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- Introduction

Bayesian Statistics and Data Analysis
Lecture 3

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Thanks to Aki Vehtari, Aalto University

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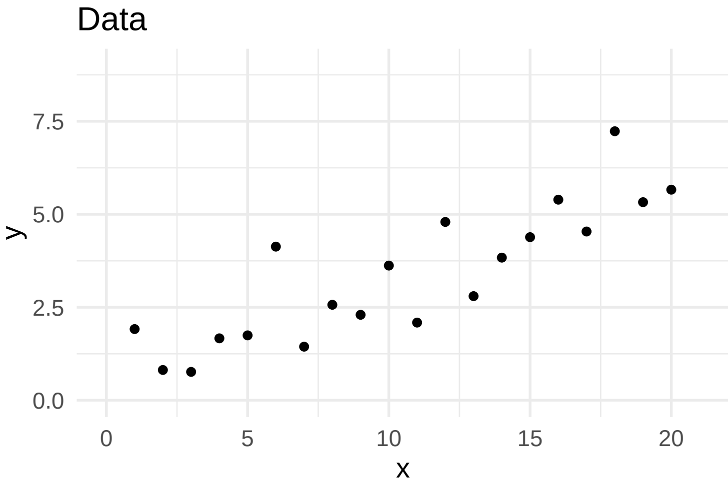
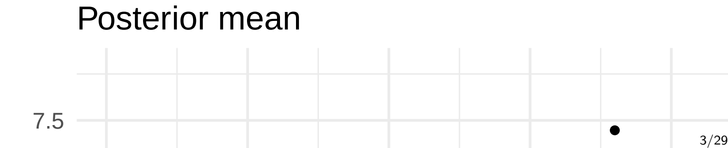
Section 1

Introduction

Example of uncertainty in modeling





Monte Carlo and posterior draws

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

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

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Marginalization

- Joint distribution of parameters

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

- 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

- Monte Carlo approximation

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

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

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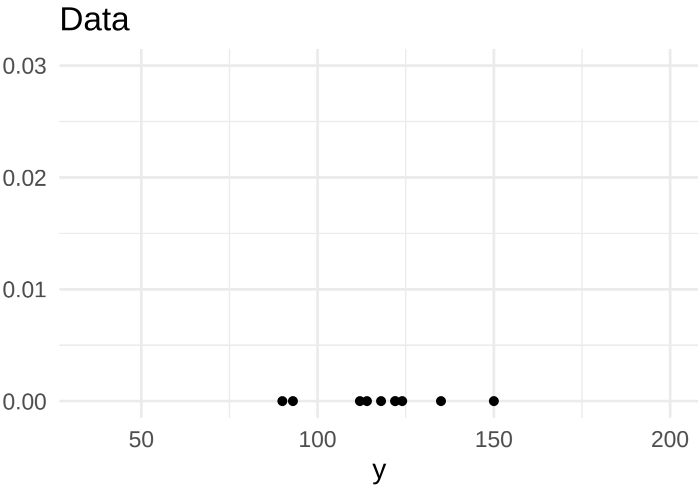
Marginalization - predictive distribution

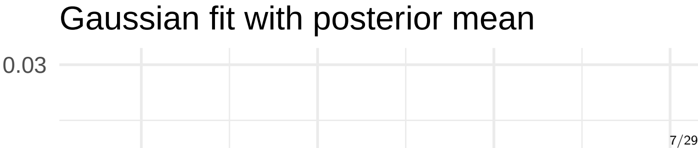
- Marginalization over posterior distribution

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

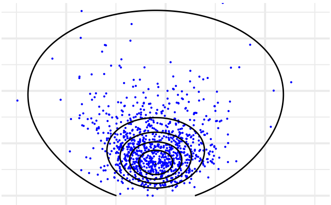
$p(\tilde{y} \mid y)$ is a predictive distribution

Gaussian example





Joint posterior



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

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

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

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

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

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

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

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

Gaussian - non-informative prior

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

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

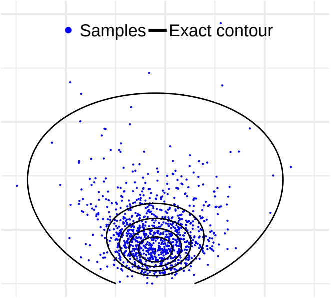
$$\sum_{i=1}^{n}(y_i^2 - 2y_i\mu + \mu^2 - \bar{y}^2 + \bar{y}^2 - 2y_i\bar{y} + 2y_i\bar{y})$$

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

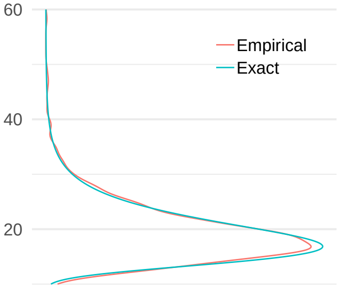
$$\sum_{i=1}^{n}(y_i - \bar{y})^2 + n(\mu^2 - 2\bar{y}\mu - \bar{y}^2 + 2\bar{y}\bar{y})$$

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

Joint posterior



Marginal of sigma



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

$$
\begin{aligned}
p(\sigma^2 \mid y) &\propto \int p(\mu, \sigma^2 \mid y) d\mu \\
&\propto \int \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}\left[(n-1)s^2 + n(\bar{y}-\mu)^2\right]\right) d\mu \\
&\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \\
&\qquad \int \exp\left(-\frac{n}{2\sigma^2}(\bar{y}-\mu)^2\right) d\mu \\
&\qquad\qquad \int \frac{1}{\sqrt{2\pi\sigma}} \exp\left(-\frac{1}{2\sigma^2}(y-\theta)^2\right) d\theta = \\
&\propto \sigma^{-n-2} \exp\left(-\frac{1}{2\sigma^2}(n-1)s^2\right) \sqrt{2\pi\sigma^2/n} \\
&\propto (\sigma^2)^{-(n+1)/2} \exp\left(-\frac{(n-1)s^2}{2\sigma^2}\right) \\
p(\sigma^2 \mid y) &= \text{Inv-}\chi^2(\sigma^2 \mid n-1, s^2)
\end{aligned}
$$

Gaussian - non-informative prior

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Known mean

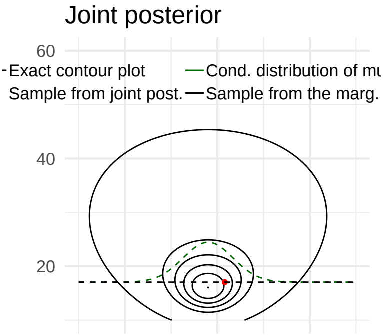
$$\sigma^2 \mid y \sim \text{Inv-}\chi^2(n, v)$$

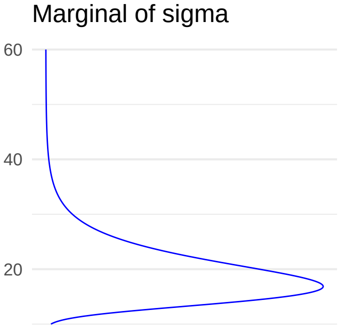
$$\text{where} \quad v = \frac{1}{n}\sum_{i=1}^{n}(y_i - \theta)^2$$

Unknown mean

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

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


Joint posterior
60
40
20
-Exact contour plot
Cond. distribution of mu
Sample from joint post.
Sample from the marg.


Marginal of sigma
60
40
20

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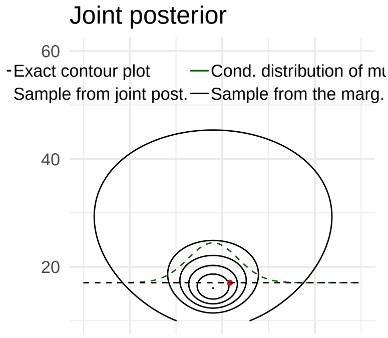

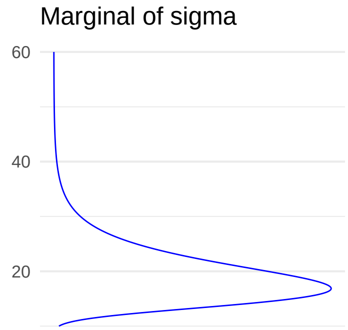

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Marginal posterior $p(\mu \mid y)$

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

Transformation

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

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

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

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

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

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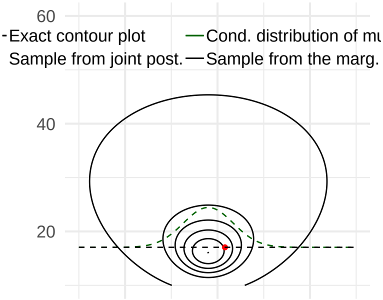
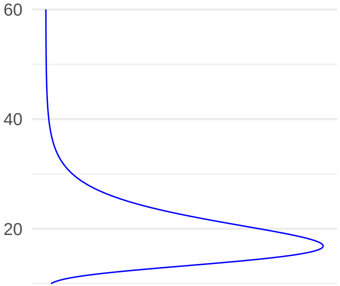
Joint posterior



Marginal of sigma



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Gaussian - posterior predictive distribution

Posterior predictive distribution given known variance

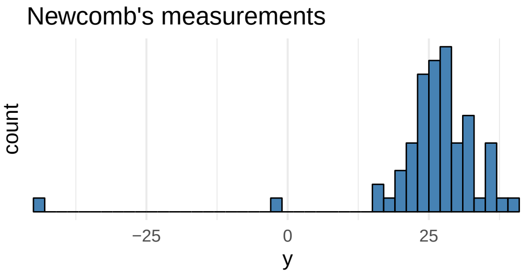
$$
\begin{aligned}
p(\tilde{y} \mid \sigma^2, y) &= \int p(\tilde{y} \mid \mu, \sigma^2) p(\mu \mid \sigma^2, y) d\mu \\
&= \int \mathcal{N}(\tilde{y} \mid \mu, \sigma^2) \mathcal{N}(\mu \mid \bar{y}, \sigma^2/n) d\mu \\
&= \mathcal{N}(\tilde{y} \mid \bar{y}, (1 + \tfrac{1}{n})\sigma^2)
\end{aligned}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

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.



Gaussian - conjugate prior

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

Gaussian - conjugate prior

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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

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

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Multinomial model for categorical data

- Extension of binomial
- Observation model

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

- BDA3 p. 69–

Multivariate Gaussian

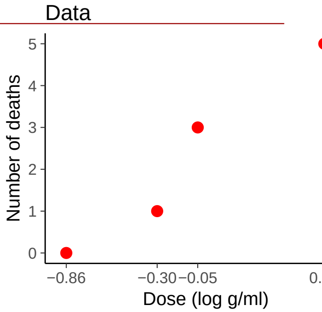
- Observation model

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

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

Bioassay

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



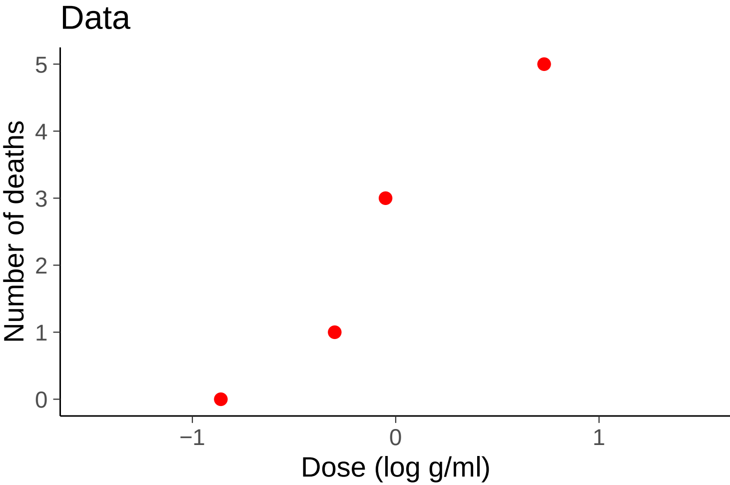
Find out lethal dose 50% (LD50)

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

Bayesian methods help to

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

Bioassay



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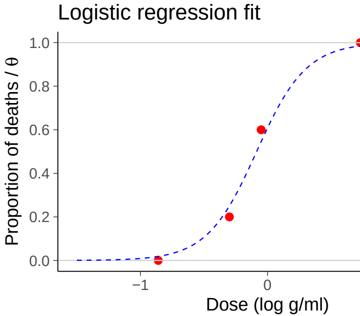
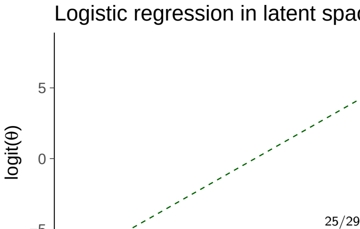
Bioassay

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

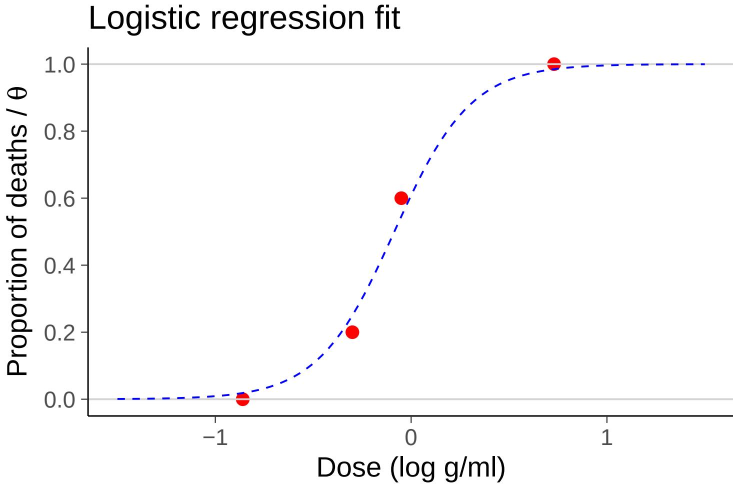
$$\text{logit}(\theta_i) = \log\left(\frac{\theta_i}{1-\theta_i}\right) = \alpha + \beta x_i$$

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





Bioassay


Logistic regression fit
Proportion of deaths / θ
1.0
0.8
0.6
0.4
0.2
0.0
−1
0
1
Dose (log g/ml)


Posterior draws
s / θ
1.0
0.8

Bioassay posterior

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Binomial model

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

Link function

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

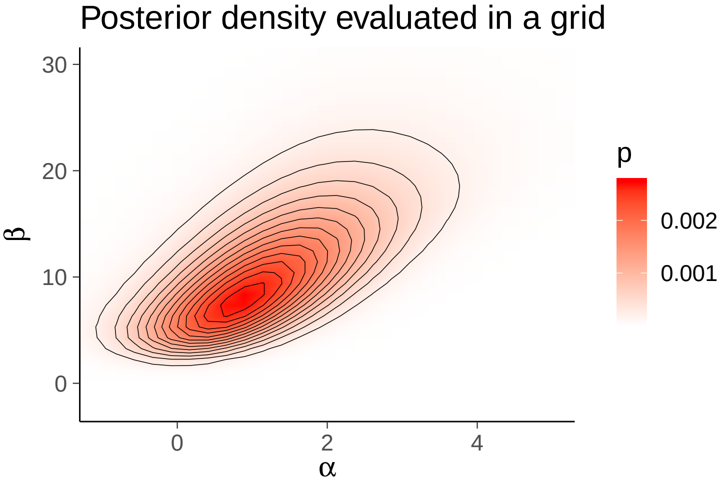
Likelihood

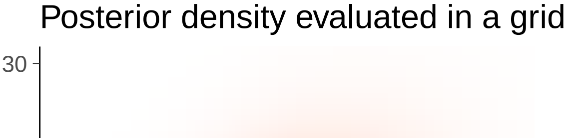
$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto \theta_i^{y_i}[1 - \theta_i]^{n_i - y_i}$$
$$p(y_i \mid \alpha, \beta, n_i, x_i) \propto [\mathrm{logit}^{-1}(\alpha + \beta x_i)]^{y_i}[1 - \mathrm{logit}^{-1}(\alpha + \beta x_i)]^{n_i - y_i}$$

Posterior (with uniform prior on α, β)

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

Bioassay


Posterior density evaluated in a grid
30
20
10
0
β
0
2
4
α
p
0.002
0.001


Posterior density evaluated in a grid
30

Grid sampling

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- 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