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

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

## Unknown mean

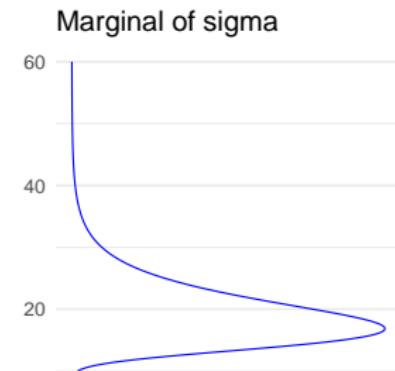
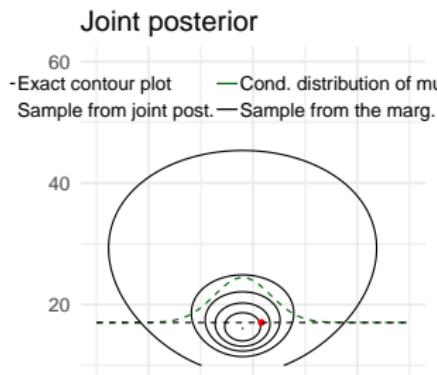
$$\sigma^2 | y \sim \text{Inv-}\chi^2(n - 1, s^2)$$

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



# UPPSALA UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



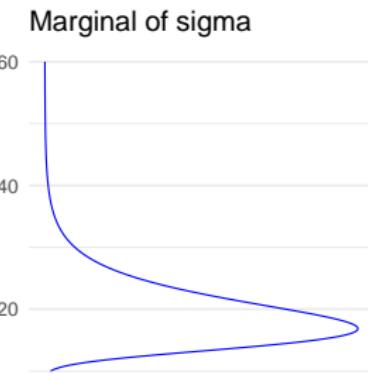
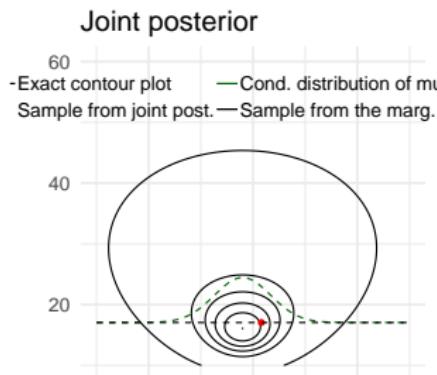
### Factorization

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



# UPPSALA UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



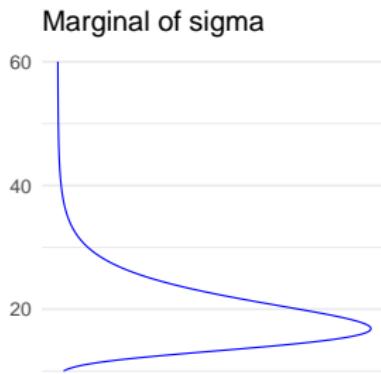
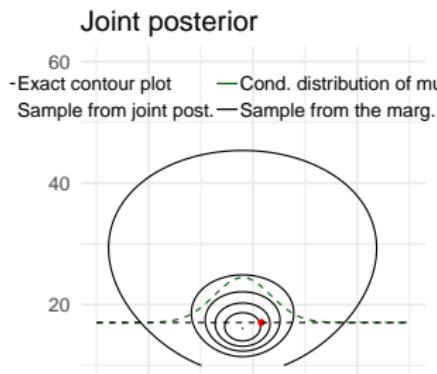
### Factorization

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



# UPPSALA UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



### Factorization

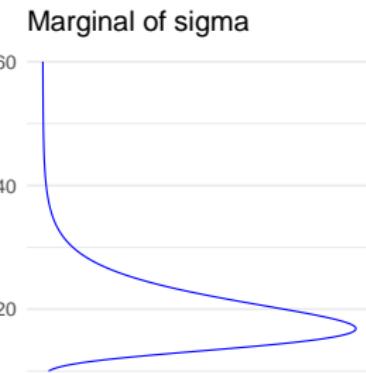
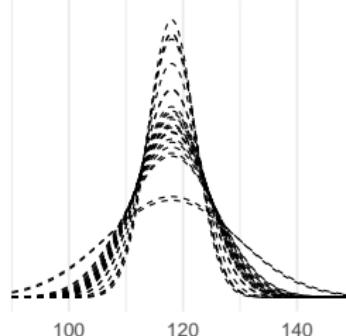
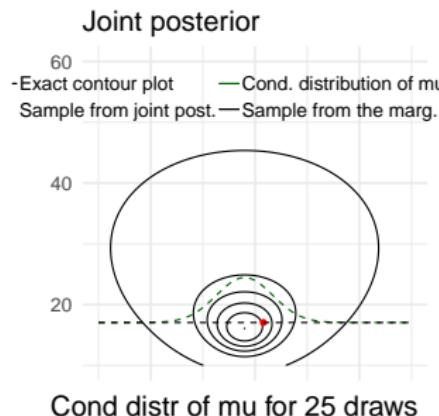
$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y) p(\sigma^2 | y)$$
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$

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



# UPPSALA UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



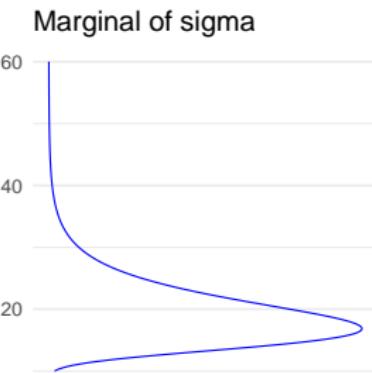
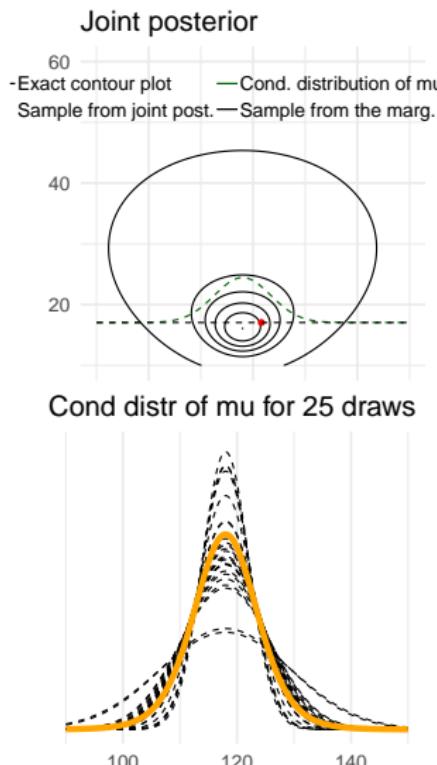
### Factorization

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

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



## Factorization

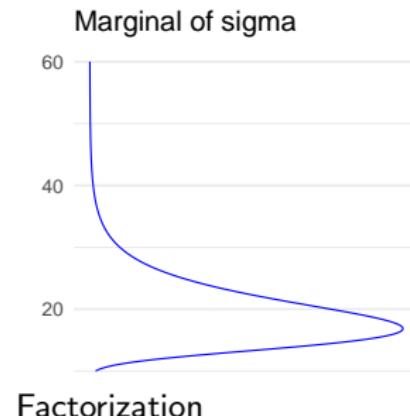
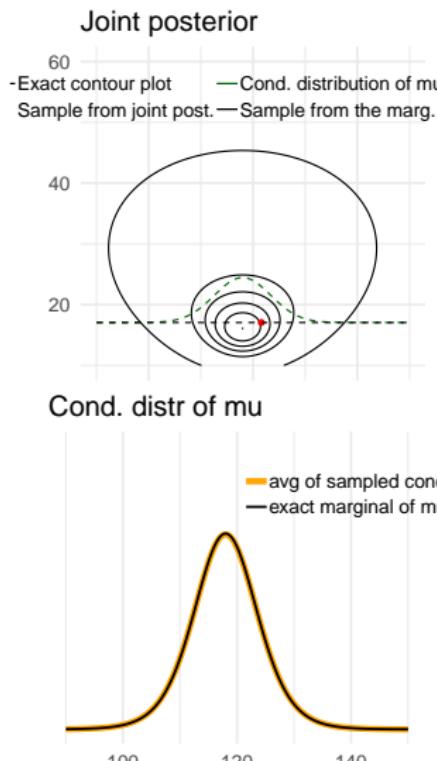
$$p(\mu, \sigma^2 | y) = p(\mu | \sigma^2, y)p(\sigma^2 | y)$$
$$(\sigma^2)^{(s)} \sim p(\sigma^2 | y)$$
$$p(\mu | (\sigma^2)^{(s)}, y) = \mathcal{N}(\mu | \bar{y}, (\sigma^2)^{(s)}/n)$$

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



# UPPSALA UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



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

---

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

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example



UPPSALA  
UNIVERSITET

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

---

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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Transformation (integration by substitution)

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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Transformation (integration by substitution)

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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Transformation (integration by substitution)

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Marginal posterior $p(\mu | y)$

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Marginal posterior $p(\mu | y)$

---

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



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

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - non-informative prior

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

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

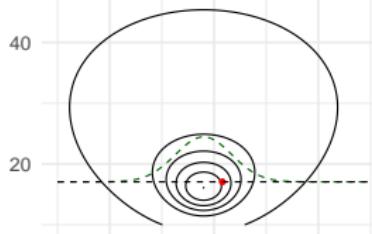
- marginal posterior of  $\mu$  a mixture of normal distributions where mixing density is the marginal posterior of  $\sigma^2$



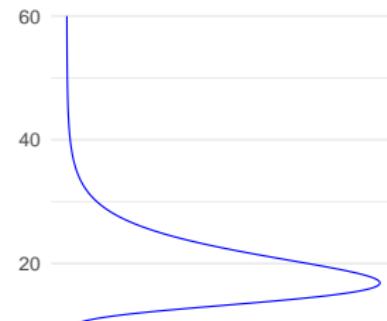
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

### Joint posterior

60  
Exact contour plot    Cond. distribution of  $\mu$   
Sample from joint post. — Sample from the marg.



### Marginal of sigma



### Predictive distribution for new $\tilde{y}$

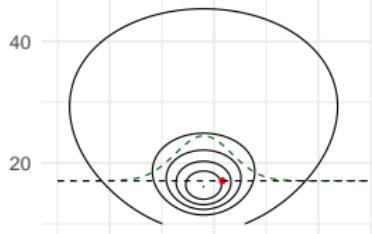
$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu, \sigma)p(\mu, \sigma|y)d\mu d\sigma$$



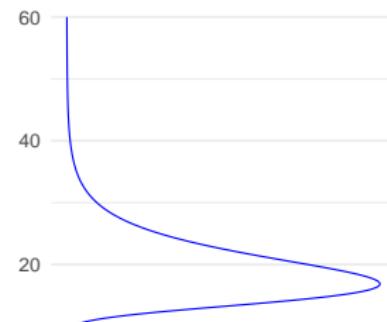
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

### Joint posterior

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Exact contour plot    Cond. distribution of  $\mu$   
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### Predictive distribution for new $\tilde{y}$

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

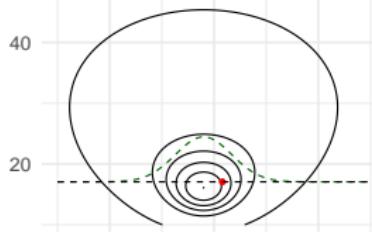
$$\mu^{(s)}, \sigma^{(s)} \sim p(\mu, \sigma|y)$$



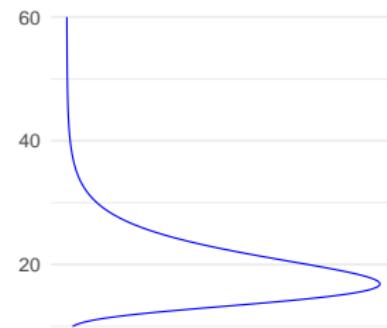
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

### Joint posterior

60  
Exact contour plot    Cond. distribution of  $\mu$   
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### Marginal of sigma



### Predictive distribution for new $\tilde{y}$

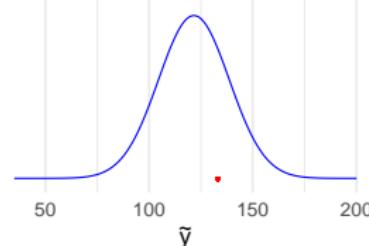
$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu, \sigma)p(\mu, \sigma|y)d\mu d\sigma$$

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

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

### Posterior predictive distribution

- Sample from the predictive distribution
- Predictive distribution given the posterior samp

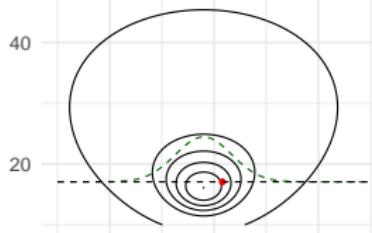




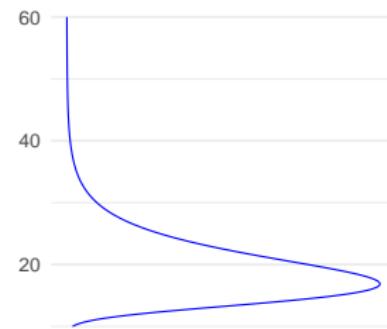
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

### Joint posterior

60  
Exact contour plot    Cond. distribution of  $\mu$   
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### Predictive distribution for new $\tilde{y}$

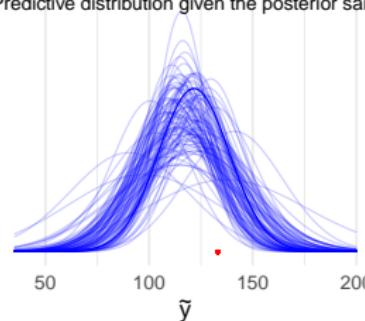
$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu, \sigma)p(\mu, \sigma|y)d\mu d\sigma$$

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

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

### Posterior predictive distribution

- Sample from the predictive distribution
- Predictive distribution given the posterior samp

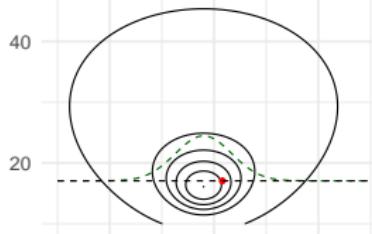




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

### Joint posterior

- Exact contour plot    — Cond. distribution of  $\mu$   
Sample from joint post. — Sample from the marg.



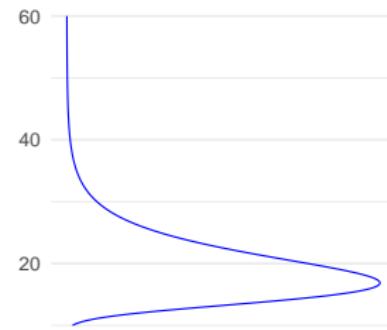
### Predictive distribution for new $\tilde{y}$

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

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

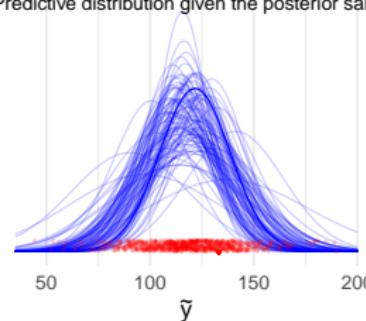
$$\tilde{y}^{(s)} \sim p(\tilde{y}|\mu^{(s)}, \sigma^{(s)})$$

### Marginal of sigma



### Posterior predictive distribution

- Sample from the predictive distribution
- Predictive distribution given the posterior samp



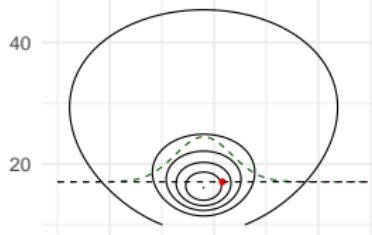


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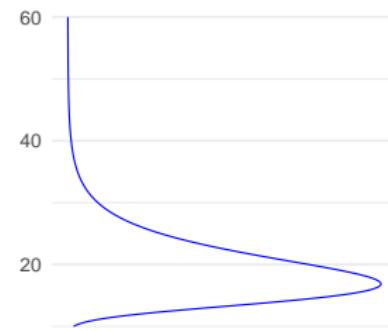
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Joint posterior

- Exact contour plot    — Cond. distribution of  $\mu$   
Sample from joint post. — Sample from the marg.



## Marginal of sigma



## Predictive distribution for new $\tilde{y}$

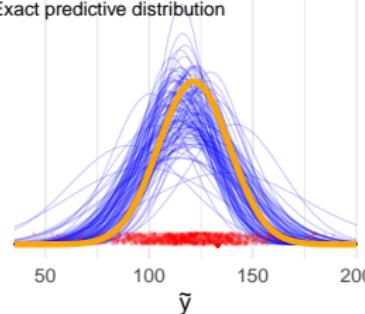
$$p(\tilde{y}|y) = \int p(\tilde{y}|\mu, \sigma)p(\mu, \sigma|y)d\mu d\sigma$$

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

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

## Posterior predictive distribution

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





# Gaussian - posterior predictive distribution

---

- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

Posterior predictive distribution given known variance

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Gaussian - posterior predictive distribution

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Posterior predictive distribution given known variance

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - posterior predictive distribution

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Posterior predictive distribution given known variance

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

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

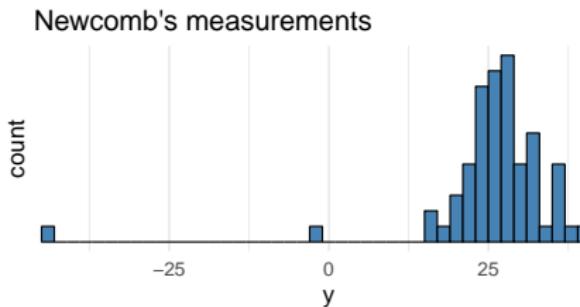
$$p(\tilde{y} \mid y) = t_{n-1}(\tilde{y} \mid \bar{y}, (1 + \frac{1}{n})s^2)$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## 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.

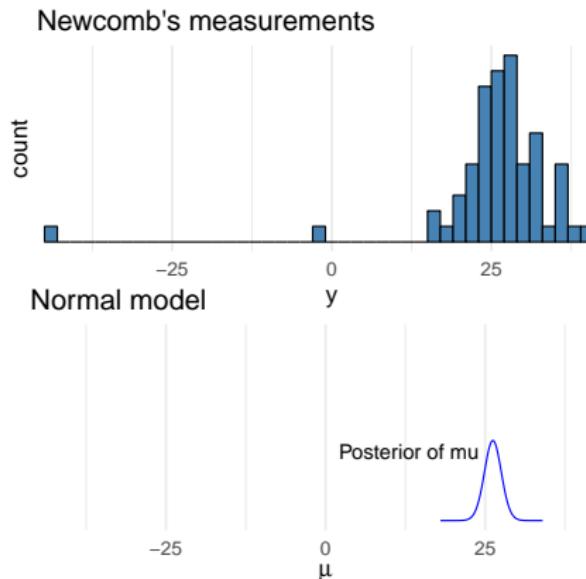




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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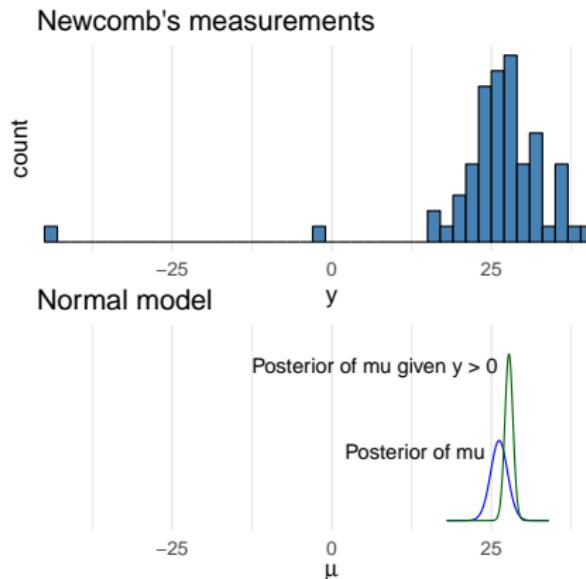




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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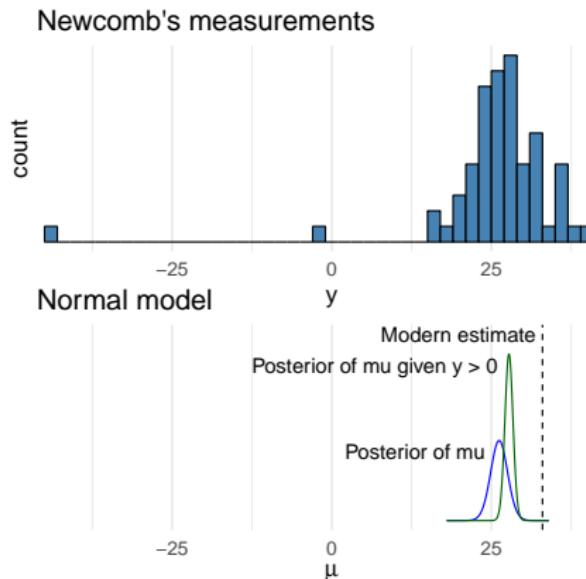




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - conjugate prior

---

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - conjugate prior

---

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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which can be written as

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

- $\mu$  and  $\sigma^2$  are a priori dependent
  - if  $\sigma^2$  is large, then  $\mu$  has wide prior



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## 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

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

$$\kappa_n = \kappa_0 + n$$

$$\nu_n = \nu_0 + n$$

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Gaussian - conjugate prior

---

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

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

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

- Marginal  $p(\mu | y)$

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - **Multinomial model**
  - Multivariate Gaussian
- Bioassay example

## 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?



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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---

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 $y_i = (0, 1, 0, 0, 0)$  - what is  $K$  here?

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

where  $\sum_k^K \theta_k = 1$ , and  $\forall \theta_k > 0$

- What is important when choosing the prior for  $\theta$ ?



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Multinomial model for categorical data

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 $y_i = (0, 1, 0, 0, 0)$  - what is  $K$  here?

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where  $\sum_k^K \theta_k = 1$ , and  $\forall \theta_k > 0$

- What is important when choosing the prior for  $\theta$ ?
- Conjugate prior: The Dirichlet distribution

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

where  $\forall \alpha_k > 0$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - **Multinomial model**
  - Multivariate Gaussian
- Bioassay example

# Multinomial model for categorical data: The posterior

---

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - **Multinomial model**
  - Multivariate Gaussian
- Bioassay example

# Multinomial model for categorical data: The posterior

---

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

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

$$\propto \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_i^n \prod_{k=1}^K \theta_k^{y_{k,i}}$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Multinomial model for categorical data: The posterior

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

$$\propto \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_i^n \prod_{k=1}^K \theta_k^{y_{k,i}}$$

$$= \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_{k=1}^K \theta_k^{\sum_i^n y_{k,i}}$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - **Multinomial model**
  - Multivariate Gaussian
- Bioassay example

# Multinomial model for categorical data: The posterior

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$$\propto \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_i^n \prod_{k=1}^K \theta_k^{y_{k,i}}$$

$$= \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_{k=1}^K \theta_k^{\sum_i^n y_{k,i}}$$

$$= \prod_{k=1}^K \theta_k^{\alpha_k-1 + \sum_i^n y_{k,i}}$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Multinomial model for categorical data: The posterior

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

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

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$$= \prod_{k=1}^K \theta_k^{\alpha_k-1} \prod_{k=1}^K \theta_k^{\sum_i^n y_{k,i}}$$

$$= \prod_{k=1}^K \theta_k^{\alpha_k-1 + \sum_i^n y_{k,i}}$$

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Multivariate Gaussian

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- Observation model

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

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

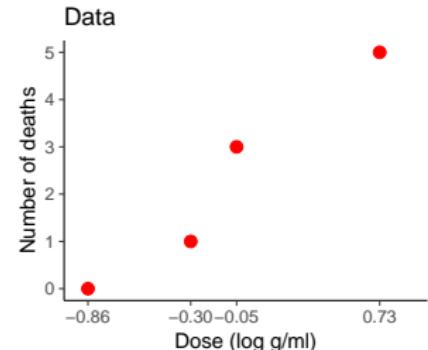
- See BDA3 p. 72–
- New recommended LKJ-prior mentioned in Appendix A,  
see more in Stan manual



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## 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

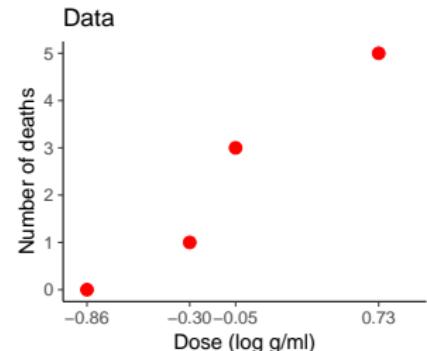




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay

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-0.05	5	3
0.73	5	5



Find out lethal dose 50% (LD50)

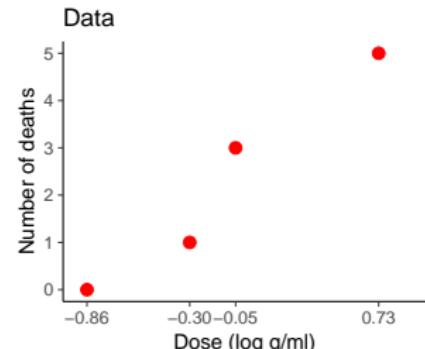
- used to classify how hazardous chemical is
- 1984 EEC directive has 4 levels



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay

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



### Find out lethal dose 50% (LD50)

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

Bayesian methods help to

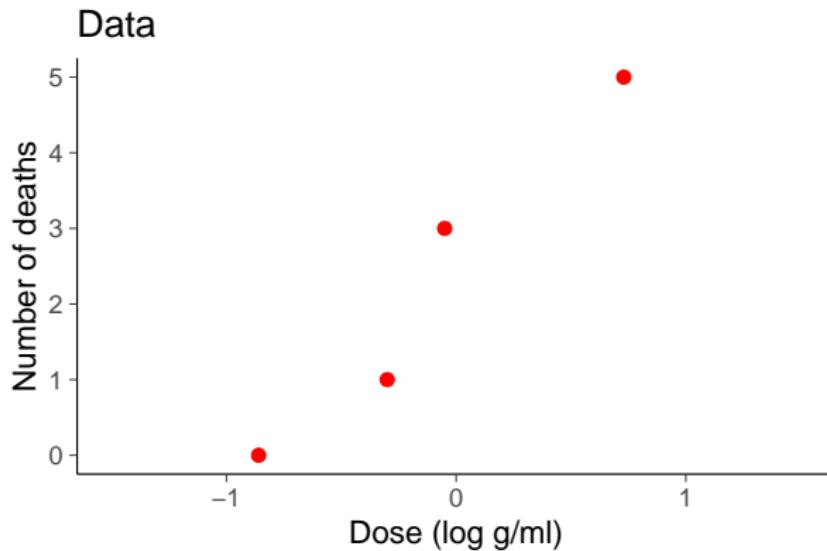
- reduce the number of animals needed
- easy to make sequential experiment and stop as soon as desired accuracy is obtained



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay

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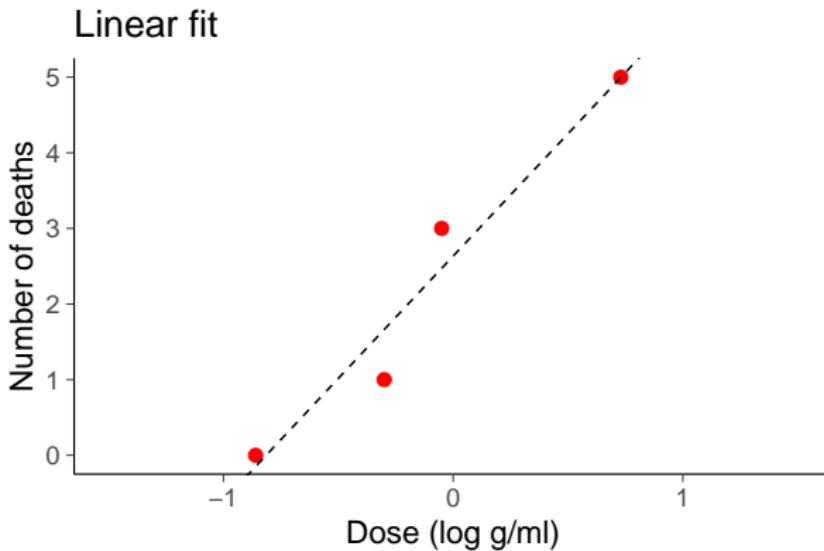




# Bioassay

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

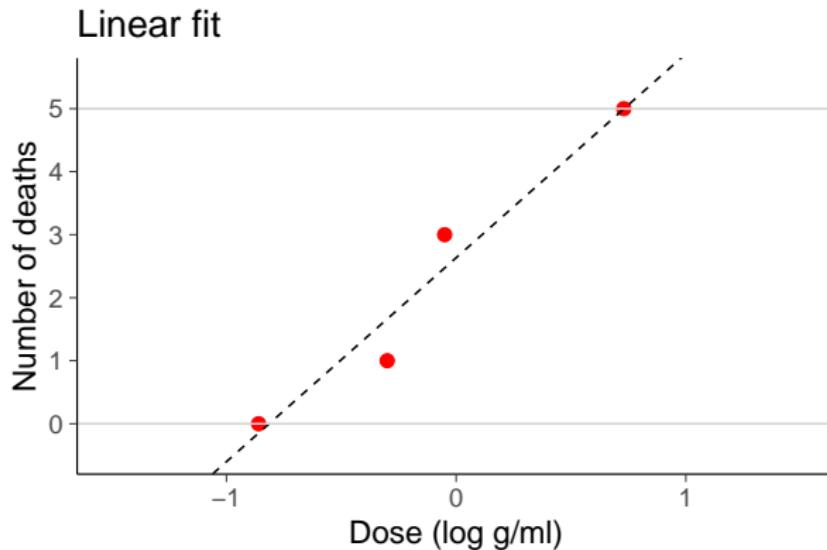




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay

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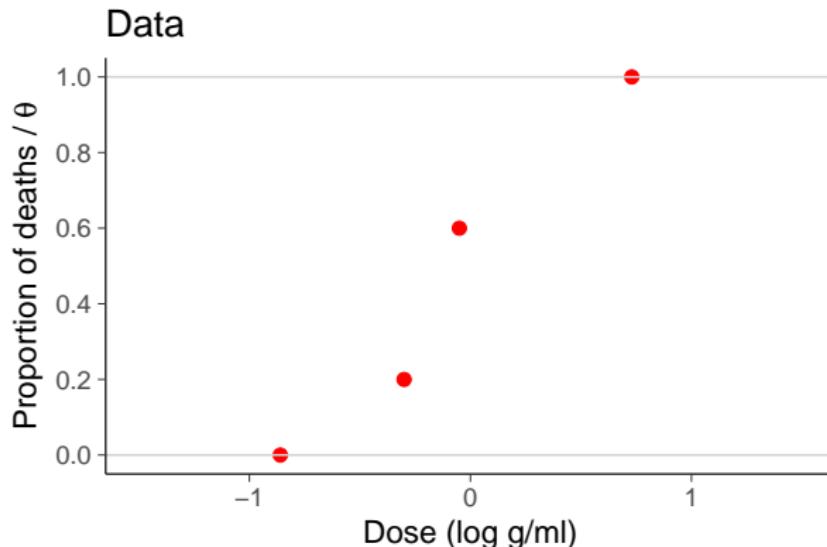




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay

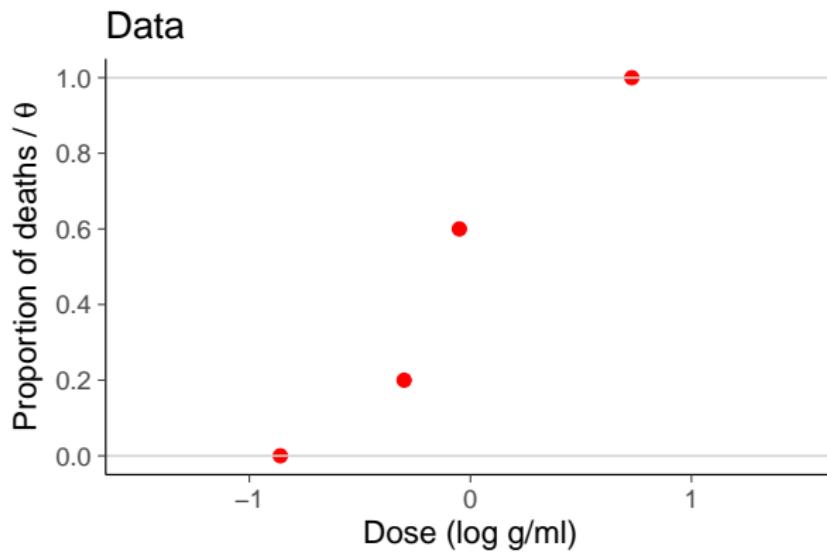
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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay



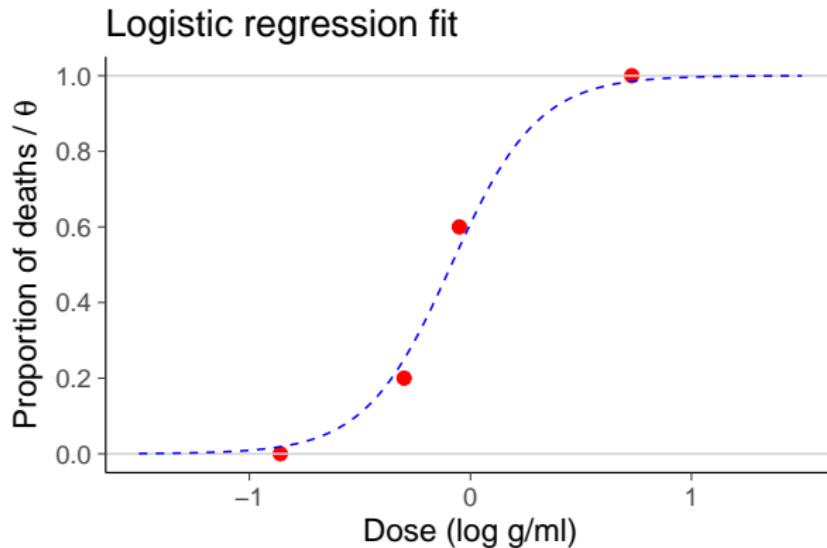
Binomial model

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay



Binomial model

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



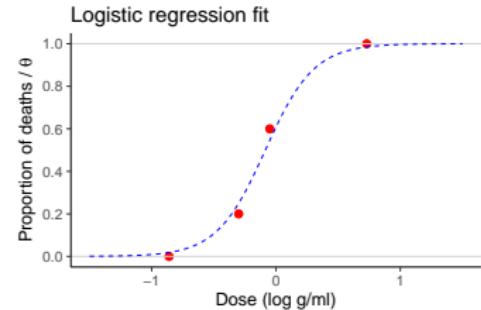
# Bioassay

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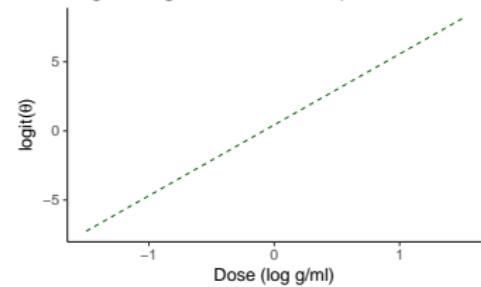
- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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



Logistic regression in latent space





# Bioassay

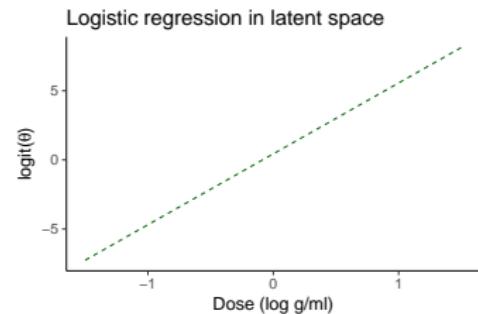
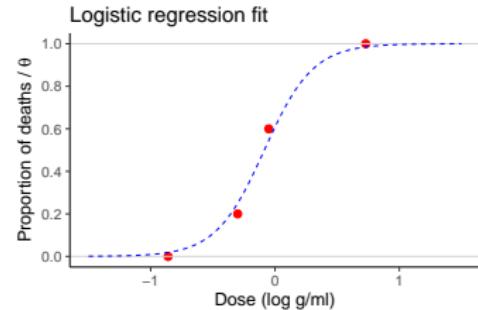
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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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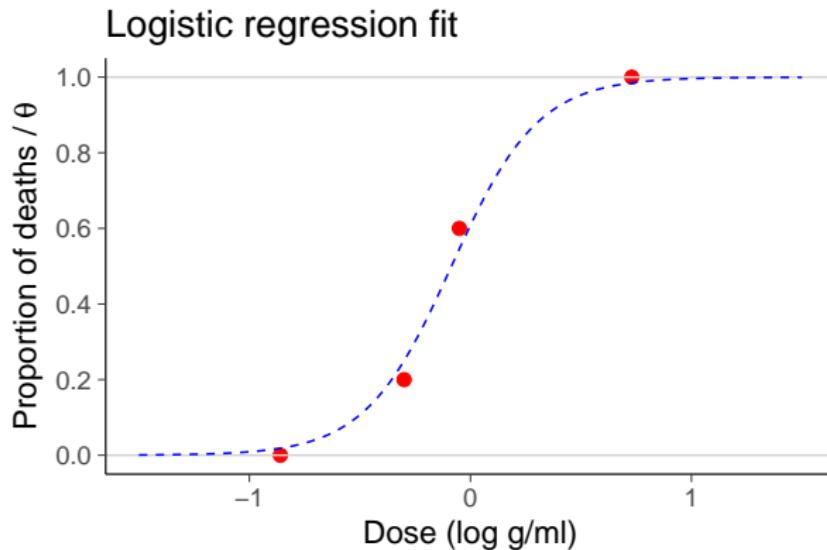
$$\theta_i = \frac{1}{1 + \exp(-(\alpha + \beta x_i))}$$





- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay: Lethal Dose 50%

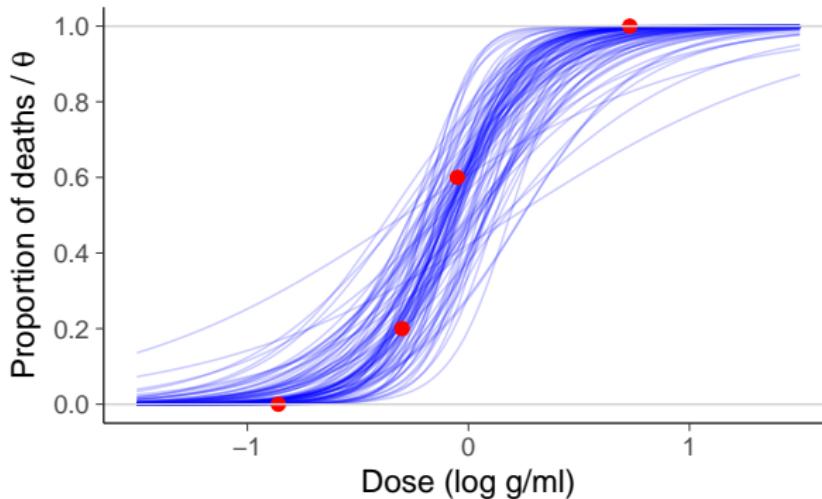




- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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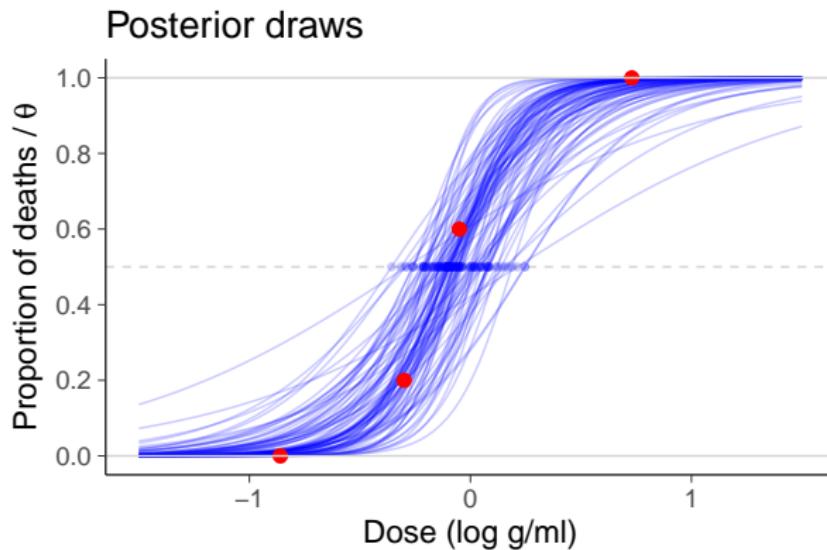
Posterior draws





- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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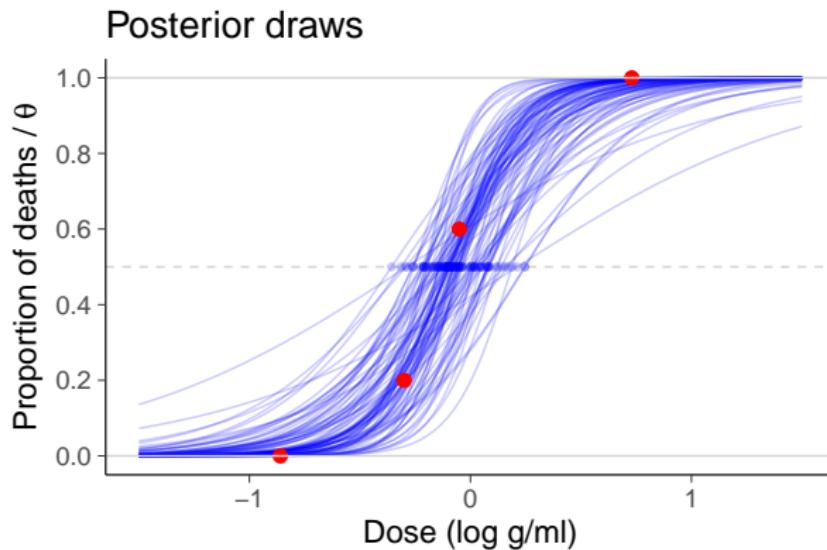


$$E\left(\frac{y}{n}\right) = \text{logit}^{-1}(\alpha + \beta x) = 0.5$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay: Lethal Dose 50%

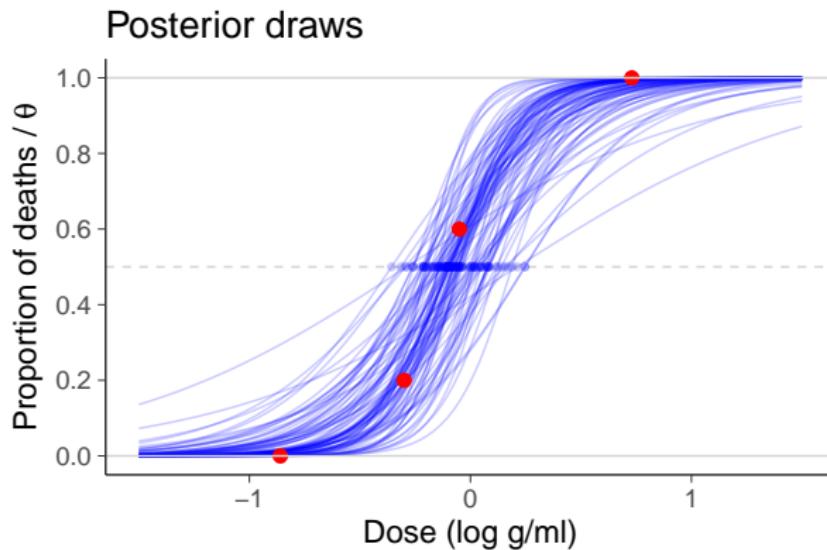


$$E\left(\frac{y}{n}\right) = \text{logit}^{-1}(\alpha + \beta x) = 0.5 \quad \Rightarrow \quad x_{LD50} = -\alpha/\beta$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay: Lethal Dose 50%



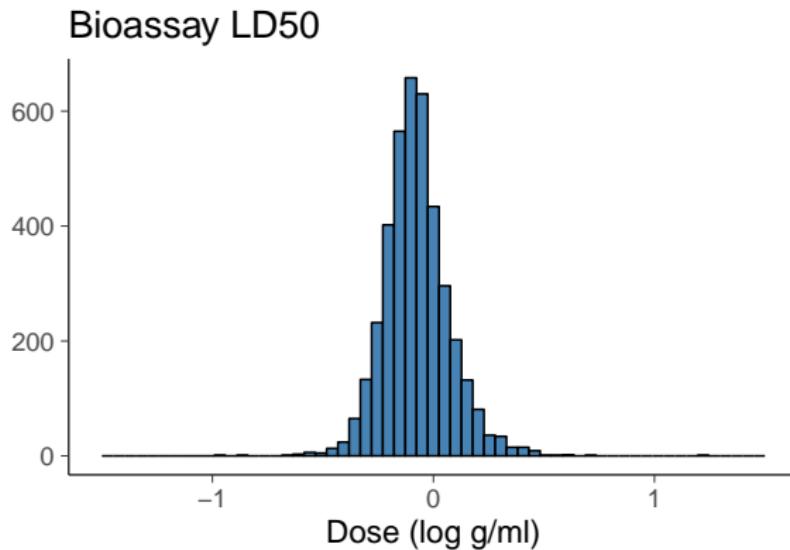
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$$x_{LD50}^{(s)} = -\alpha^{(s)}/\beta^{(s)}$$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay posterior

---

## Binomial model

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

## Link function

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

# Bioassay posterior

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## Binomial model

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## Link function

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

## Likelihood

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

## 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?



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Grid evaluation

---

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Grid evaluation

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1. Setup an area (can be hard) for  $\alpha$  and  $\beta$  that capture most mass (here  $\alpha = [-1, 5]$  and  $\beta = [0, 30]$ )
2. Compute unnormalized  $p(\alpha^{(g)}, \beta^{(g)} | y, n, x)$ , here  $\tilde{p}$ , at the grid points  $g$



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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3. Sum up  $\tilde{p}$  over the whole grid (for all  $g \in \{1, \dots, G\}$ )



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Grid evaluation

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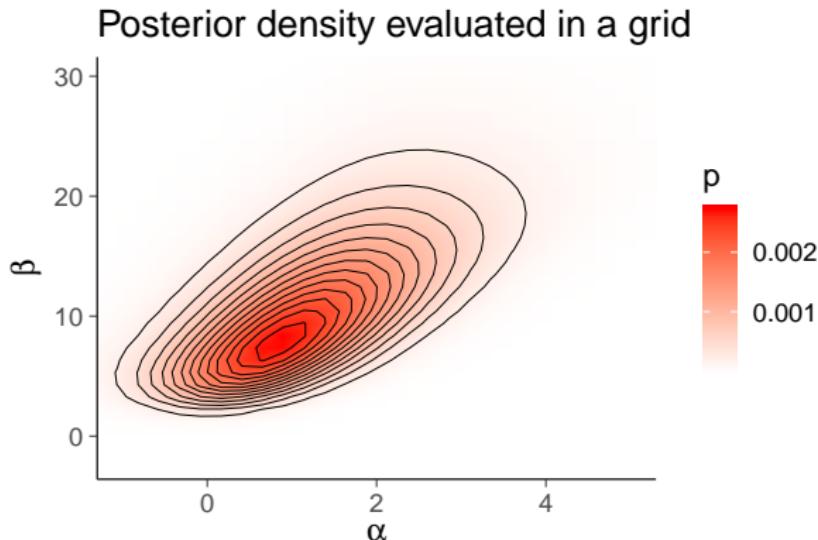
1. Setup an area (can be hard) for  $\alpha$  and  $\beta$  that capture most mass (here  $\alpha = [-1, 5]$  and  $\beta = [0, 30]$ )
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3. Sum up  $\tilde{p}$  over the whole grid (for all  $g \in \{1, \dots, G\}$ )
4. Compute (normalize) the pmf approximation 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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

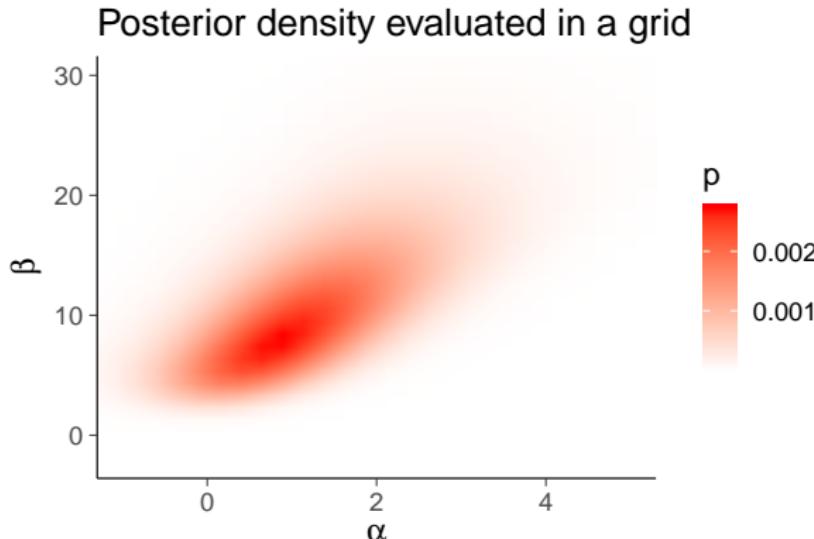
## Bioassay (with uniform prior on $\alpha, \beta$ )





- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

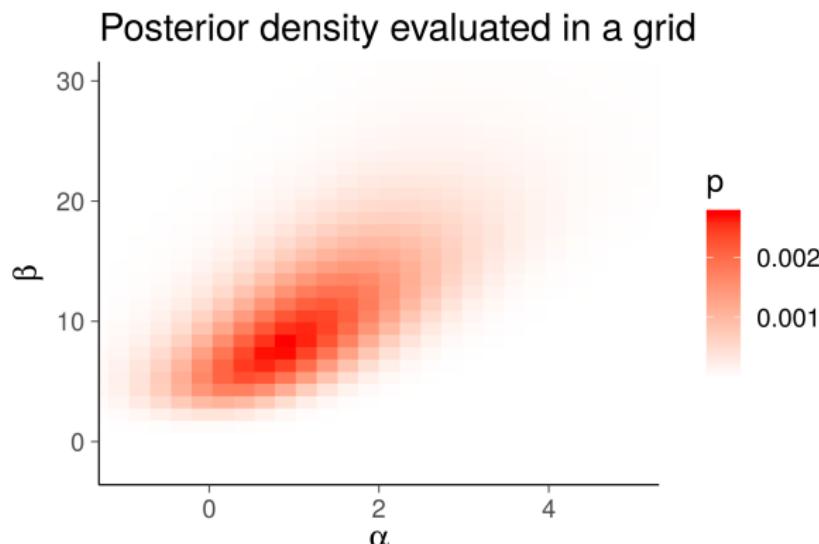


Density evaluated in grid, but plotted using interpolation



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )



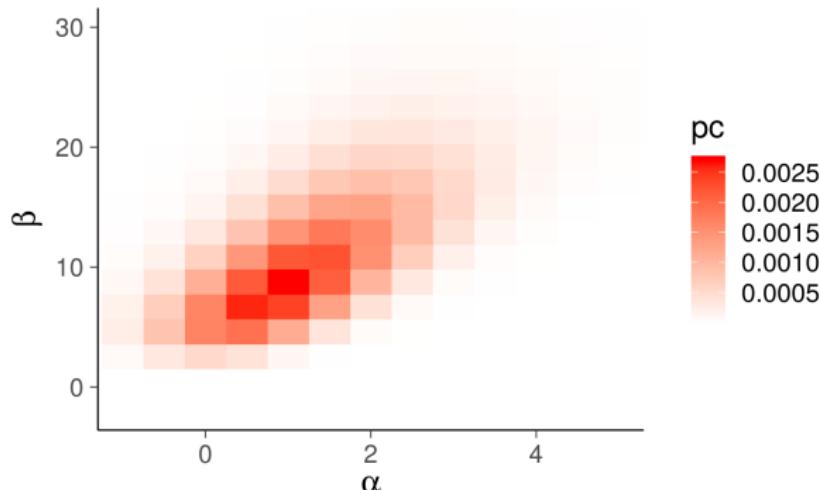
Density evaluated in grid, and plotted without interpolation



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

Posterior density evaluated in a grid

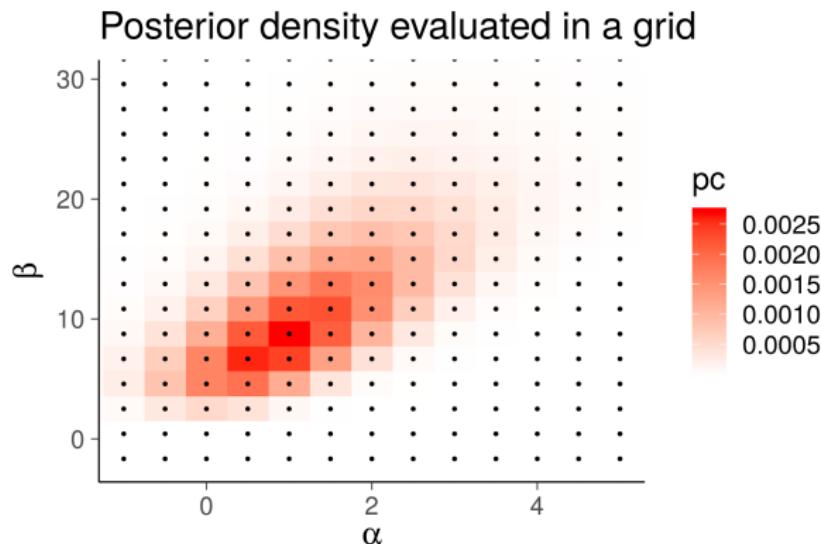


Density evaluated in a coarser grid



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

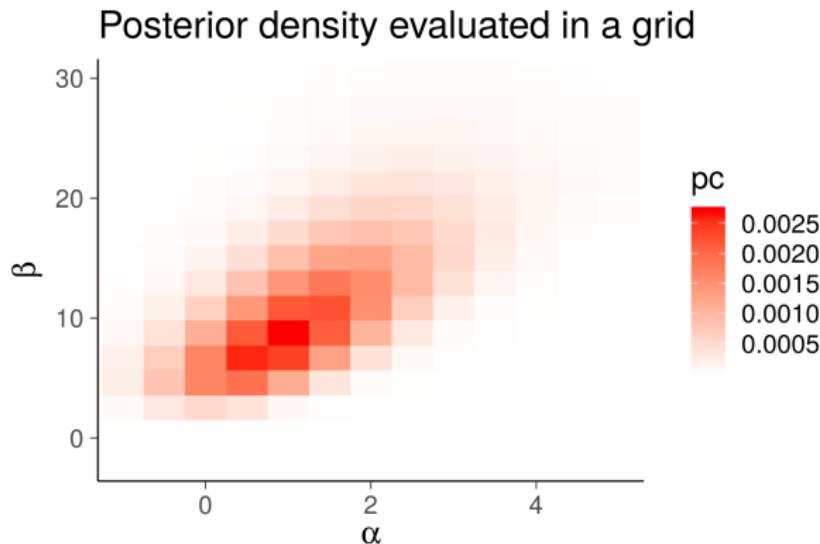


- Approximate the density as piecewise constant function
- Evaluate density in a grid over some finite region
- Density times cell area gives probability mass in each cell



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

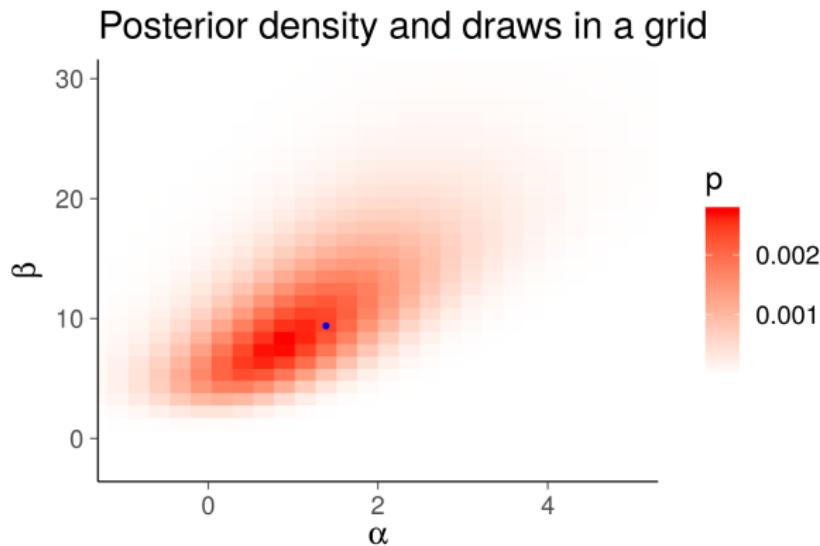


- Densities at 1, 2, and 3: 0.0027 0.0010 0.0001
- Probabilities of cells 1, 2, and 3: 0.0431 0.0166 0.0010
- Probabilities of cells sum to 1



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

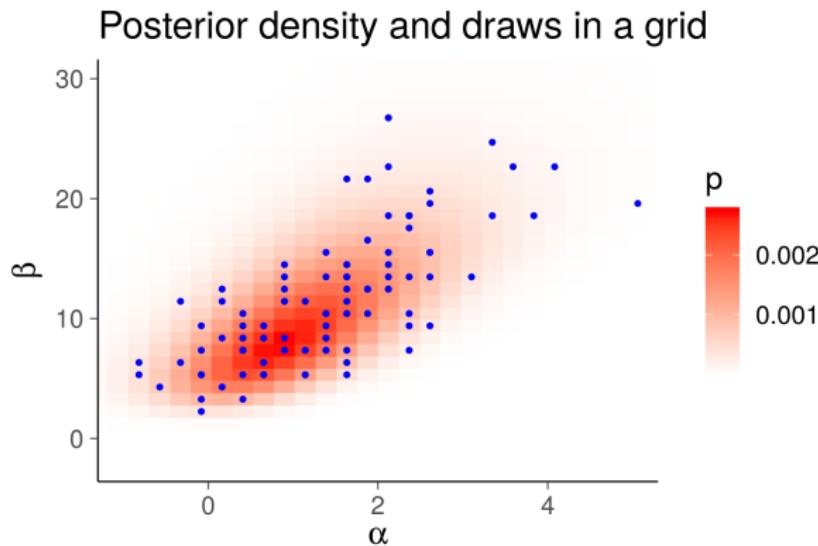


- Sample according to grid cell probabilities



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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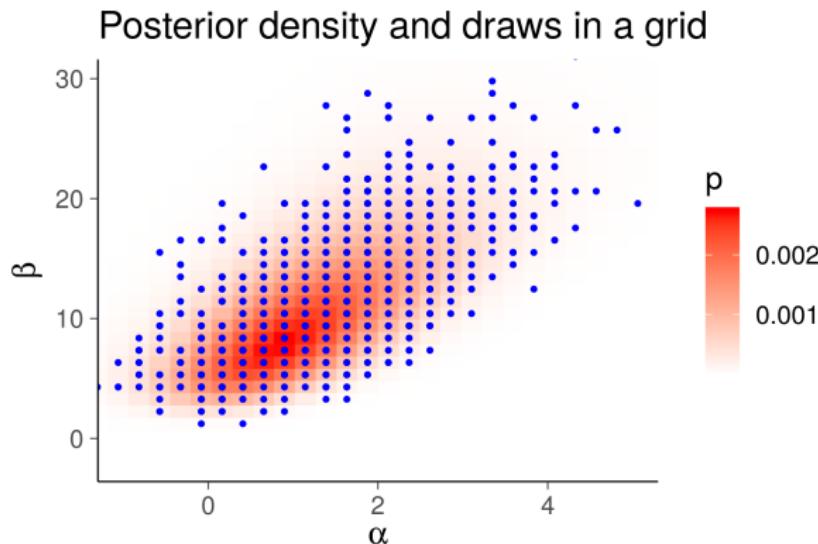


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- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )

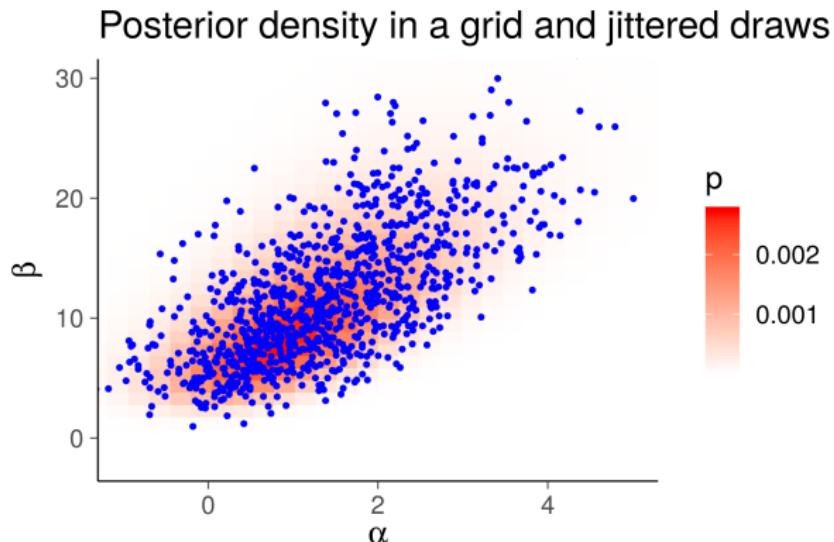


- Sample according to grid cell probabilities
- Several draws can be from the same grid cell



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Bioassay (with uniform prior on $\alpha, \beta$ )



- Jitter can be added to improve visualization



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

## Grid sampling

---

- Draws can be used to estimate expectations, for example

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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

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

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



- Introduction
- Multiple parameter models
  - Marginalization
  - Gaussian
  - Example
  - Gaussian - conjugate prior
  - Multinomial model
  - Multivariate Gaussian
- Bioassay example

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- Grid sampling gets computationally too expensive in high dimensions